Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 04:34 PM EST

PDB ID	:	5EBZ
Title	:	Crystal structure of human IKK1
Authors	:	Polley, S.; Passos, D.; Huang, D.; Biswas, T.; Verma, I.; Lyumkis, D.; Ghosh, G.
Deposited on	:	2015-10-20
Resolution	:	4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

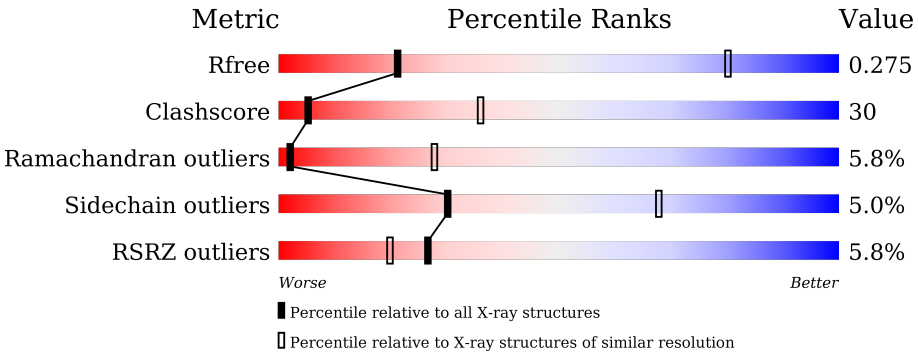
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	4% 46% 47% 6%
1	B	655	6% 44% 49% 6%
1	C	655	3% 44% 50% 5%
1	D	655	7% 44% 51% 5%
1	E	655	4% 43% 51% 6%
1	F	655	7% 44% 51%

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Mol	Chain	Length	Quality of chain
1	G	655	3% 44% 50% 5%
1	H	655	8% 44% 50% 6%
1	I	655	6% 43% 51% 5%
1	J	655	8% 44% 50% 5%
1	K	655	7% 42% 52% 5%
1	L	655	6% 43% 52% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	Z4K	C	709	-	-	-	X
2	5TL	A	701	-	-	-	X
2	5TL	B	701	-	-	-	X
2	5TL	C	701	-	-	-	X
2	5TL	D	701	-	-	-	X
2	5TL	E	701	-	-	-	X
2	5TL	F	701	-	-	-	X
2	5TL	H	701	-	-	-	X
2	5TL	I	701	-	-	-	X
2	5TL	J	701	-	-	-	X
2	5TL	K	701	-	-	-	X
2	5TL	L	701	-	-	-	X
3	5LS	B	707	-	-	-	X
3	5LS	D	702	-	-	-	X
3	5LS	G	702	-	-	-	X
3	5LS	K	702	-	-	-	X
3	5LS	L	704	-	-	-	X
4	GLC	J	705	-	-	X	-
4	GLC	K	703	-	-	-	X
5	PDX	G	704	-	-	-	X
5	PDX	K	707	-	-	-	X
5	PDX	L	709	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 65132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inhibitor of nuclear factor kappa-B kinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	B	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	C	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	D	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	E	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	F	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	G	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	H	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	I	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	J	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	K	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	L	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASP	-	expression tag	UNP O15111
A	7	PRO	-	expression tag	UNP O15111
A	8	GLU	-	expression tag	UNP O15111
A	9	PHE	-	expression tag	UNP O15111
A	176	GLU	SER	engineered mutation	UNP O15111

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Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	UNP O15111
B	180	GLU	SER	engineered mutation	UNP O15111
B	268	ILE	VAL	variant	UNP O15111
C	6	ASP	-	expression tag	UNP O15111
C	7	PRO	-	expression tag	UNP O15111
C	8	GLU	-	expression tag	UNP O15111
C	9	PHE	-	expression tag	UNP O15111
C	176	GLU	SER	engineered mutation	UNP O15111
C	180	GLU	SER	engineered mutation	UNP O15111
C	268	ILE	VAL	variant	UNP O15111
D	6	ASP	-	expression tag	UNP O15111
D	7	PRO	-	expression tag	UNP O15111
D	8	GLU	-	expression tag	UNP O15111
D	9	PHE	-	expression tag	UNP O15111
D	176	GLU	SER	engineered mutation	UNP O15111
D	180	GLU	SER	engineered mutation	UNP O15111
D	268	ILE	VAL	variant	UNP O15111
E	6	ASP	-	expression tag	UNP O15111
E	7	PRO	-	expression tag	UNP O15111
E	8	GLU	-	expression tag	UNP O15111
E	9	PHE	-	expression tag	UNP O15111
E	176	GLU	SER	engineered mutation	UNP O15111
E	180	GLU	SER	engineered mutation	UNP O15111
E	268	ILE	VAL	variant	UNP O15111
F	6	ASP	-	expression tag	UNP O15111
F	7	PRO	-	expression tag	UNP O15111
F	8	GLU	-	expression tag	UNP O15111
F	9	PHE	-	expression tag	UNP O15111
F	176	GLU	SER	engineered mutation	UNP O15111
F	180	GLU	SER	engineered mutation	UNP O15111
F	268	ILE	VAL	variant	UNP O15111
G	6	ASP	-	expression tag	UNP O15111
G	7	PRO	-	expression tag	UNP O15111
G	8	GLU	-	expression tag	UNP O15111
G	9	PHE	-	expression tag	UNP O15111
G	176	GLU	SER	engineered mutation	UNP O15111

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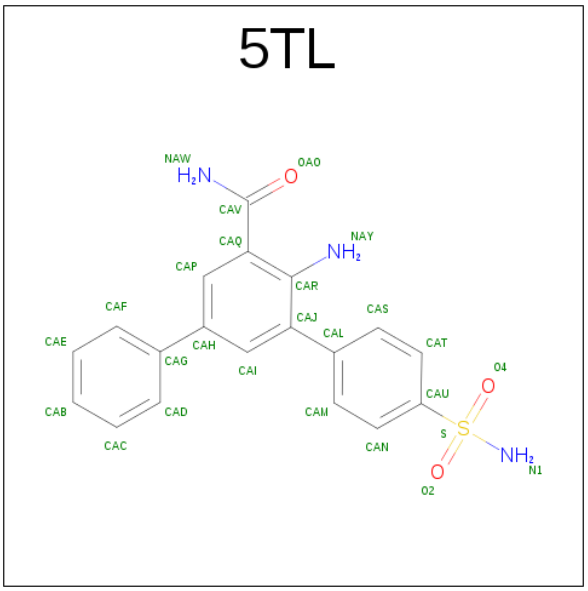
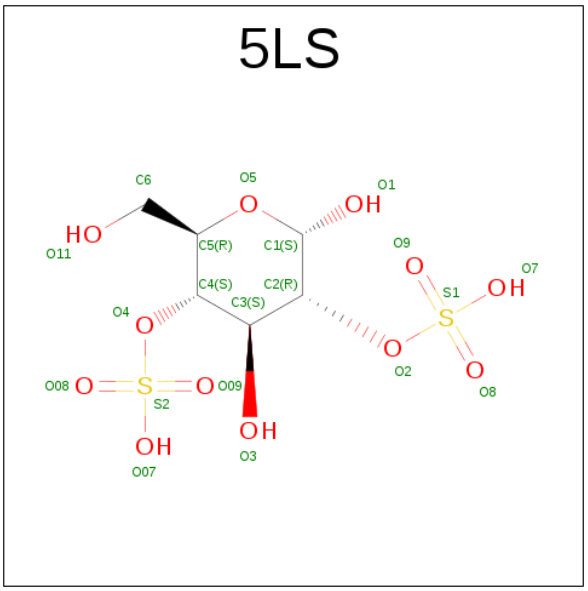
Chain	Residue	Modelled	Actual	Comment	Reference
G	180	GLU	SER	engineered mutation	UNP O15111
G	268	ILE	VAL	variant	UNP O15111
H	6	ASP	-	expression tag	UNP O15111
H	7	PRO	-	expression tag	UNP O15111
H	8	GLU	-	expression tag	UNP O15111
H	9	PHE	-	expression tag	UNP O15111
H	176	GLU	SER	engineered mutation	UNP O15111
H	180	GLU	SER	engineered mutation	UNP O15111
H	268	ILE	VAL	variant	UNP O15111
I	6	ASP	-	expression tag	UNP O15111
I	7	PRO	-	expression tag	UNP O15111
I	8	GLU	-	expression tag	UNP O15111
I	9	PHE	-	expression tag	UNP O15111
I	176	GLU	SER	engineered mutation	UNP O15111
I	180	GLU	SER	engineered mutation	UNP O15111
I	268	ILE	VAL	variant	UNP O15111
J	6	ASP	-	expression tag	UNP O15111
J	7	PRO	-	expression tag	UNP O15111
J	8	GLU	-	expression tag	UNP O15111
J	9	PHE	-	expression tag	UNP O15111
J	176	GLU	SER	engineered mutation	UNP O15111
J	180	GLU	SER	engineered mutation	UNP O15111
J	268	ILE	VAL	variant	UNP O15111
K	6	ASP	-	expression tag	UNP O15111
K	7	PRO	-	expression tag	UNP O15111
K	8	GLU	-	expression tag	UNP O15111
K	9	PHE	-	expression tag	UNP O15111
K	176	GLU	SER	engineered mutation	UNP O15111
K	180	GLU	SER	engineered mutation	UNP O15111
K	268	ILE	VAL	variant	UNP O15111
L	6	ASP	-	expression tag	UNP O15111
L	7	PRO	-	expression tag	UNP O15111
L	8	GLU	-	expression tag	UNP O15111
L	9	PHE	-	expression tag	UNP O15111
L	176	GLU	SER	engineered mutation	UNP O15111
L	180	GLU	SER	engineered mutation	UNP O15111
L	268	ILE	VAL	variant	UNP O15111

- Molecule 2 is 2-azanyl-5-phenyl-3-(4-sulfamoylphenyl)benzamide (three-letter code: 5TL) (formula: $C_{19}H_{17}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	G	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	H	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	I	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	J	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	K	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	L	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

- Molecule 3 is [(2 {R},3 {S},4 {S},5 {R},6 {S})-2-(hydroxymethyl)-4,6-bis(oxidanyl)-5-sulfooxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5LS) (formula: $C_6H_{12}O_{12}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			20	6	12	2		
3	A	1	Total	C	O	S	0	0
			20	6	12	2		
3	B	1	Total	C	O	S	0	0
			20	6	12	2		
3	B	1	Total	C	O	S	0	0
			20	6	12	2		
3	C	1	Total	C	O	S	0	0
			20	6	12	2		
3	C	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	E	1	Total	C	O	S	0	0
			20	6	12	2		
3	E	1	Total	C	O	S	0	0
			20	6	12	2		
3	F	1	Total	C	O	S	0	0
			20	6	12	2		
3	F	1	Total	C	O	S	0	0
			20	6	12	2		

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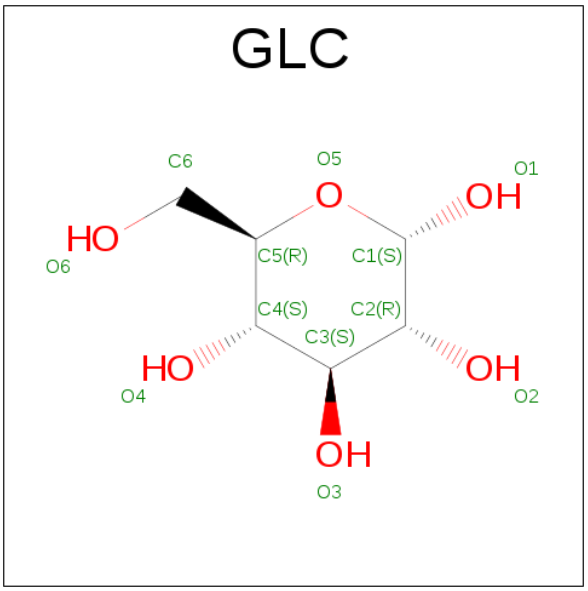
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	O	S	0	0
			20	6	12	2		
3	G	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	I	1	Total	C	O	S	0	0
			20	6	12	2		
3	I	1	Total	C	O	S	0	0
			20	6	12	2		
3	J	1	Total	C	O	S	0	0
			20	6	12	2		
3	J	1	Total	C	O	S	0	0
			20	6	12	2		
3	K	1	Total	C	O	S	0	0
			20	6	12	2		
3	K	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		

- Molecule 4 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	F	1	Total C O 11 6 5	0	0
4	F	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0

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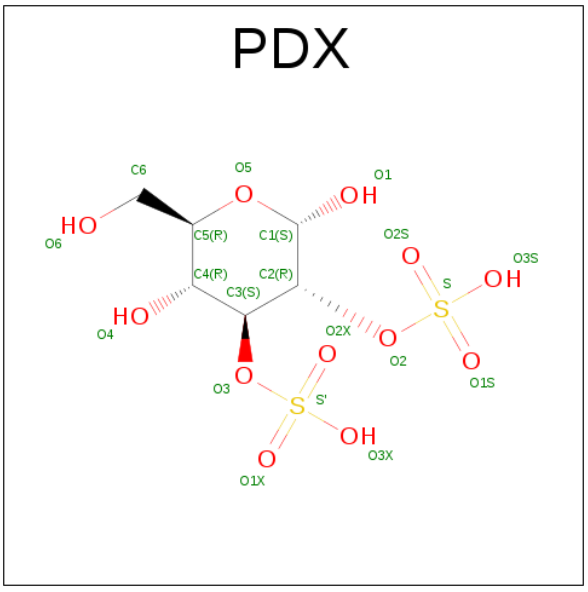
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 11 6 5	0	0
4	H	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	J	1	Total C O 11 6 5	0	0
4	J	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0
4	L	1	Total C O 11 6 5	0	0
4	L	1	Total C O 11 6 5	0	0

- Molecule 5 is 2,3-DI-O-SULFO-ALPHA-D-GLUCOPYRANOSE (three-letter code: PDX) (formula: $C_6H_{12}O_{12}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 19 6 11 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			19	6	11	2		
5	B	1	Total	C	O	S	0	0
			19	6	11	2		
5	B	1	Total	C	O	S	0	0
			19	6	11	2		
5	C	1	Total	C	O	S	0	0
			19	6	11	2		
5	C	1	Total	C	O	S	0	0
			19	6	11	2		
5	D	1	Total	C	O	S	0	0
			19	6	11	2		
5	D	1	Total	C	O	S	0	0
			19	6	11	2		
5	E	1	Total	C	O	S	0	0
			19	6	11	2		
5	E	1	Total	C	O	S	0	0
			19	6	11	2		
5	F	1	Total	C	O	S	0	0
			19	6	11	2		
5	F	1	Total	C	O	S	0	0
			19	6	11	2		
5	G	1	Total	C	O	S	0	0
			19	6	11	2		
5	G	1	Total	C	O	S	0	0
			19	6	11	2		
5	H	1	Total	C	O	S	0	0
			19	6	11	2		
5	I	1	Total	C	O	S	0	0
			19	6	11	2		
5	I	1	Total	C	O	S	0	0
			19	6	11	2		
5	J	1	Total	C	O	S	0	0
			19	6	11	2		
5	J	1	Total	C	O	S	0	0
			19	6	11	2		
5	K	1	Total	C	O	S	0	0
			19	6	11	2		
5	K	1	Total	C	O	S	0	0
			19	6	11	2		
5	L	1	Total	C	O	S	0	0
			19	6	11	2		

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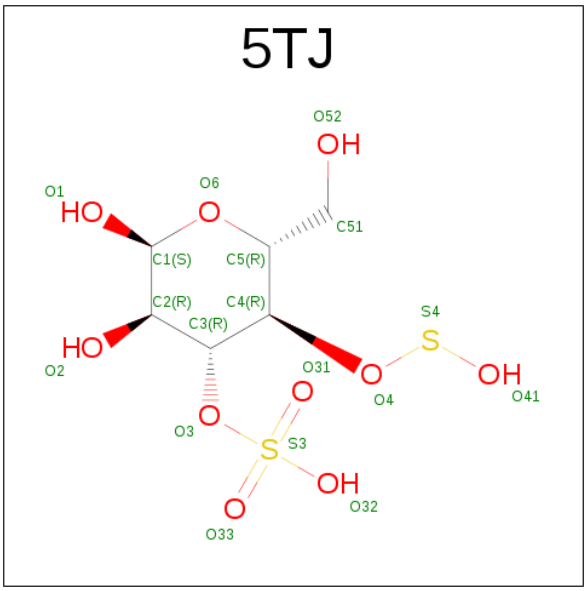
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O S 19 6 11 2	0	0
5	L	1	Total C O S 19 6 11 2	0	0

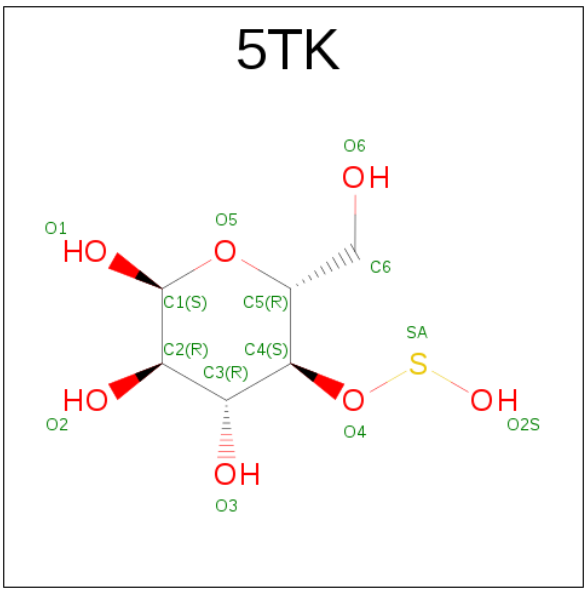
- Molecule 6 is [(2 {R},3 {R},4 {R},5 {R},6 {S})-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate (three-letter code: 5TJ) (formula: $C_6H_{12}O_{10}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 17 6 9 2	0	0
6	A	1	Total C O S 17 6 9 2	0	0
6	D	1	Total C O S 17 6 9 2	0	0
6	D	1	Total C O S 17 6 9 2	0	0
6	H	1	Total C O S 17 6 9 2	0	0
6	H	1	Total C O S 17 6 9 2	0	0
6	I	1	Total C O S 17 6 9 2	0	0
6	I	1	Total C O S 17 6 9 2	0	0

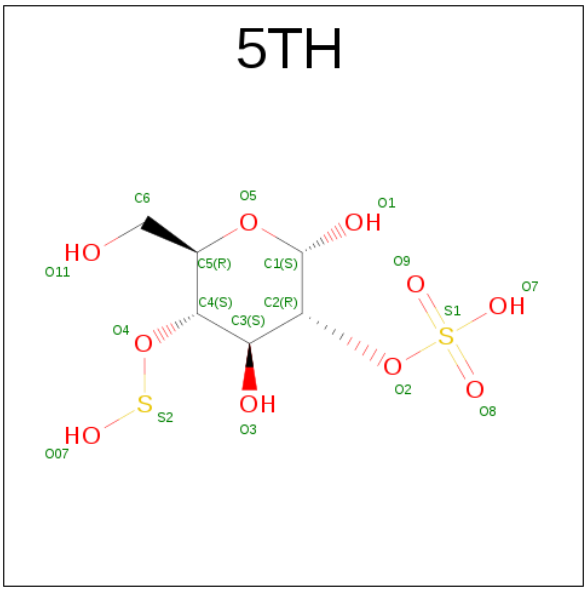
- Molecule 7 is (2 {S},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-ox

ane-2,3,4-triol (three-letter code: 5TK) (formula: $C_6H_{12}O_7S$).



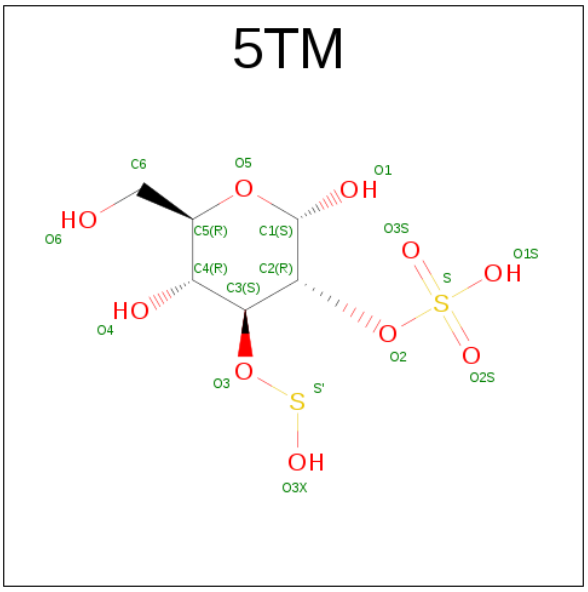
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			13	6	6	1		
7	C	1	Total	C	O	S	0	0
			13	6	6	1		
7	G	1	Total	C	O	S	0	0
			13	6	6	1		
7	I	1	Total	C	O	S	0	0
			13	6	6	1		

- Molecule 8 is [(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5TH) (formula: $C_6H_{12}O_{10}S_2$).



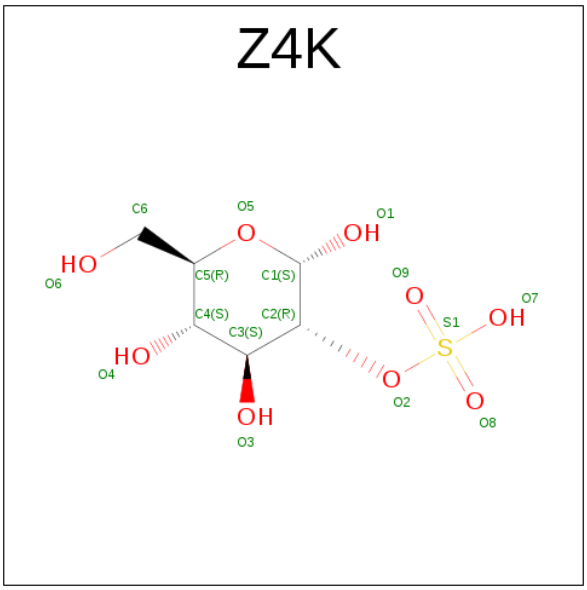
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 17 6 9 2	0	0
8	C	1	Total C O S 17 6 9 2	0	0
8	G	1	Total C O S 17 6 9 2	0	0
8	I	1	Total C O S 17 6 9 2	0	0

- Molecule 9 is [(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5TM) (formula: $C_6H_{12}O_{10}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O S 17 6 9 2	0	0
9	C	1	Total C O S 17 6 9 2	0	0
9	G	1	Total C O S 17 6 9 2	0	0
9	J	1	Total C O S 17 6 9 2	0	0

- Molecule 10 is 2-O-sulfo-alpha-D-glucopyranose (three-letter code: Z4K) (formula: $C_6H_{12}O_9S$).



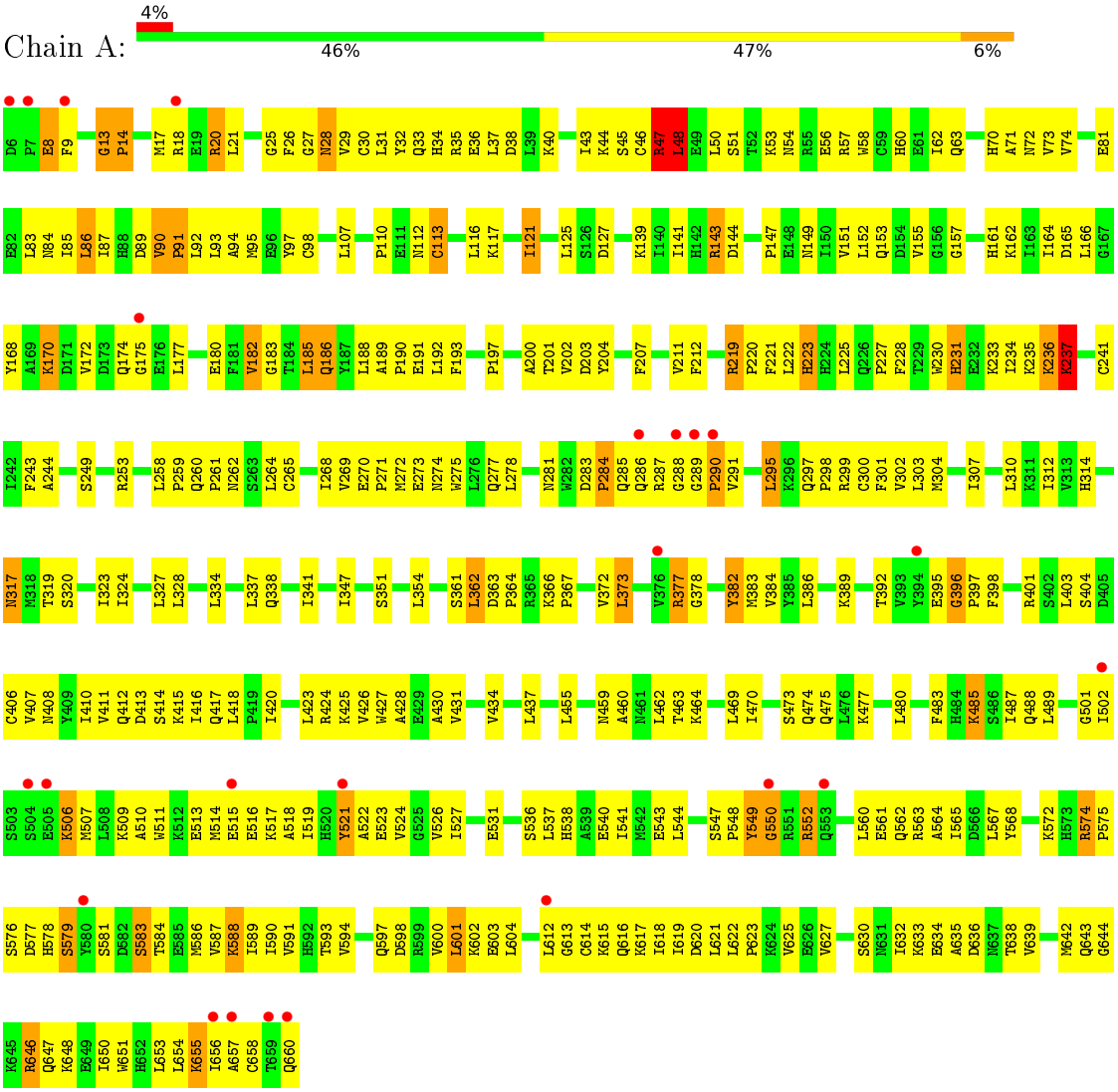
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O S 15 6 8 1	0	0
10	C	1	Total C O S 15 6 8 1	0	0
10	H	1	Total C O S 15 6 8 1	0	0
10	J	1	Total C O S 15 6 8 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

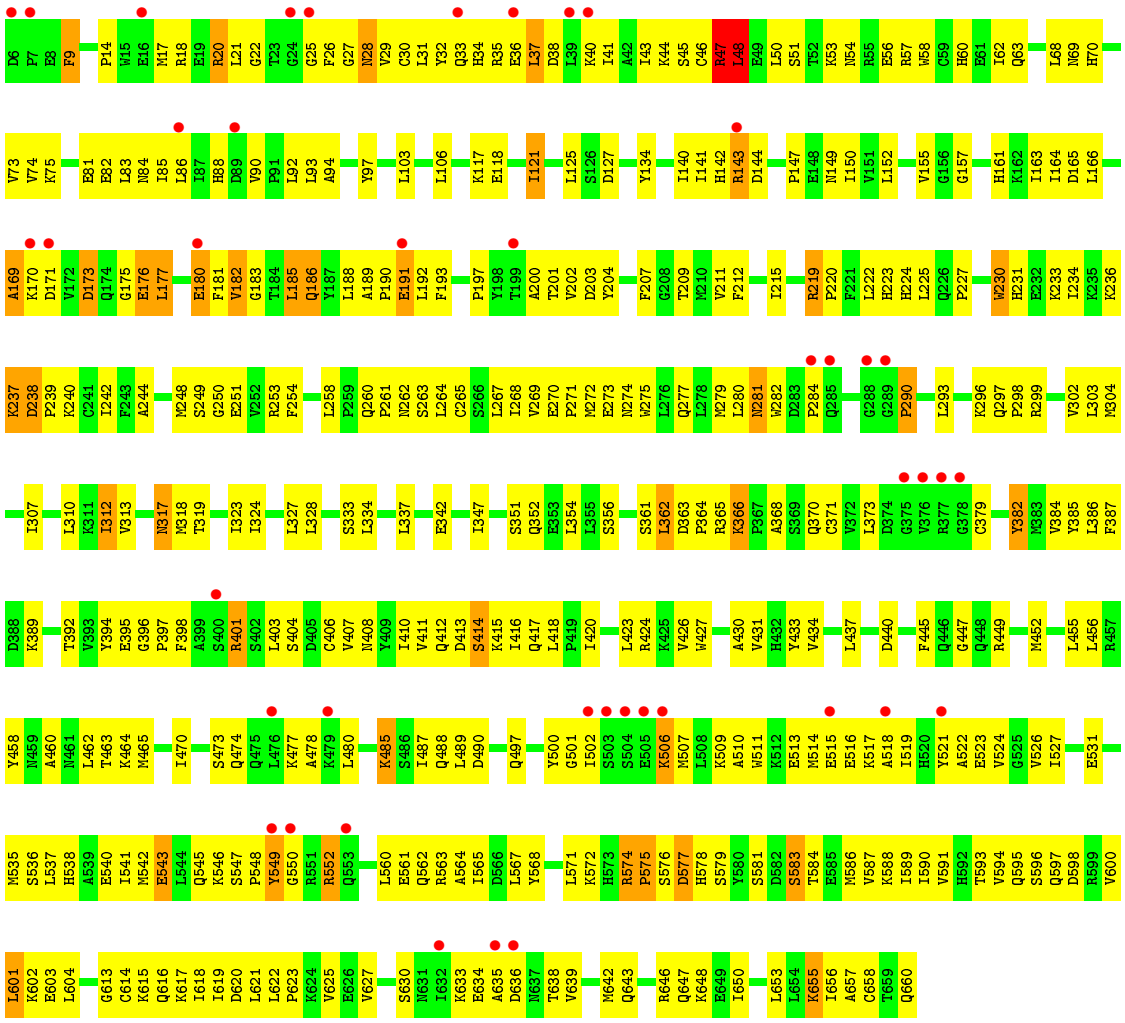
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain A:



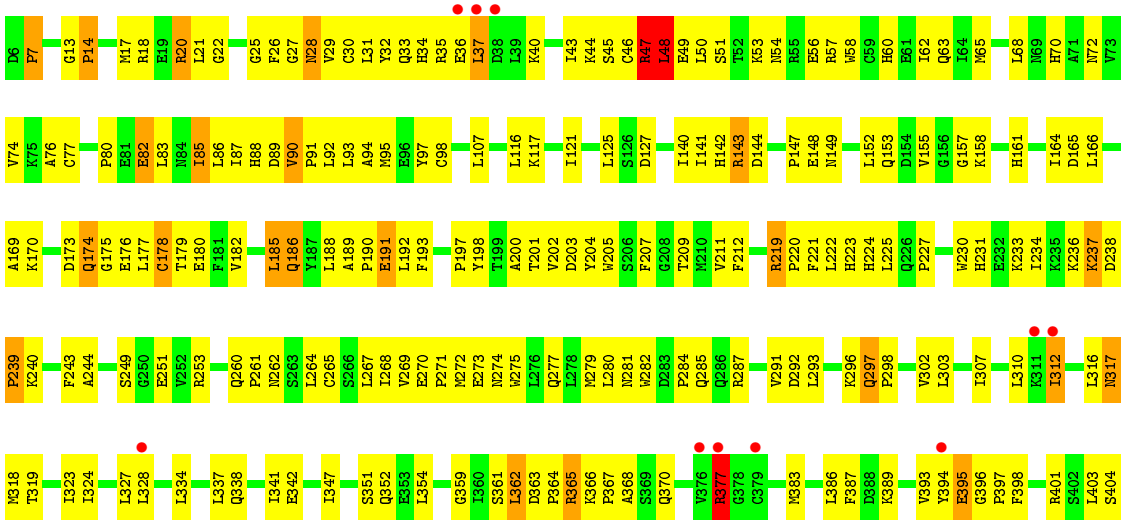
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

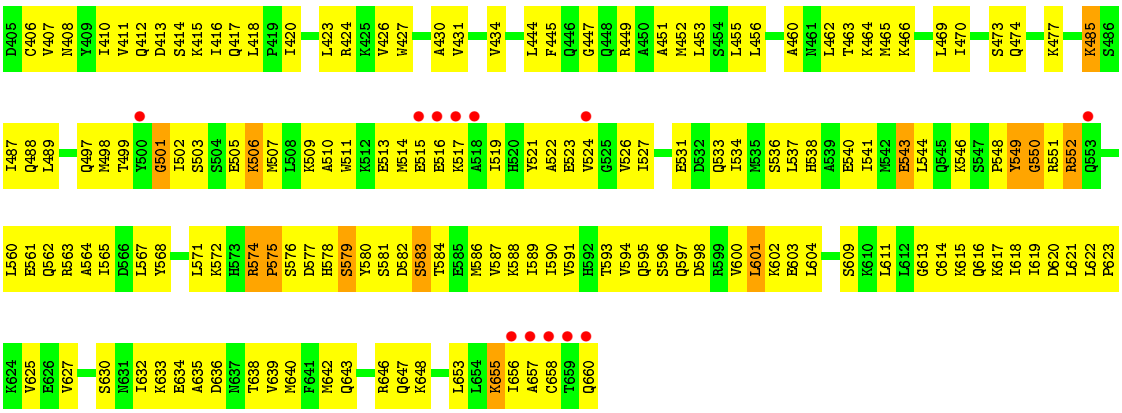
Chain B:



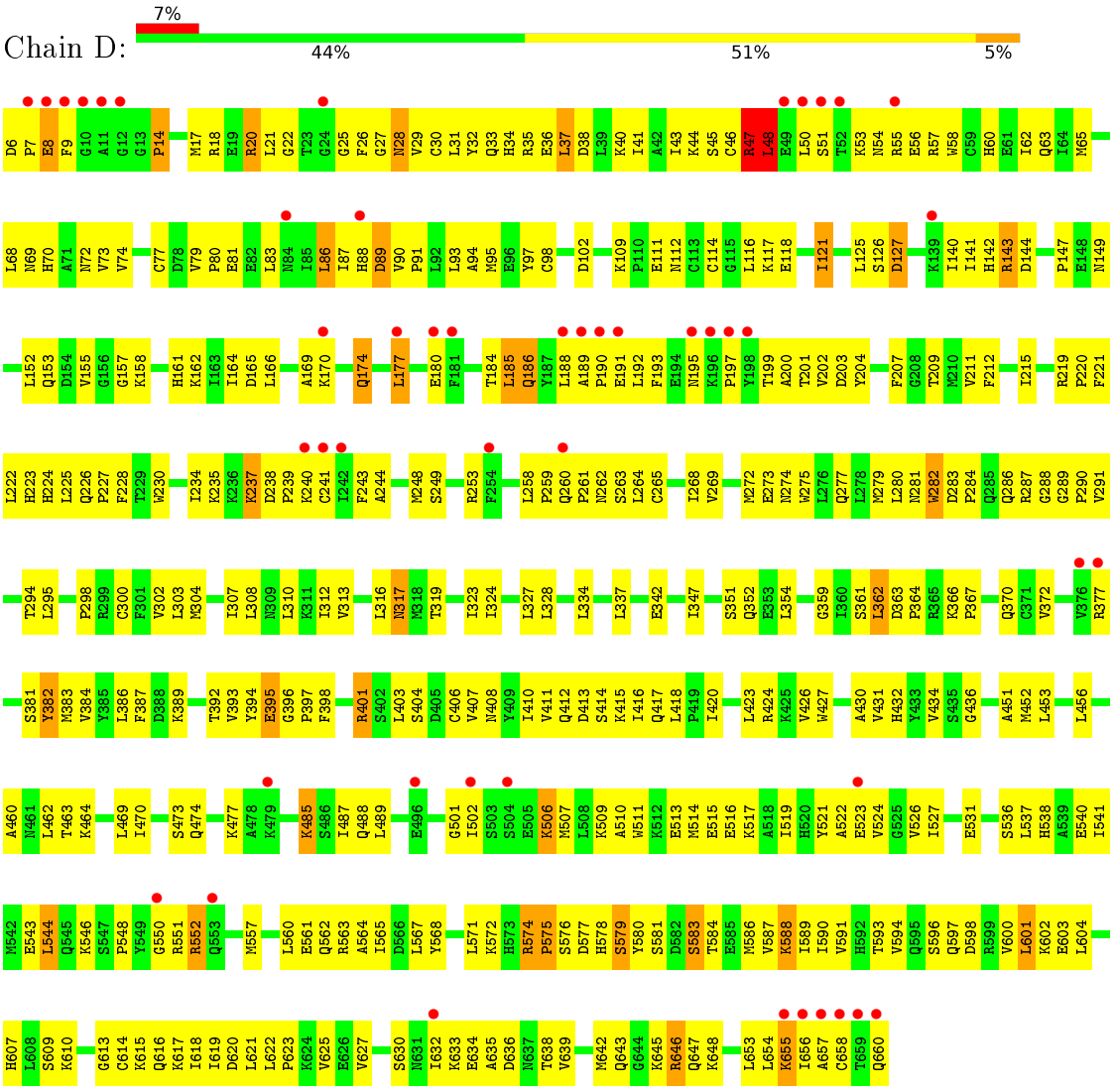
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain C:

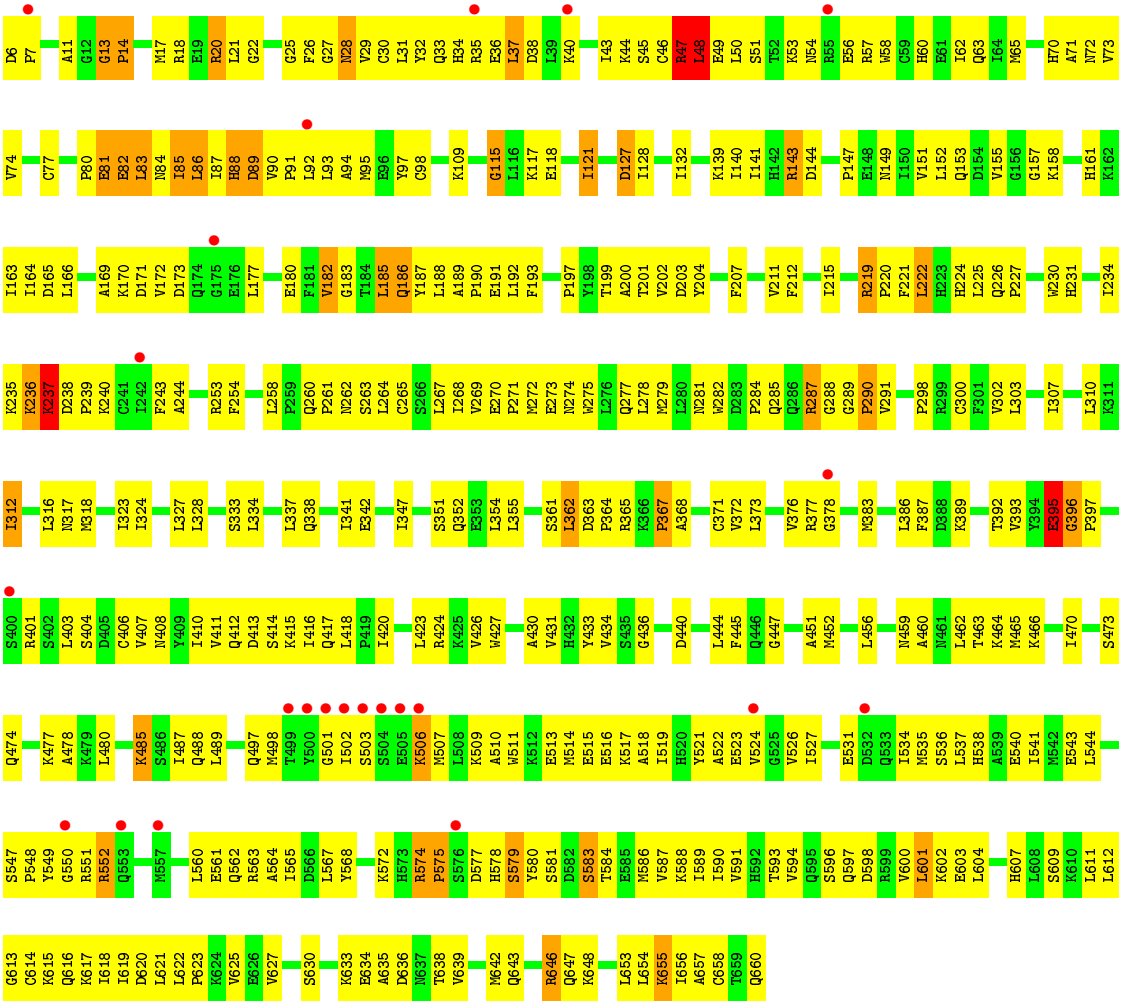




• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

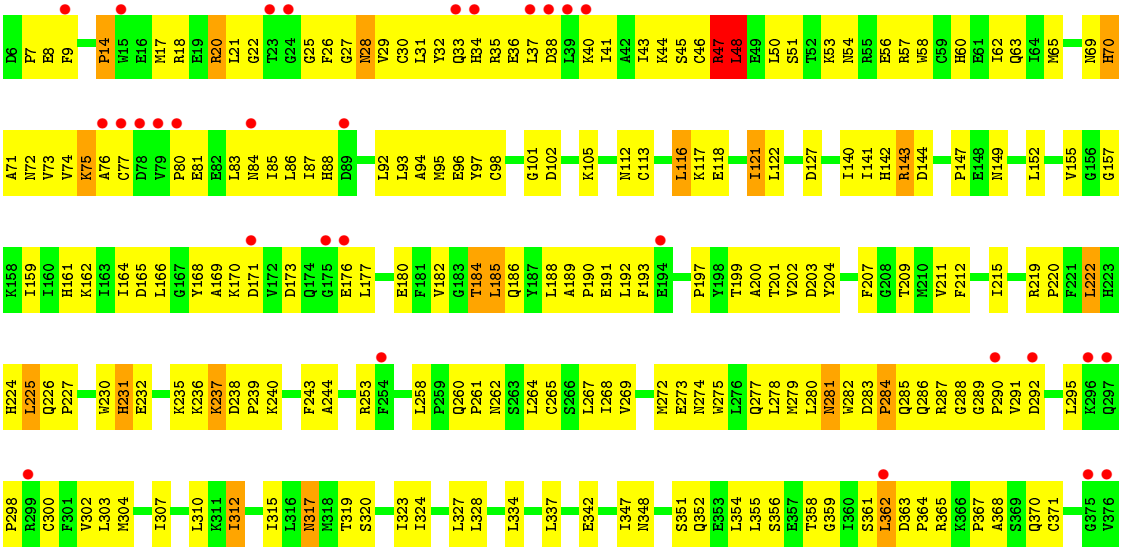


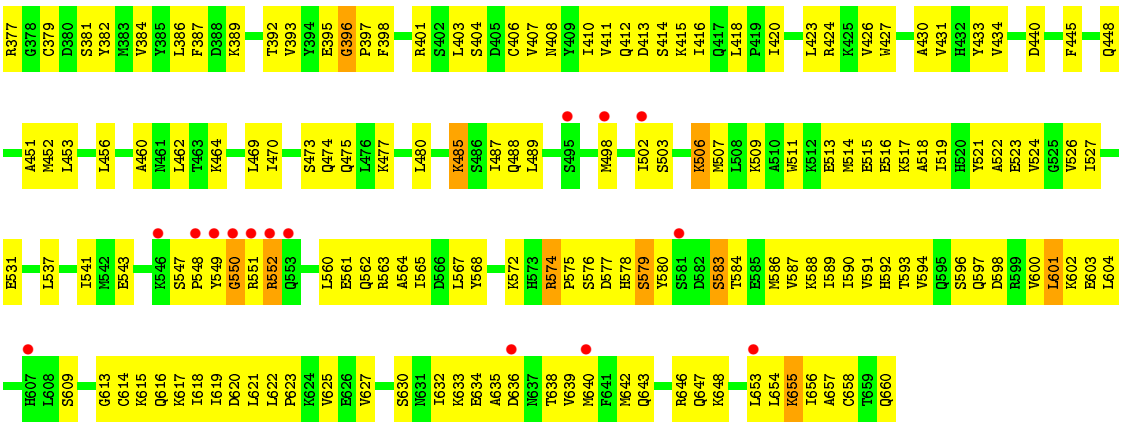
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

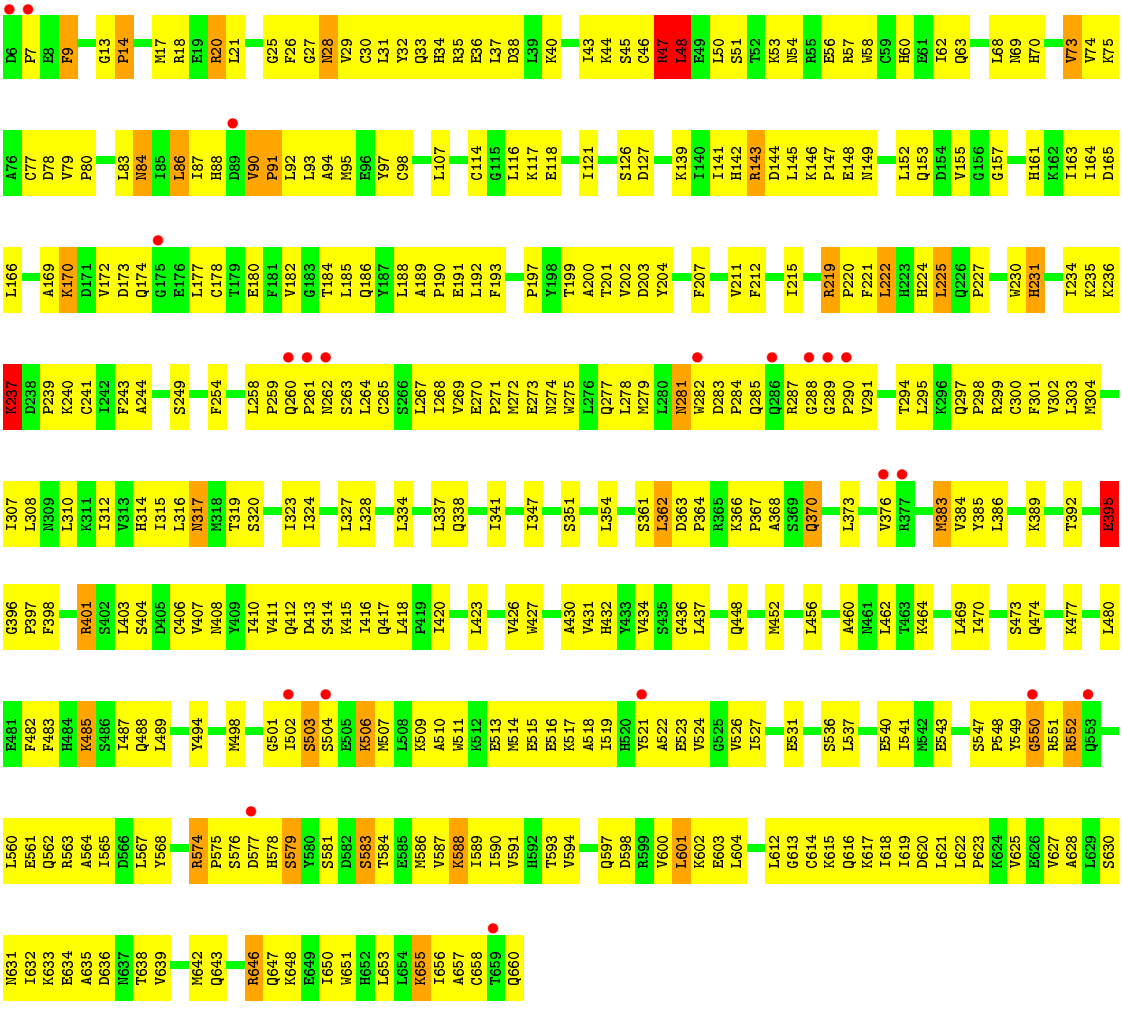
Chain F:





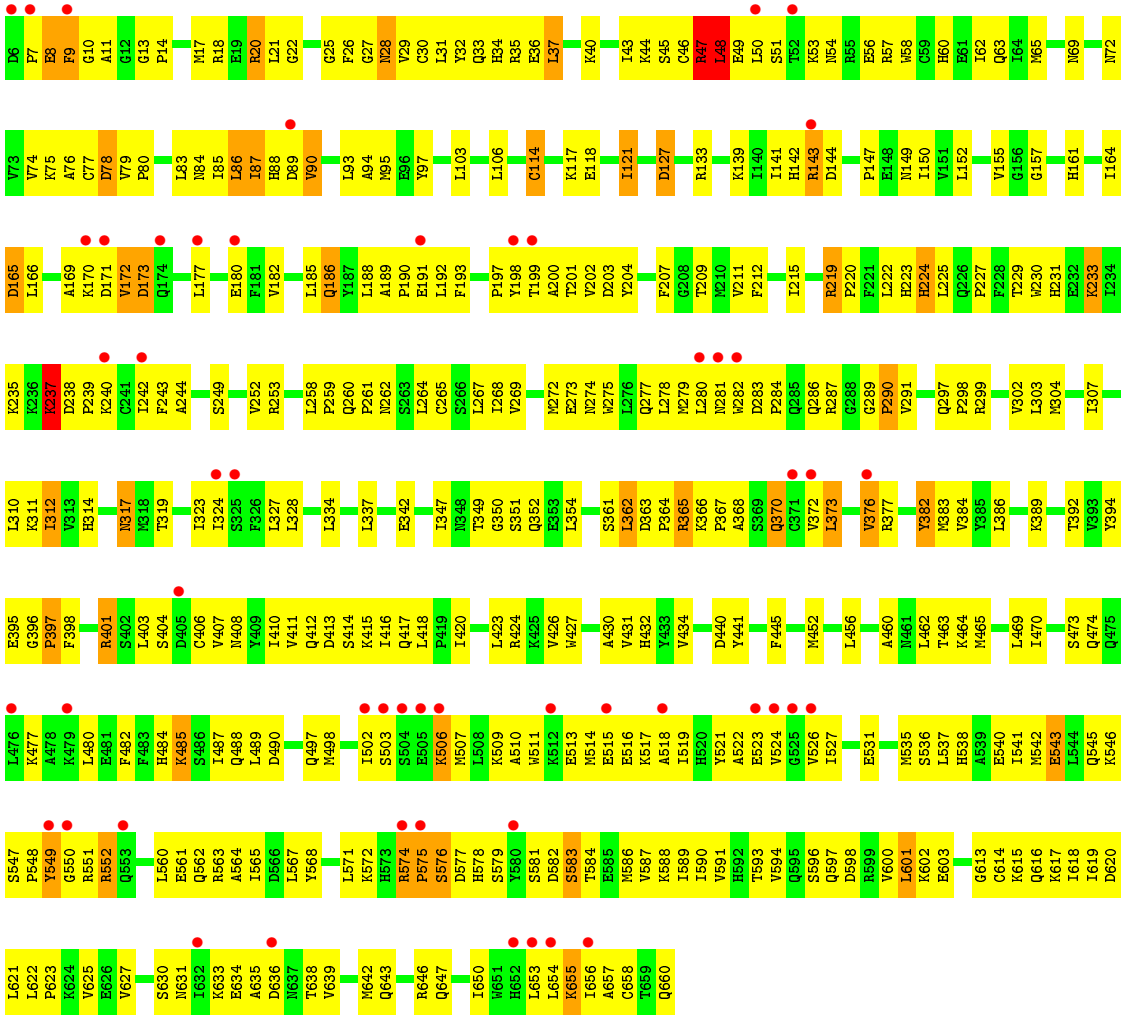
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain G:



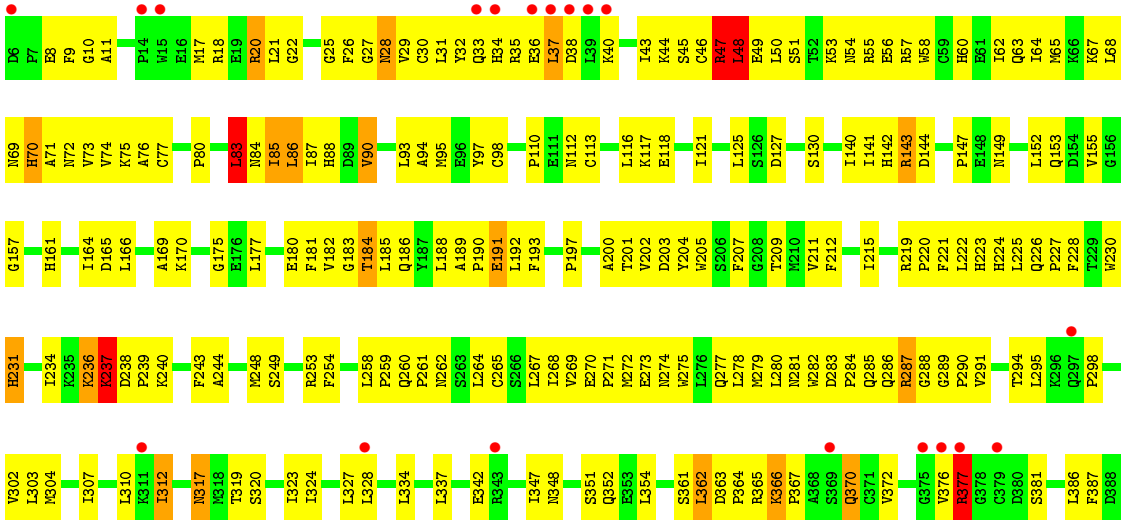
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

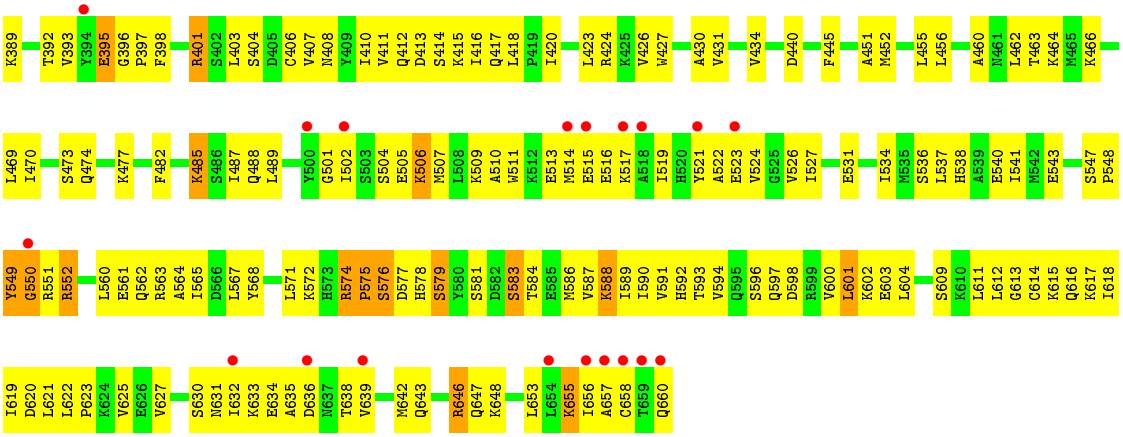
Chain H:



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

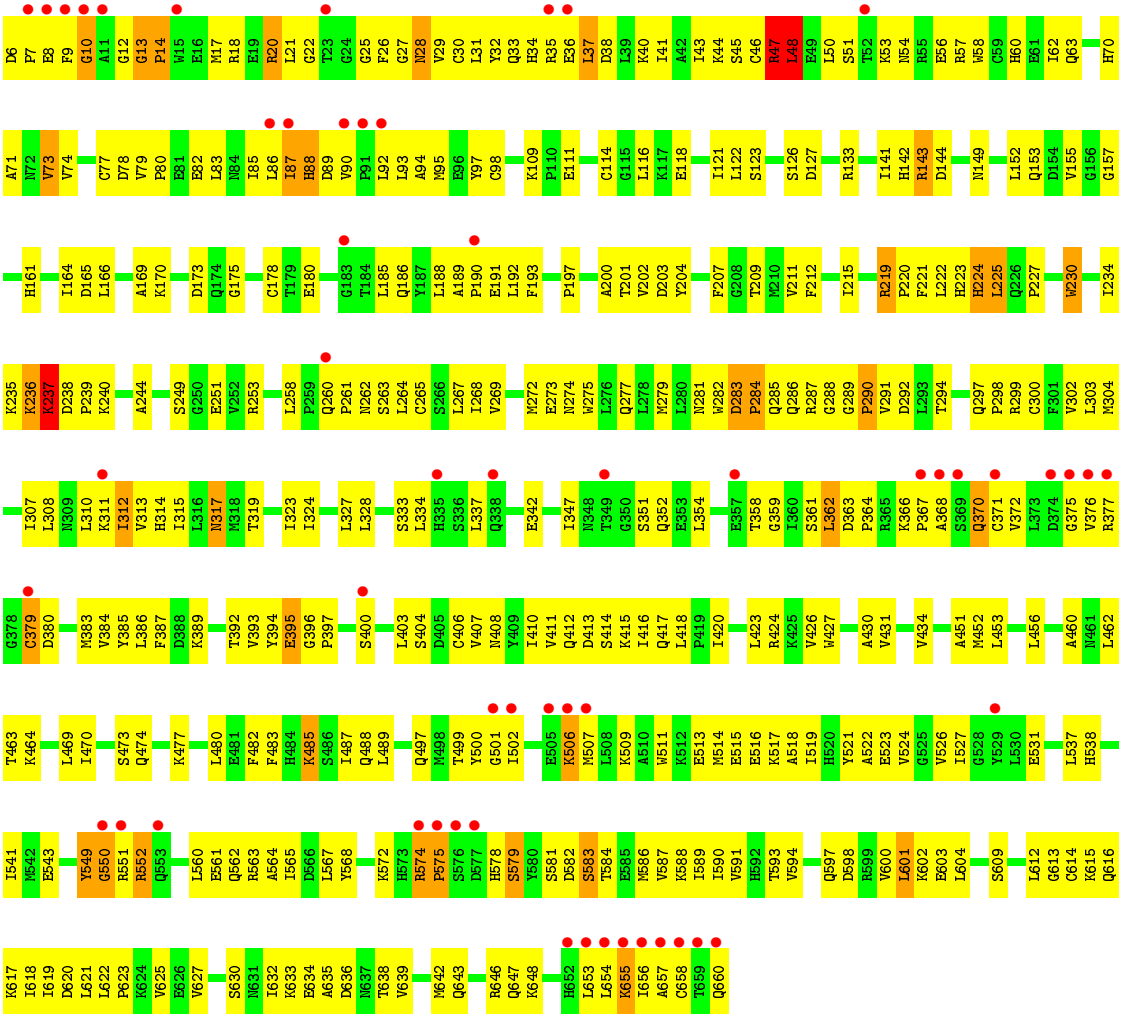
Chain I:





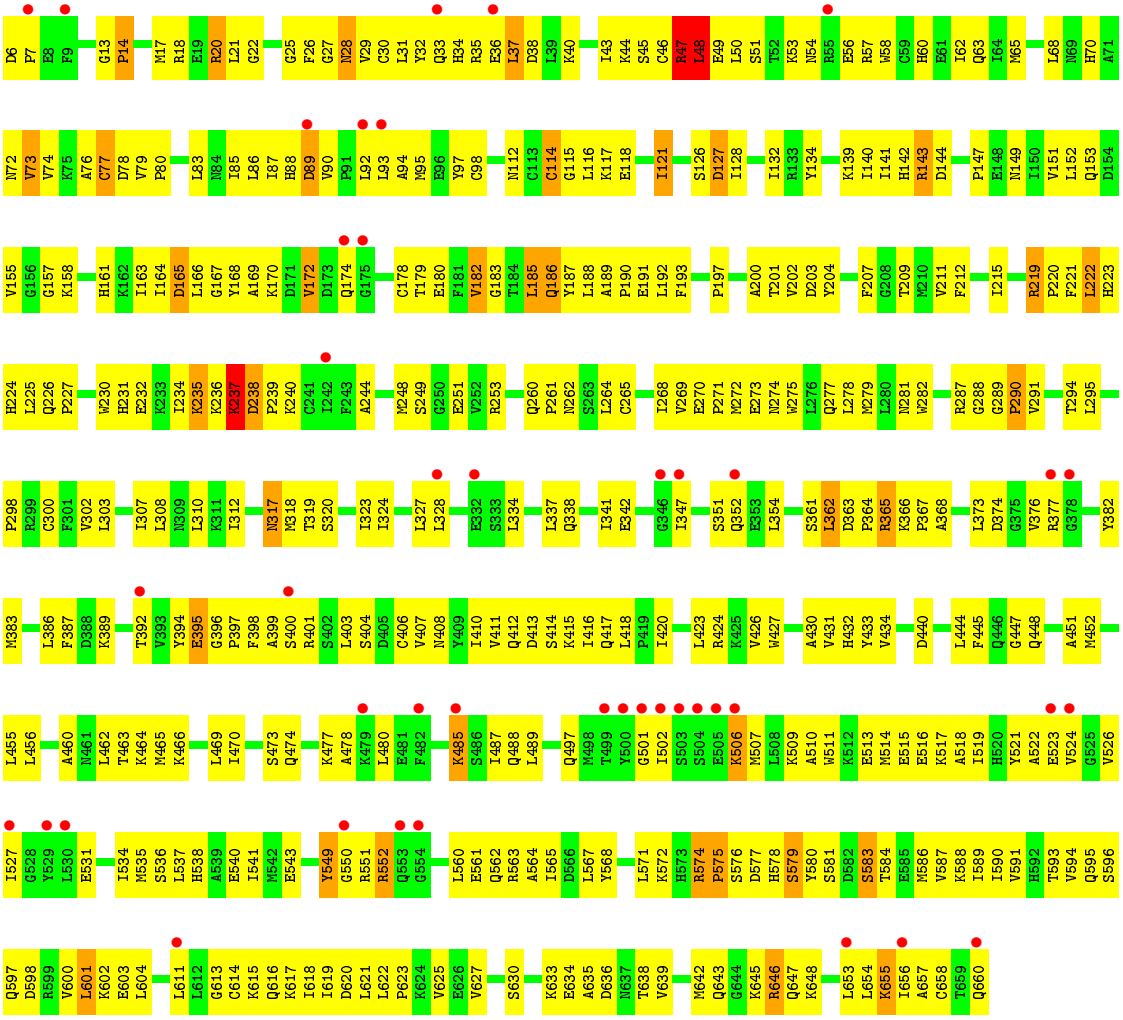
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain J:



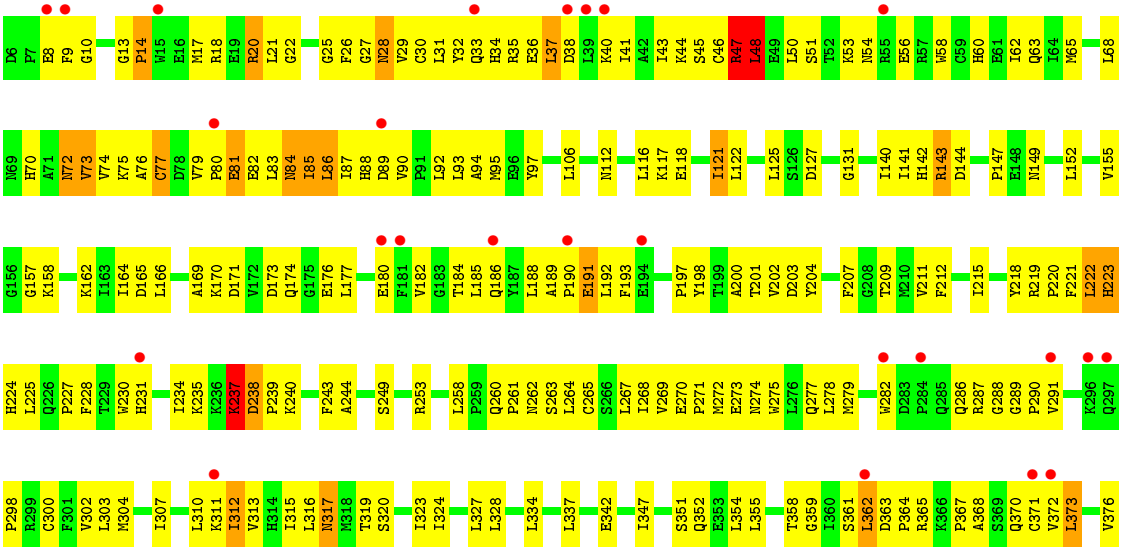
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

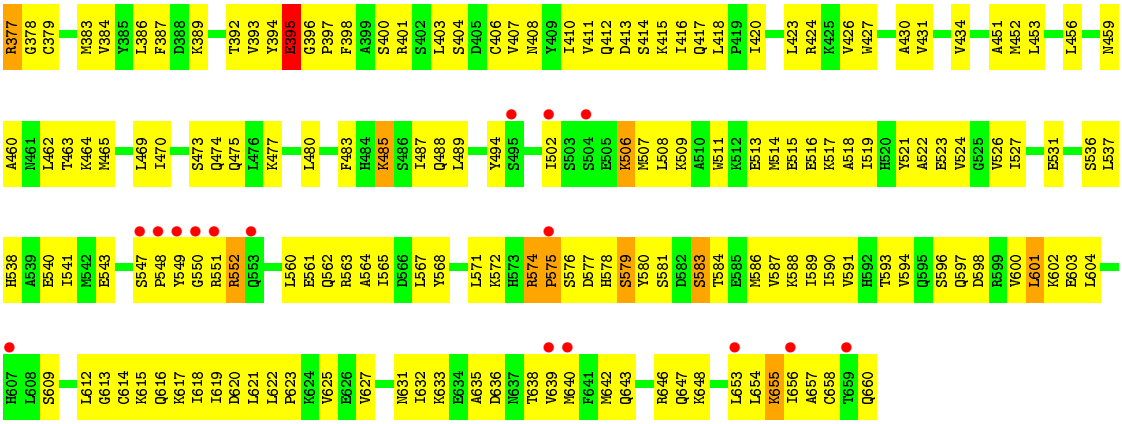
Chain K:



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain L:




R377 G378 C379 M383 V384 Y385 L386 F387 D388 K389 T392 V393 Y394 E395 G396 P397 F398 A399 S400 R401 S402 L403 S404 D405 C406 V407 N408 Y409 I410 V411 Q412 D413 S414 K415 I416 Q417 L418 P419 I420 L423 R424 K425 V426 W427 A430 V431 V434 A451 M452 L453 L456 N459
A460 N461 L462 T463 K464 M465 L469 I470 S473 Q474 Q475 L476 K477 L480 F483 H484 K485 S486 I487 Q488 L489 Y494 S495 I502 S503 S504 E505 K506 M507 L508 K509 A510 W511 K512 E513 M514 E515 E516 K517 A518 I519 H520 Y521 A522 E523 V524 G525 V526 I527 E531 S536 L537
H538 A539 E540 I541 M542 E543 S547 P548 Y549 G550 R551 R552 Q553 L560 E561 Q562 R563 A564 I565 D566 L567 Y568 L571 K572 H573 R574 P575 S576 D577 H578 S579 Y580 S581 D582 S583 T584 E585 M586 V587 K588 I589 I590 V591 H592 T593 V594 Q595 S596 Q597 D598 R599 V600 L601 K602 E603 L604
H607 L608 S609 L612 G613 C614 K615 Q616 K617 I618 I619 D620 L621 L622 P623 K624 V625 E626 V627 N631 I632 K633 E634 A635 D636 N637 T638 V639 M640 F641 W642 Q643 R646 Q647 K648 L653 L654 K655 I656 A657 C658 I659 Q660

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	174.51Å 186.94Å 275.83Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	29.94 – 4.50 44.79 – 4.44	Depositor EDS
% Data completeness (in resolution range)	68.1 (29.94-4.50) 80.6 (44.79-4.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.276 0.241 , 0.275	Depositor DCC
R_{free} test set	3450 reflections (4.02%)	DCC
Wilson B-factor (Å^2)	178.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 311.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	65132	wwPDB-VP
Average B, all atoms (Å^2)	267.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5998e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z4K, PDX, 5TJ, 5LS, 5TH, GLC, 5TL, 5TM, 5TK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/5370	0.43	0/7239
1	B	0.27	0/5370	0.42	0/7239
1	C	0.27	0/5370	0.43	0/7239
1	D	0.27	0/5370	0.43	0/7239
1	E	0.28	0/5370	0.43	0/7239
1	F	0.27	0/5370	0.43	0/7239
1	G	0.31	0/5370	0.44	0/7239
1	H	0.27	0/5370	0.42	0/7239
1	I	0.27	0/5370	0.43	0/7239
1	J	0.27	0/5370	0.43	0/7239
1	K	0.28	0/5370	0.43	0/7239
1	L	0.26	0/5370	0.42	0/7239
All	All	0.28	0/64440	0.43	0/86868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5263	0	5320	348	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5263	0	5320	349	0
1	C	5263	0	5320	334	0
1	D	5263	0	5320	341	0
1	E	5263	0	5320	343	0
1	F	5263	0	5320	325	0
1	G	5263	0	5320	362	0
1	H	5263	0	5320	325	0
1	I	5263	0	5320	326	0
1	J	5263	0	5320	325	0
1	K	5263	0	5320	344	0
1	L	5263	0	5320	346	0
2	A	26	0	0	3	0
2	B	26	0	0	2	0
2	C	26	0	0	4	0
2	D	26	0	0	2	0
2	E	26	0	0	3	0
2	F	26	0	0	6	0
2	G	26	0	0	5	0
2	H	26	0	0	2	0
2	I	26	0	0	6	0
2	J	26	0	0	2	0
2	K	26	0	0	3	0
2	L	26	0	0	2	0
3	A	40	0	0	1	0
3	B	40	0	0	2	0
3	C	40	0	0	1	0
3	D	80	0	0	1	0
3	E	40	0	0	0	0
3	F	40	0	0	0	0
3	G	40	0	0	0	0
3	H	60	0	0	1	0
3	I	40	0	0	0	0
3	J	40	0	0	2	0
3	K	40	0	0	0	0
3	L	60	0	0	0	0
4	A	22	0	18	1	0
4	B	22	0	18	3	0
4	C	22	0	18	3	0
4	D	22	0	18	0	0
4	E	22	0	18	3	0
4	F	22	0	18	2	0
4	G	22	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	22	0	18	1	0
4	I	22	0	18	4	0
4	J	22	0	18	7	0
4	K	22	0	18	0	0
4	L	22	0	18	4	0
5	A	38	0	20	0	0
5	B	38	0	20	2	0
5	C	38	0	20	1	0
5	D	38	0	20	0	0
5	E	38	0	20	0	0
5	F	38	0	20	0	0
5	G	38	0	20	0	0
5	H	19	0	10	0	0
5	I	38	0	20	0	0
5	J	38	0	20	4	0
5	K	38	0	20	1	0
5	L	57	0	30	2	0
6	A	34	0	0	0	0
6	D	34	0	0	1	0
6	H	34	0	0	0	0
6	I	34	0	0	0	0
7	A	13	0	0	0	0
7	C	13	0	0	1	0
7	G	13	0	0	0	0
7	I	13	0	0	0	0
8	A	17	0	0	0	0
8	C	17	0	0	1	0
8	G	17	0	0	0	0
8	I	17	0	0	0	0
9	B	17	0	0	0	0
9	C	17	0	0	1	0
9	G	17	0	0	0	0
9	J	17	0	0	0	0
10	B	15	0	0	0	0
10	C	15	0	0	2	0
10	H	15	0	0	0	0
10	J	15	0	0	0	0
All	All	65132	0	64296	3919	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (3919) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:701:5TL:CAS	2:J:701:5TL:NAY	1.99	1.20
2:G:701:5TL:NAY	2:G:701:5TL:CAS	2.00	1.18
2:D:701:5TL:CAS	2:D:701:5TL:NAY	1.99	1.17
2:K:701:5TL:CAS	2:K:701:5TL:NAY	2.00	1.17
2:A:701:5TL:NAY	2:A:701:5TL:CAS	2.00	1.16
2:B:701:5TL:NAY	2:B:701:5TL:CAS	2.00	1.16
2:F:701:5TL:NAY	2:F:701:5TL:CAS	1.98	1.15
2:E:701:5TL:CAS	2:E:701:5TL:NAY	1.99	1.14
2:I:701:5TL:NAY	2:I:701:5TL:CAS	1.99	1.14
2:H:701:5TL:NAY	2:H:701:5TL:CAS	2.00	1.13
2:C:701:5TL:CAS	2:C:701:5TL:NAY	1.99	1.12
2:L:701:5TL:CAS	2:L:701:5TL:NAY	1.99	1.12
1:I:185:LEU:HD11	1:I:188:LEU:HB3	1.38	1.03
1:C:477:LYS:HB2	1:C:524:VAL:HG21	1.43	1.01
1:J:227:PRO:HA	1:J:230:TRP:HB2	1.44	1.00
1:L:185:LEU:HD11	1:L:188:LEU:HB3	1.42	1.00
1:A:227:PRO:HA	1:A:230:TRP:HB3	1.42	0.99
1:L:563:ARG:HH12	4:L:708:GLC:H2	1.27	0.99
1:L:222:LEU:HB3	1:L:225:LEU:HD12	1.42	0.98
1:J:13:GLY:H	1:J:14:PRO:HD3	1.26	0.96
1:F:434:VAL:HG13	1:F:593:THR:HG21	1.46	0.96
1:H:142:HIS:ND1	1:H:169:ALA:HB2	1.81	0.96
1:A:13:GLY:H	1:A:14:PRO:HD3	1.30	0.95
1:L:434:VAL:HG13	1:L:593:THR:HG21	1.46	0.95
1:C:434:VAL:HG13	1:C:593:THR:HG21	1.47	0.95
1:F:260:GLN:HE21	1:F:261:PRO:HA	1.32	0.95
1:B:185:LEU:HD11	1:B:188:LEU:HB3	1.47	0.94
1:A:185:LEU:HD11	1:A:188:LEU:HB3	1.47	0.94
1:C:260:GLN:HE21	1:C:261:PRO:HA	1.33	0.94
1:K:260:GLN:HE21	1:K:261:PRO:HA	1.32	0.94
1:L:477:LYS:HB2	1:L:524:VAL:HG21	1.50	0.94
1:I:260:GLN:HE21	1:I:261:PRO:HA	1.33	0.94
1:A:396:GLY:H	1:A:397:PRO:HD3	1.29	0.94
1:E:260:GLN:HE21	1:E:261:PRO:HA	1.33	0.94
1:G:260:GLN:HE21	1:G:261:PRO:HA	1.32	0.94
1:L:260:GLN:HE21	1:L:261:PRO:HA	1.33	0.93
1:C:227:PRO:HA	1:C:230:TRP:HB3	1.49	0.93
1:I:477:LYS:HB2	1:I:524:VAL:HG21	1.48	0.93
1:J:477:LYS:HB2	1:J:524:VAL:HG21	1.50	0.93
1:E:328:LEU:HD13	1:E:368:ALA:HB1	1.48	0.93
1:A:260:GLN:HE21	1:A:261:PRO:HA	1.34	0.92
1:G:328:LEU:HD13	1:G:368:ALA:HB1	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASP:H	1:F:579:SER:HB3	1.32	0.92
1:H:260:GLN:HE21	1:H:261:PRO:HA	1.34	0.92
1:B:260:GLN:HE21	1:B:261:PRO:HA	1.35	0.92
1:B:434:VAL:HG13	1:B:593:THR:HG21	1.52	0.91
1:A:462:LEU:HD22	1:A:618:ILE:HG23	1.52	0.91
1:H:50:LEU:HD22	1:H:90:VAL:HG11	1.51	0.91
1:D:185:LEU:HD11	1:D:188:LEU:HB3	1.53	0.91
1:D:260:GLN:HE21	1:D:261:PRO:HA	1.34	0.91
1:K:185:LEU:HD11	1:K:188:LEU:HB3	1.53	0.90
1:J:260:GLN:HE21	1:J:261:PRO:HA	1.34	0.90
1:B:290:PRO:HB2	1:B:299:ARG:HB2	1.53	0.90
1:C:74:VAL:HG21	1:C:95:MET:HE3	1.53	0.90
1:F:462:LEU:HD22	1:F:618:ILE:HG23	1.52	0.90
1:F:477:LYS:HB2	1:F:524:VAL:HG21	1.53	0.89
1:C:395:GLU:HG2	1:C:397:PRO:HD3	1.52	0.89
1:I:278:LEU:HD23	1:I:288:GLY:HA2	1.51	0.89
1:H:434:VAL:HG13	1:H:593:THR:HG21	1.55	0.89
1:E:373:LEU:HB2	1:E:378:GLY:HA3	1.56	0.88
1:F:186:GLN:HE22	1:F:227:PRO:HD3	1.38	0.88
1:I:366:LYS:HD2	1:I:367:PRO:HD2	1.54	0.88
1:E:477:LYS:HB2	1:E:524:VAL:HG21	1.55	0.88
1:H:373:LEU:HD21	1:H:382:TYR:HB2	1.55	0.87
1:D:219:ARG:HD3	1:D:224:HIS:H	1.39	0.87
1:D:395:GLU:HG3	1:D:397:PRO:HD3	1.57	0.87
1:K:477:LYS:HB2	1:K:524:VAL:HG21	1.57	0.86
4:L:705:GLC:H62	5:L:706:PDX:H5	1.57	0.86
1:B:363:ASP:HB3	1:B:370:GLN:HE22	1.39	0.86
1:F:278:LEU:HD23	1:F:288:GLY:HA2	1.57	0.86
1:L:462:LEU:HD22	1:L:618:ILE:HG23	1.56	0.86
1:A:112:ASN:HD22	1:A:116:LEU:HA	1.40	0.86
1:B:227:PRO:HA	1:B:230:TRP:HB2	1.58	0.86
1:I:434:VAL:HG13	1:I:593:THR:HG21	1.54	0.86
1:E:396:GLY:H	1:E:397:PRO:HD3	1.40	0.85
1:F:219:ARG:HE	1:F:224:HIS:H	1.23	0.85
1:B:73:VAL:HG23	1:B:163:ILE:HB	1.55	0.85
1:J:222:LEU:HD23	1:J:234:ILE:HD11	1.59	0.85
1:K:595:GLN:HE21	5:K:707:PDX:H6C1	1.42	0.84
1:E:434:VAL:HG13	1:E:593:THR:HG21	1.59	0.84
1:F:237:LYS:HG3	1:F:282:TRP:HB2	1.57	0.84
1:C:185:LEU:HD11	1:C:188:LEU:HB3	1.57	0.84
1:H:477:LYS:HB2	1:H:524:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:PRO:HA	1:F:230:TRP:HB3	1.60	0.84
1:C:219:ARG:HH21	1:C:223:HIS:HB2	1.43	0.84
1:D:434:VAL:HG13	1:D:593:THR:HG21	1.60	0.83
1:H:577:ASP:H	1:L:579:SER:HB3	1.43	0.83
1:K:434:VAL:HG13	1:K:593:THR:HG21	1.58	0.83
1:A:434:VAL:HG13	1:A:593:THR:HG21	1.59	0.83
1:D:477:LYS:HB2	1:D:524:VAL:HG21	1.60	0.83
1:K:654:LEU:HD12	1:L:654:LEU:HD12	1.61	0.83
1:C:219:ARG:HE	1:C:223:HIS:HA	1.44	0.82
1:K:502:ILE:HD12	1:L:654:LEU:HD11	1.59	0.82
1:C:86:LEU:HD23	1:C:92:LEU:HD11	1.61	0.82
1:I:502:ILE:HD11	1:J:654:LEU:HD11	1.61	0.82
1:A:477:LYS:HB2	1:A:524:VAL:HG21	1.61	0.82
1:J:462:LEU:HD22	1:J:618:ILE:HG23	1.62	0.82
1:L:65:MET:HB3	1:L:76:ALA:HB2	1.61	0.82
1:G:222:LEU:H	1:G:230:TRP:HE1	1.25	0.81
1:C:577:ASP:H	1:E:579:SER:HB3	1.46	0.81
1:K:48:LEU:HD13	1:K:48:LEU:H	1.45	0.81
1:B:396:GLY:H	1:B:397:PRO:HD3	1.46	0.81
1:K:185:LEU:HD13	1:K:186:GLN:H	1.45	0.81
1:J:408:ASN:HD21	1:L:26:PHE:HD1	1.27	0.81
1:G:199:THR:HG21	1:G:285:GLN:HE22	1.45	0.81
1:E:13:GLY:H	1:E:14:PRO:HD3	1.45	0.81
1:A:395:GLU:HG3	1:A:397:PRO:HD3	1.62	0.81
1:G:220:PRO:O	1:G:243:PHE:HA	1.80	0.81
1:B:48:LEU:HD13	1:B:48:LEU:H	1.46	0.81
1:G:434:VAL:HG13	1:G:593:THR:HG21	1.62	0.80
1:B:477:LYS:HB2	1:B:524:VAL:HG21	1.62	0.80
1:E:654:LEU:HD12	1:F:654:LEU:HD12	1.64	0.80
1:I:48:LEU:HD13	1:I:48:LEU:H	1.47	0.80
1:C:297:GLN:HG3	1:C:298:PRO:HD2	1.63	0.80
1:C:48:LEU:H	1:C:48:LEU:HD13	1.47	0.80
1:G:48:LEU:HD13	1:G:48:LEU:H	1.47	0.80
1:J:434:VAL:HG13	1:J:593:THR:HG21	1.64	0.80
1:K:86:LEU:HD13	1:K:92:LEU:HD11	1.63	0.80
1:H:86:LEU:HD23	1:H:87:ILE:HG13	1.63	0.80
1:D:142:HIS:ND1	1:D:169:ALA:HB2	1.96	0.80
1:G:222:LEU:HB2	1:G:230:TRP:CD1	2.16	0.80
1:L:50:LEU:HD22	1:L:90:VAL:HG11	1.63	0.80
1:G:501:GLY:HA3	1:H:655:LYS:HE2	1.64	0.80
1:G:290:PRO:HB2	1:G:299:ARG:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:431:VAL:HG21	1:J:568:TYR:HB2	1.63	0.79
1:A:236:LYS:HD3	1:A:236:LYS:H	1.46	0.79
1:E:48:LEU:HD13	1:E:48:LEU:H	1.47	0.79
1:H:48:LEU:H	1:H:48:LEU:HD13	1.48	0.79
1:H:238:ASP:HB3	1:H:239:PRO:HD2	1.65	0.79
1:A:48:LEU:HD13	1:A:48:LEU:H	1.48	0.79
1:K:240:LYS:HD2	1:K:277:GLN:HB3	1.63	0.79
1:L:227:PRO:HA	1:L:230:TRP:HB3	1.63	0.79
1:I:577:ASP:H	1:K:579:SER:HB3	1.48	0.78
1:A:222:LEU:HB2	1:A:230:TRP:HD1	1.46	0.78
1:C:462:LEU:HD22	1:C:618:ILE:HG23	1.63	0.78
1:D:589:ILE:HD12	1:D:589:ILE:H	1.49	0.78
1:G:477:LYS:HB2	1:G:524:VAL:HG21	1.63	0.78
1:J:395:GLU:HG3	1:J:397:PRO:HD3	1.65	0.78
1:L:13:GLY:H	1:L:14:PRO:HD3	1.48	0.78
1:L:237:LYS:HD2	1:L:238:ASP:H	1.47	0.78
1:K:73:VAL:HG23	1:K:163:ILE:HB	1.64	0.78
1:F:395:GLU:HG2	1:F:396:GLY:H	1.49	0.78
1:J:48:LEU:H	1:J:48:LEU:HD13	1.48	0.78
1:G:502:ILE:HD12	1:H:654:LEU:HD11	1.64	0.78
1:I:219:ARG:HE	1:I:223:HIS:HA	1.49	0.78
1:L:328:LEU:HD21	1:L:337:LEU:HD13	1.66	0.78
1:A:320:SER:HA	1:A:398:PHE:HB3	1.66	0.77
1:D:48:LEU:H	1:D:48:LEU:HD13	1.48	0.77
1:K:46:CYS:H	1:K:86:LEU:HD23	1.48	0.77
1:L:311:LYS:HD2	1:L:372:VAL:HG21	1.65	0.77
1:F:48:LEU:H	1:F:48:LEU:HD13	1.48	0.77
1:F:420:ILE:HB	1:F:580:TYR:HB3	1.65	0.77
1:H:142:HIS:HA	1:H:169:ALA:HB1	1.64	0.77
1:D:408:ASN:HD21	1:F:26:PHE:HD1	1.32	0.77
1:I:221:PHE:HB2	1:I:230:TRP:HE1	1.50	0.77
1:J:589:ILE:HD12	1:J:589:ILE:H	1.50	0.77
1:L:219:ARG:HH21	1:L:224:HIS:H	1.28	0.77
1:B:589:ILE:HD12	1:B:589:ILE:H	1.49	0.77
1:G:185:LEU:HD13	1:G:186:GLN:N	1.99	0.77
1:H:589:ILE:HD12	1:H:589:ILE:H	1.49	0.77
1:F:328:LEU:HD21	1:F:337:LEU:HD13	1.67	0.77
1:E:288:GLY:HA3	1:E:300:CYS:SG	2.25	0.76
1:A:579:SER:HB3	1:E:577:ASP:H	1.49	0.76
1:L:48:LEU:HD13	1:L:48:LEU:H	1.49	0.76
1:C:237:LYS:HD3	1:C:282:TRP:HB2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:GLN:HE22	1:F:7:PRO:HB3	1.50	0.76
1:H:227:PRO:HA	1:H:230:TRP:HB3	1.67	0.76
1:K:589:ILE:H	1:K:589:ILE:HD12	1.51	0.76
1:G:73:VAL:HG22	1:G:74:VAL:H	1.49	0.76
1:L:33:GLN:HG3	1:L:40:LYS:HG2	1.67	0.76
1:C:328:LEU:HD21	1:C:337:LEU:HD13	1.68	0.76
1:C:589:ILE:HD12	1:C:589:ILE:H	1.51	0.76
1:G:33:GLN:HG3	1:G:40:LYS:HG2	1.68	0.76
1:L:589:ILE:H	1:L:589:ILE:HD12	1.50	0.76
1:F:33:GLN:HG3	1:F:40:LYS:HG2	1.67	0.75
1:G:46:CYS:H	1:G:86:LEU:HG	1.51	0.75
1:A:33:GLN:HG3	1:A:40:LYS:HG2	1.68	0.75
1:A:473:SER:HB2	1:A:524:VAL:HA	1.68	0.75
1:I:33:GLN:HG3	1:I:40:LYS:HG2	1.66	0.75
1:D:83:LEU:HG	1:D:86:LEU:HD11	1.67	0.75
1:G:462:LEU:HD22	1:G:618:ILE:HG23	1.66	0.75
1:B:33:GLN:HG3	1:B:40:LYS:HG2	1.69	0.75
1:G:185:LEU:HD11	1:G:188:LEU:HB3	1.69	0.75
1:G:589:ILE:H	1:G:589:ILE:HD12	1.50	0.75
1:H:33:GLN:HG3	1:H:40:LYS:HG2	1.69	0.75
1:B:417:GLN:HB3	1:B:581:SER:HB3	1.68	0.75
1:I:589:ILE:H	1:I:589:ILE:HD12	1.51	0.75
1:K:231:HIS:HB3	1:K:282:TRP:HH2	1.51	0.75
1:A:487:ILE:HG12	1:A:515:GLU:HB2	1.68	0.75
1:I:284:PRO:HA	1:I:287:ARG:HH21	1.52	0.75
1:F:589:ILE:HD12	1:F:589:ILE:H	1.51	0.74
1:G:91:PRO:C	1:G:92:LEU:HD12	2.08	0.74
1:K:224:HIS:O	1:K:225:LEU:HD22	1.86	0.74
1:K:79:VAL:HG11	1:K:83:LEU:HD13	1.68	0.74
1:A:589:ILE:HD12	1:A:589:ILE:H	1.51	0.74
1:K:403:LEU:H	1:K:403:LEU:HD23	1.52	0.74
1:D:328:LEU:HD21	1:D:337:LEU:HD13	1.68	0.74
1:D:420:ILE:HG21	1:D:578:HIS:H	1.50	0.74
1:E:563:ARG:HH12	4:E:706:GLC:H2	1.51	0.74
1:J:328:LEU:HD21	1:J:337:LEU:HD13	1.69	0.74
1:E:237:LYS:HE2	1:E:282:TRP:H	1.52	0.74
1:G:73:VAL:HG23	1:G:163:ILE:HB	1.70	0.74
1:C:33:GLN:HG3	1:C:40:LYS:HG2	1.67	0.74
1:H:328:LEU:HD21	1:H:337:LEU:HD13	1.70	0.74
1:J:33:GLN:HG3	1:J:40:LYS:HG2	1.68	0.74
1:D:33:GLN:HG3	1:D:40:LYS:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:ILE:H	1:E:589:ILE:HD12	1.53	0.74
1:F:65:MET:HB3	1:F:76:ALA:HB3	1.70	0.74
1:H:170:LYS:HG2	1:H:177:LEU:HG	1.68	0.74
1:G:222:LEU:HD22	1:G:230:TRP:HD1	1.52	0.74
1:H:240:LYS:HD2	1:H:277:GLN:HB3	1.69	0.74
1:H:564:ALA:HB2	1:H:589:ILE:HG21	1.69	0.74
1:I:328:LEU:HD21	1:I:337:LEU:HD13	1.69	0.74
1:I:423:LEU:HA	1:I:426:VAL:HG22	1.70	0.74
1:A:328:LEU:HD21	1:A:337:LEU:HD13	1.70	0.73
1:B:328:LEU:HD21	1:B:337:LEU:HD13	1.69	0.73
1:J:13:GLY:H	1:J:14:PRO:CD	2.01	0.73
1:J:18:ARG:HH21	1:J:33:GLN:HE22	1.36	0.73
1:L:18:ARG:HH21	1:L:33:GLN:HE22	1.36	0.73
1:B:334:LEU:HD22	1:B:366:LYS:O	1.88	0.73
1:E:564:ALA:HB2	1:E:589:ILE:HG21	1.70	0.73
1:G:328:LEU:HD21	1:G:337:LEU:HD13	1.70	0.73
1:H:424:ARG:NH1	1:H:572:LYS:HG2	2.03	0.73
1:D:63:GLN:HE22	1:D:174:GLN:HE22	1.33	0.73
1:G:231:HIS:HB3	1:G:282:TRP:HH2	1.53	0.73
1:B:415:LYS:HA	1:B:584:THR:HB	1.70	0.73
1:D:462:LEU:HD22	1:D:618:ILE:HG23	1.70	0.73
1:G:395:GLU:HG3	1:G:397:PRO:HD3	1.69	0.73
1:K:33:GLN:HG3	1:K:40:LYS:HG2	1.69	0.73
1:D:18:ARG:HH21	1:D:33:GLN:HE22	1.37	0.73
1:F:431:VAL:HG21	1:F:568:TYR:HB2	1.71	0.73
1:K:423:LEU:HA	1:K:426:VAL:HG22	1.70	0.73
1:C:501:GLY:HA3	1:D:655:LYS:HE2	1.69	0.73
1:I:462:LEU:HD22	1:I:618:ILE:HG23	1.68	0.73
1:G:18:ARG:HH21	1:G:33:GLN:HE22	1.37	0.73
4:J:705:GLC:H61	5:J:706:PDX:H3	1.71	0.73
1:G:502:ILE:HD13	1:G:656:ILE:HD12	1.70	0.73
1:K:328:LEU:HD21	1:K:337:LEU:HD13	1.71	0.73
1:B:564:ALA:HB2	1:B:589:ILE:HG21	1.70	0.73
1:E:423:LEU:HA	1:E:426:VAL:HG22	1.71	0.73
1:C:185:LEU:HD13	1:C:186:GLN:H	1.53	0.72
1:D:238:ASP:HB3	1:D:239:PRO:HD2	1.72	0.72
1:F:18:ARG:HH21	1:F:33:GLN:HE22	1.37	0.72
1:D:564:ALA:HB2	1:D:589:ILE:HG21	1.70	0.72
1:E:328:LEU:HD21	1:E:337:LEU:HD13	1.71	0.72
1:E:401:ARG:HH21	1:E:436:GLY:C	1.93	0.72
1:I:112:ASN:HB3	1:I:116:LEU:HD23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HH21	1:C:33:GLN:HE22	1.38	0.72
1:E:392:THR:HG22	1:E:616:GLN:HE22	1.54	0.72
1:G:221:PHE:HB2	1:G:230:TRP:HE1	1.55	0.72
1:K:564:ALA:HB2	1:K:589:ILE:HG21	1.71	0.72
1:G:579:SER:HB3	1:K:577:ASP:H	1.55	0.72
1:C:527:ILE:HG22	1:C:531:GLU:HG3	1.72	0.72
1:C:564:ALA:HB2	1:C:589:ILE:HG21	1.72	0.72
1:E:33:GLN:HG3	1:E:40:LYS:HG2	1.70	0.72
1:G:487:ILE:HG12	1:G:515:GLU:HB2	1.70	0.72
1:J:564:ALA:HB2	1:J:589:ILE:HG21	1.71	0.72
1:B:363:ASP:HB3	1:B:370:GLN:NE2	2.04	0.72
1:I:18:ARG:HH21	1:I:33:GLN:HE22	1.38	0.72
1:J:118:GLU:HB2	1:J:263:SER:O	1.90	0.72
1:L:564:ALA:HB2	1:L:589:ILE:HG21	1.70	0.72
1:A:564:ALA:HB2	1:A:589:ILE:HG21	1.72	0.71
1:D:310:LEU:HD22	1:D:327:LEU:HD21	1.72	0.71
1:G:396:GLY:H	1:G:397:PRO:HD3	1.54	0.71
1:H:290:PRO:HB2	1:H:299:ARG:HB2	1.72	0.71
1:A:523:GLU:HB2	1:A:632:ILE:HG12	1.73	0.71
1:C:423:LEU:HA	1:C:426:VAL:HG22	1.72	0.71
1:E:527:ILE:HG22	1:E:531:GLU:HG3	1.72	0.71
1:J:240:LYS:HD2	1:J:277:GLN:HB3	1.71	0.71
1:D:209:THR:HG22	1:D:220:PRO:HG3	1.70	0.71
1:E:73:VAL:HG23	1:E:163:ILE:HB	1.71	0.71
1:K:18:ARG:HH21	1:K:33:GLN:HE22	1.38	0.71
1:L:310:LEU:HD22	1:L:327:LEU:HD21	1.71	0.71
1:G:47:ARG:O	1:G:87:ILE:HD12	1.91	0.71
1:J:238:ASP:HB3	1:J:239:PRO:HD2	1.72	0.71
1:K:328:LEU:HD13	1:K:368:ALA:HB1	1.72	0.71
1:A:18:ARG:HH21	1:A:33:GLN:HE22	1.38	0.71
1:B:240:LYS:HB3	1:B:277:GLN:HB3	1.71	0.71
1:F:237:LYS:HE2	1:F:281:ASN:HA	1.72	0.71
1:F:396:GLY:H	1:F:397:PRO:HD3	1.55	0.71
1:L:13:GLY:N	1:L:14:PRO:HD3	2.05	0.71
1:F:310:LEU:HD22	1:F:327:LEU:HD21	1.71	0.71
1:F:564:ALA:HB2	1:F:589:ILE:HG21	1.70	0.71
1:L:141:ILE:HG23	1:L:170:LYS:HB2	1.72	0.71
1:B:18:ARG:HH21	1:B:33:GLN:HE22	1.38	0.71
1:F:83:LEU:HA	1:F:86:LEU:HD12	1.72	0.71
1:H:142:HIS:HA	1:H:169:ALA:CB	2.21	0.71
1:E:18:ARG:HH21	1:E:33:GLN:HE22	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LYS:HG2	1:G:177:LEU:HG	1.72	0.71
1:H:18:ARG:HH21	1:H:33:GLN:HE22	1.38	0.71
1:J:473:SER:HB2	1:J:524:VAL:HA	1.73	0.71
1:L:403:LEU:HD23	1:L:403:LEU:H	1.56	0.71
1:L:516:GLU:HA	1:L:519:ILE:HD12	1.73	0.71
1:C:48:LEU:HA	1:C:87:ILE:HG21	1.73	0.71
1:F:423:LEU:HA	1:F:426:VAL:HG22	1.72	0.71
1:F:516:GLU:HA	1:F:519:ILE:HD12	1.73	0.71
1:K:219:ARG:HH12	1:K:224:HIS:H	1.36	0.71
1:A:91:PRO:C	1:A:92:LEU:HD12	2.11	0.70
1:E:310:LEU:HD22	1:E:327:LEU:HD21	1.73	0.70
1:E:551:ARG:HB3	1:E:552:ARG:HH21	1.54	0.70
1:D:579:SER:HB3	1:F:577:ASP:H	1.55	0.70
1:F:328:LEU:HD13	1:F:368:ALA:HB1	1.73	0.70
1:K:310:LEU:HD22	1:K:327:LEU:HD21	1.73	0.70
1:B:392:THR:HG22	1:B:616:GLN:HE22	1.56	0.70
1:I:527:ILE:HG22	1:I:531:GLU:HG3	1.73	0.70
1:J:310:LEU:HD22	1:J:327:LEU:HD21	1.73	0.70
1:J:424:ARG:NH1	1:J:572:LYS:HG2	2.06	0.70
1:J:502:ILE:HD13	1:J:656:ILE:HD12	1.73	0.70
1:K:527:ILE:HG22	1:K:531:GLU:HG3	1.74	0.70
1:C:403:LEU:H	1:C:403:LEU:HD23	1.55	0.70
1:D:423:LEU:HA	1:D:426:VAL:HG22	1.72	0.70
1:E:550:GLY:HA3	1:E:604:LEU:HD13	1.74	0.70
1:G:231:HIS:HB3	1:G:282:TRP:CH2	2.26	0.70
1:D:431:VAL:HG21	1:D:568:TYR:HB2	1.72	0.70
1:B:403:LEU:HD23	1:B:403:LEU:H	1.56	0.70
1:E:403:LEU:H	1:E:403:LEU:HD23	1.57	0.70
1:G:564:ALA:HB2	1:G:589:ILE:HG21	1.73	0.70
1:I:564:ALA:HB2	1:I:589:ILE:HG21	1.74	0.70
1:G:516:GLU:HA	1:G:519:ILE:HD12	1.74	0.70
1:I:144:ASP:OD1	1:I:182:VAL:HG11	1.92	0.70
1:L:423:LEU:HA	1:L:426:VAL:HG22	1.73	0.70
1:A:112:ASN:ND2	1:A:116:LEU:HA	2.06	0.69
1:C:310:LEU:HD22	1:C:327:LEU:HD21	1.72	0.69
1:A:185:LEU:HD13	1:A:186:GLN:N	2.07	0.69
1:A:298:PRO:O	1:A:302:VAL:HG23	1.91	0.69
1:B:516:GLU:HA	1:B:519:ILE:HD12	1.74	0.69
1:E:417:GLN:HB3	1:E:581:SER:HB3	1.74	0.69
1:B:420:ILE:HD12	1:B:423:LEU:HB2	1.74	0.69
1:F:403:LEU:HD23	1:F:403:LEU:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLN:HG2	1:G:219:ARG:HD2	1.74	0.69
1:G:310:LEU:HD22	1:G:327:LEU:HD21	1.74	0.69
1:H:310:LEU:HD22	1:H:327:LEU:HD21	1.74	0.69
1:A:562:GLN:HA	1:A:565:ILE:HD12	1.74	0.69
1:D:29:VAL:HA	1:D:44:LYS:HA	1.75	0.69
1:K:72:ASN:HD21	1:K:127:ASP:HA	1.56	0.69
1:B:310:LEU:HD22	1:B:327:LEU:HD21	1.74	0.69
1:F:560:LEU:HD13	1:F:593:THR:HA	1.74	0.69
1:G:514:MET:HA	1:G:642:MET:HE1	1.75	0.69
1:H:502:ILE:HG21	1:H:656:ILE:HG21	1.75	0.69
1:J:423:LEU:HA	1:J:426:VAL:HG22	1.73	0.69
1:K:448:GLN:OE1	1:K:549:TYR:HB3	1.92	0.69
1:A:527:ILE:HG22	1:A:531:GLU:HG3	1.74	0.69
1:E:278:LEU:HD23	1:E:288:GLY:HA2	1.73	0.69
1:G:527:ILE:HG22	1:G:531:GLU:HG3	1.74	0.69
1:H:516:GLU:HA	1:H:519:ILE:HD12	1.74	0.69
1:L:186:GLN:NE2	1:L:227:PRO:HD3	2.08	0.69
1:A:420:ILE:HD12	1:A:423:LEU:HB2	1.73	0.69
1:B:423:LEU:HA	1:B:426:VAL:HG22	1.73	0.69
1:G:396:GLY:N	1:G:397:PRO:HD3	2.06	0.69
1:L:230:TRP:O	1:L:234:ILE:HG12	1.93	0.69
1:C:550:GLY:HA3	1:C:604:LEU:HD13	1.74	0.69
1:D:420:ILE:HG21	1:D:577:ASP:HB3	1.74	0.69
1:J:516:GLU:HA	1:J:519:ILE:HD12	1.75	0.69
1:J:46:CYS:SG	1:J:86:LEU:HD12	2.33	0.69
1:H:29:VAL:HA	1:H:44:LYS:HA	1.75	0.69
1:A:501:GLY:HA3	1:B:655:LYS:HE2	1.74	0.69
1:D:527:ILE:HG22	1:D:531:GLU:HG3	1.75	0.69
1:A:577:ASP:H	1:C:579:SER:HB2	1.58	0.69
1:A:516:GLU:HA	1:A:519:ILE:HD12	1.75	0.68
1:B:328:LEU:HD13	1:B:368:ALA:HB1	1.75	0.68
1:B:427:TRP:HZ3	1:B:567:LEU:HB3	1.59	0.68
1:G:577:ASP:H	1:I:579:SER:HB3	1.58	0.68
1:K:29:VAL:HA	1:K:44:LYS:HA	1.75	0.68
1:L:420:ILE:HD12	1:L:423:LEU:HB2	1.73	0.68
1:L:527:ILE:HG22	1:L:531:GLU:HG3	1.75	0.68
1:H:420:ILE:HD12	1:H:423:LEU:HB2	1.75	0.68
1:H:527:ILE:HG22	1:H:531:GLU:HG3	1.74	0.68
1:A:221:PHE:HB2	1:A:230:TRP:HE1	1.59	0.68
1:C:516:GLU:HA	1:C:519:ILE:HD12	1.74	0.68
1:G:420:ILE:HD12	1:G:423:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:LEU:HD11	1:I:188:LEU:CB	2.20	0.68
1:I:403:LEU:HD23	1:I:403:LEU:H	1.57	0.68
1:I:516:GLU:HA	1:I:519:ILE:HD12	1.74	0.68
1:K:288:GLY:HA3	1:K:300:CYS:SG	2.33	0.68
1:A:288:GLY:HA3	1:A:300:CYS:SG	2.32	0.68
1:G:221:PHE:HB2	1:G:230:TRP:NE1	2.08	0.68
1:G:423:LEU:HA	1:G:426:VAL:HG22	1.73	0.68
1:I:424:ARG:NH1	1:I:572:LYS:HG2	2.08	0.68
1:L:359:GLY:HA3	1:L:453:LEU:HB2	1.74	0.68
1:A:310:LEU:HD22	1:A:327:LEU:HD21	1.75	0.68
1:D:516:GLU:HA	1:D:519:ILE:HD12	1.75	0.68
1:E:540:GLU:O	1:E:544:LEU:HG	1.94	0.68
1:H:328:LEU:HD13	1:H:368:ALA:HB1	1.75	0.68
1:I:395:GLU:HG2	1:I:397:PRO:HD3	1.75	0.68
1:D:420:ILE:HD12	1:D:423:LEU:HB2	1.75	0.68
1:G:180:GLU:HB3	1:G:192:LEU:HD23	1.74	0.68
1:H:427:TRP:HZ3	1:H:567:LEU:HB3	1.59	0.68
1:L:185:LEU:HD13	1:L:186:GLN:N	2.07	0.68
1:J:46:CYS:H	1:J:86:LEU:HD12	1.59	0.68
1:L:560:LEU:HD13	1:L:593:THR:HA	1.75	0.68
1:L:562:GLN:HA	1:L:565:ILE:HD12	1.76	0.68
1:A:110:PRO:O	1:A:113:CYS:HB3	1.94	0.68
1:B:527:ILE:HG22	1:B:531:GLU:HG3	1.75	0.68
1:H:423:LEU:HA	1:H:426:VAL:HG22	1.73	0.68
1:J:420:ILE:HD12	1:J:423:LEU:HB2	1.75	0.68
1:I:575:PRO:HB3	1:K:574:ARG:NH1	2.08	0.68
1:B:29:VAL:HA	1:B:44:LYS:HA	1.76	0.68
1:D:189:ALA:HB3	1:D:202:VAL:HG13	1.76	0.68
1:J:222:LEU:HD22	1:J:244:ALA:O	1.94	0.68
1:L:186:GLN:HE21	1:L:227:PRO:HD3	1.58	0.68
1:L:288:GLY:HA3	1:L:300:CYS:SG	2.34	0.68
1:L:420:ILE:HB	1:L:580:TYR:HB3	1.74	0.68
1:J:29:VAL:HA	1:J:44:LYS:HA	1.76	0.68
1:A:473:SER:HB3	1:A:632:ILE:HD13	1.76	0.67
1:B:401:ARG:HH22	1:B:440:ASP:HB2	1.59	0.67
1:D:415:LYS:HA	1:D:584:THR:HB	1.76	0.67
1:H:560:LEU:HD13	1:H:593:THR:HA	1.76	0.67
1:L:431:VAL:HG21	1:L:568:TYR:HB2	1.75	0.67
1:A:201:THR:HB	1:A:287:ARG:HH12	1.58	0.67
1:A:403:LEU:HD23	1:A:403:LEU:H	1.59	0.67
1:A:423:LEU:HA	1:A:426:VAL:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:HD22	1:A:518:ALA:HB1	1.77	0.67
1:D:396:GLY:N	1:D:397:PRO:HD3	2.10	0.67
1:I:267:LEU:HD12	1:I:312:ILE:HG23	1.76	0.67
1:J:527:ILE:HG22	1:J:531:GLU:HG3	1.76	0.67
1:D:334:LEU:HD11	1:D:364:PRO:HA	1.75	0.67
1:H:283:ASP:OD1	1:H:286:GLN:HG2	1.95	0.67
1:I:310:LEU:HD22	1:I:327:LEU:HD21	1.75	0.67
1:L:48:LEU:HA	1:L:87:ILE:HD12	1.75	0.67
1:B:267:LEU:HD12	1:B:312:ILE:HG23	1.76	0.67
1:B:463:THR:HG21	1:B:538:HIS:HD2	1.60	0.67
1:C:551:ARG:HB3	1:C:552:ARG:HH21	1.58	0.67
1:D:560:LEU:HD13	1:D:593:THR:HA	1.75	0.67
1:D:424:ARG:NH1	1:D:572:LYS:HG2	2.08	0.67
1:F:527:ILE:HG22	1:F:531:GLU:HG3	1.77	0.67
1:A:29:VAL:HA	1:A:44:LYS:HA	1.76	0.67
1:G:143:ARG:NH1	1:G:180:GLU:HA	2.08	0.67
1:G:562:GLN:HA	1:G:565:ILE:HD12	1.76	0.67
1:H:249:SER:HB3	1:J:185:LEU:H	1.59	0.67
1:H:311:LYS:HD2	1:H:372:VAL:HG11	1.77	0.67
1:H:74:VAL:HG11	1:H:164:ILE:HA	1.77	0.67
1:J:189:ALA:HB3	1:J:202:VAL:HG13	1.77	0.67
1:E:29:VAL:HA	1:E:44:LYS:HA	1.77	0.67
1:F:74:VAL:HG21	1:F:164:ILE:HG13	1.76	0.67
1:L:377:ARG:HA	1:L:377:ARG:HE	1.58	0.67
1:C:420:ILE:HD12	1:C:423:LEU:HB2	1.76	0.67
1:F:141:ILE:HD12	1:F:200:ALA:HA	1.76	0.67
1:F:29:VAL:HA	1:F:44:LYS:HA	1.77	0.67
1:K:516:GLU:HA	1:K:519:ILE:HD12	1.75	0.67
1:B:396:GLY:N	1:B:397:PRO:HD3	2.10	0.67
1:B:643:GLN:HE21	1:B:647:GLN:HG3	1.59	0.67
1:C:185:LEU:HD13	1:C:186:GLN:N	2.09	0.67
1:D:427:TRP:HZ3	1:D:567:LEU:HB3	1.59	0.67
1:E:498:MET:HA	1:E:503:SER:HB3	1.75	0.67
1:E:487:ILE:HA	1:E:646:ARG:HD2	1.77	0.67
1:G:116:LEU:HD12	1:G:116:LEU:H	1.58	0.67
1:G:560:LEU:HD13	1:G:593:THR:HA	1.77	0.67
1:C:265:CYS:SG	1:C:268:ILE:HG13	2.35	0.67
1:D:463:THR:HG21	1:D:538:HIS:HD2	1.60	0.67
1:H:514:MET:HA	1:H:517:LYS:HD2	1.77	0.67
1:I:74:VAL:HG11	1:I:164:ILE:HG13	1.76	0.67
1:J:396:GLY:N	1:J:397:PRO:HD3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:209:THR:HG22	1:K:220:PRO:HG3	1.77	0.67
1:D:141:ILE:HD12	1:D:200:ALA:HA	1.77	0.67
1:G:29:VAL:HA	1:G:44:LYS:HA	1.76	0.67
1:J:212:PHE:CD2	1:J:220:PRO:HA	2.30	0.67
1:K:643:GLN:HE21	1:K:647:GLN:HG3	1.60	0.67
1:A:395:GLU:HG3	1:A:396:GLY:H	1.60	0.66
1:B:189:ALA:HB3	1:B:202:VAL:HG13	1.77	0.66
1:D:227:PRO:HA	1:D:230:TRP:HB3	1.77	0.66
1:G:473:SER:HB2	1:G:524:VAL:HA	1.77	0.66
1:G:473:SER:HB3	1:G:632:ILE:HD13	1.77	0.66
1:A:182:VAL:HG12	1:A:183:GLY:H	1.59	0.66
1:A:514:MET:HA	1:A:517:LYS:HD2	1.77	0.66
1:E:516:GLU:HA	1:E:519:ILE:HD12	1.76	0.66
1:J:403:LEU:HD23	1:J:403:LEU:H	1.60	0.66
1:L:29:VAL:HA	1:L:44:LYS:HA	1.77	0.66
1:B:560:LEU:HD13	1:B:593:THR:HA	1.77	0.66
1:B:449:ARG:HH22	3:B:707:5LS:C3	2.08	0.66
1:C:562:GLN:HA	1:C:565:ILE:HD12	1.78	0.66
1:D:70:HIS:HB3	1:D:73:VAL:HG22	1.76	0.66
1:E:643:GLN:HE21	1:E:647:GLN:HG3	1.61	0.66
1:G:219:ARG:NH2	1:G:224:HIS:H	1.93	0.66
1:G:91:PRO:O	1:G:92:LEU:HD12	1.96	0.66
1:D:249:SER:HB3	1:F:184:THR:HA	1.77	0.66
1:J:560:LEU:HD13	1:J:593:THR:HA	1.76	0.66
1:L:141:ILE:HD12	1:L:200:ALA:HA	1.76	0.66
1:A:473:SER:OG	1:A:524:VAL:HG13	1.95	0.66
1:F:514:MET:HA	1:F:517:LYS:HD2	1.78	0.66
1:J:410:ILE:HG23	1:J:583:SER:OG	1.95	0.66
1:K:142:HIS:ND1	1:K:169:ALA:HB2	2.11	0.66
1:J:412:GLN:CD	1:L:27:GLY:HA2	2.16	0.66
1:A:265:CYS:SG	1:A:268:ILE:HG13	2.34	0.66
1:D:562:GLN:HA	1:D:565:ILE:HD12	1.77	0.66
1:F:420:ILE:HD12	1:F:423:LEU:HB2	1.75	0.66
1:J:579:SER:HB3	1:L:577:ASP:H	1.61	0.66
1:A:560:LEU:HD13	1:A:593:THR:HA	1.78	0.66
1:D:260:GLN:NE2	1:D:261:PRO:HA	2.11	0.66
1:F:238:ASP:HB3	1:F:239:PRO:HD2	1.78	0.66
1:G:219:ARG:NH1	1:G:224:HIS:H	1.94	0.66
1:H:417:GLN:HB3	1:H:581:SER:HB3	1.78	0.66
1:J:417:GLN:HB3	1:J:581:SER:HB3	1.76	0.66
1:J:562:GLN:HA	1:J:565:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:560:LEU:HD13	1:K:593:THR:HA	1.76	0.66
1:A:549:TYR:H	1:A:552:ARG:HD2	1.61	0.66
1:C:189:ALA:HB3	1:C:202:VAL:HG13	1.78	0.66
1:G:514:MET:HA	1:G:517:LYS:HD2	1.78	0.66
1:I:562:GLN:HA	1:I:565:ILE:HD12	1.78	0.66
1:L:514:MET:HA	1:L:517:LYS:HD2	1.78	0.66
1:B:141:ILE:HD12	1:B:200:ALA:HA	1.77	0.65
1:C:396:GLY:N	1:C:397:PRO:HD3	2.10	0.65
1:E:227:PRO:HA	1:E:230:TRP:CB	2.26	0.65
1:E:560:LEU:HD13	1:E:593:THR:HA	1.76	0.65
1:H:396:GLY:N	1:H:397:PRO:HD3	2.11	0.65
1:J:209:THR:HG22	1:J:220:PRO:HG3	1.77	0.65
1:C:514:MET:HA	1:C:517:LYS:HD2	1.79	0.65
1:D:212:PHE:CD2	1:D:220:PRO:HA	2.31	0.65
1:J:141:ILE:HD12	1:J:200:ALA:HA	1.78	0.65
1:C:560:LEU:HD13	1:C:593:THR:HA	1.78	0.65
1:E:141:ILE:HD12	1:E:200:ALA:HA	1.78	0.65
1:F:562:GLN:HA	1:F:565:ILE:HD12	1.79	0.65
1:H:396:GLY:H	1:H:397:PRO:HD3	1.61	0.65
1:I:420:ILE:HD12	1:I:423:LEU:HB2	1.77	0.65
1:K:141:ILE:HD12	1:K:200:ALA:HA	1.78	0.65
1:K:189:ALA:HB3	1:K:202:VAL:HG13	1.79	0.65
1:F:209:THR:HG22	1:F:220:PRO:HG3	1.77	0.65
1:H:141:ILE:HD12	1:H:200:ALA:HA	1.77	0.65
1:H:643:GLN:HE21	1:H:647:GLN:HG3	1.61	0.65
1:I:395:GLU:CD	1:I:395:GLU:H	1.98	0.65
1:C:29:VAL:HA	1:C:44:LYS:HA	1.76	0.65
1:F:189:ALA:HB3	1:F:202:VAL:HG13	1.79	0.65
1:H:562:GLN:HA	1:H:565:ILE:HD12	1.76	0.65
1:I:396:GLY:N	1:I:397:PRO:HD3	2.10	0.65
1:J:328:LEU:HD13	1:J:368:ALA:HB1	1.78	0.65
1:G:227:PRO:HA	1:G:230:TRP:HB2	1.78	0.65
1:H:267:LEU:HD12	1:H:312:ILE:HG23	1.77	0.65
1:I:514:MET:HA	1:I:517:LYS:HD2	1.79	0.65
1:I:560:LEU:HD13	1:I:593:THR:HA	1.78	0.65
1:J:46:CYS:H	1:J:86:LEU:CD1	2.09	0.65
1:K:238:ASP:CG	1:K:239:PRO:HD2	2.17	0.65
1:K:420:ILE:HD12	1:K:423:LEU:HB2	1.77	0.65
1:C:595:GLN:HB3	4:C:706:GLC:H3	1.79	0.65
1:I:141:ILE:HD12	1:I:200:ALA:HA	1.77	0.65
1:J:290:PRO:HB2	1:J:299:ARG:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLN:NE2	1:C:261:PRO:HA	2.09	0.65
1:C:424:ARG:NH1	1:C:572:LYS:HG2	2.12	0.65
1:C:420:ILE:HB	1:C:580:TYR:HB3	1.76	0.65
1:D:551:ARG:HB3	1:D:552:ARG:HH21	1.62	0.65
1:G:219:ARG:CZ	1:G:224:HIS:H	2.08	0.65
1:A:189:ALA:HB3	1:A:202:VAL:HG13	1.78	0.65
1:F:112:ASN:HB3	1:F:116:LEU:HD22	1.79	0.65
1:L:74:VAL:HG12	1:L:75:LYS:H	1.61	0.65
1:A:643:GLN:HE21	1:A:647:GLN:HG3	1.61	0.65
1:F:643:GLN:HE21	1:F:647:GLN:HG3	1.62	0.65
1:G:265:CYS:SG	1:G:268:ILE:HG13	2.36	0.65
1:H:403:LEU:H	1:H:403:LEU:HD23	1.61	0.65
1:I:260:GLN:NE2	1:I:261:PRO:HA	2.09	0.65
1:K:139:LYS:HD2	1:K:172:VAL:HG11	1.77	0.65
1:A:48:LEU:HA	1:A:87:ILE:HG21	1.79	0.64
1:C:477:LYS:HE3	1:C:524:VAL:HG11	1.77	0.64
1:E:222:LEU:HD22	1:E:222:LEU:H	1.61	0.64
1:I:29:VAL:HA	1:I:44:LYS:HA	1.76	0.64
1:B:227:PRO:HA	1:B:230:TRP:CB	2.26	0.64
1:B:514:MET:HA	1:B:517:LYS:HD2	1.80	0.64
1:E:463:THR:HG21	1:E:538:HIS:HD2	1.61	0.64
1:F:469:LEU:HD12	1:F:625:VAL:HG13	1.78	0.64
1:H:265:CYS:SG	1:H:268:ILE:HG13	2.38	0.64
1:I:324:ILE:H	1:I:324:ILE:HD12	1.63	0.64
1:J:366:LYS:HE3	1:J:367:PRO:HD2	1.80	0.64
1:J:424:ARG:HH11	1:J:572:LYS:HG2	1.62	0.64
1:L:209:THR:HG22	1:L:220:PRO:HG3	1.79	0.64
1:L:415:LYS:HA	1:L:584:THR:HB	1.79	0.64
1:A:185:LEU:HD13	1:A:186:GLN:H	1.62	0.64
1:F:359:GLY:HA3	1:F:453:LEU:HB2	1.78	0.64
1:I:643:GLN:HE21	1:I:647:GLN:HG3	1.60	0.64
1:J:215:ILE:HD13	1:J:264:LEU:HD11	1.79	0.64
1:A:324:ILE:H	1:A:324:ILE:HD12	1.63	0.64
1:A:401:ARG:HH21	1:A:437:LEU:HD23	1.63	0.64
1:G:643:GLN:HE21	1:G:647:GLN:HG3	1.61	0.64
1:J:514:MET:HA	1:J:517:LYS:HD2	1.78	0.64
1:H:26:PHE:HD1	1:L:408:ASN:HD21	1.46	0.64
1:K:489:LEU:HD21	1:L:648:LYS:HG3	1.78	0.64
1:B:209:THR:HG22	1:B:220:PRO:HG3	1.80	0.64
1:A:502:ILE:HG13	1:B:658:CYS:SG	2.37	0.64
1:C:351:SER:HA	1:C:389:LYS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:420:ILE:HD12	1:E:423:LEU:HB2	1.77	0.64
1:H:141:ILE:HG23	1:H:170:LYS:HB2	1.78	0.64
1:I:351:SER:HA	1:I:389:LYS:HD2	1.80	0.64
1:I:477:LYS:HE3	1:I:524:VAL:HG11	1.78	0.64
1:K:562:GLN:HA	1:K:565:ILE:HD12	1.80	0.64
1:B:265:CYS:SG	1:B:268:ILE:HG13	2.38	0.64
1:B:324:ILE:HD12	1:B:324:ILE:H	1.62	0.64
1:D:291:VAL:HA	1:D:298:PRO:HA	1.79	0.64
1:D:324:ILE:H	1:D:324:ILE:HD12	1.63	0.64
1:D:643:GLN:HE21	1:D:647:GLN:HG3	1.62	0.64
1:E:562:GLN:HA	1:E:565:ILE:HD12	1.80	0.64
1:G:237:LYS:HE2	1:G:282:TRP:H	1.61	0.64
1:K:424:ARG:NH1	1:K:572:LYS:HG2	2.12	0.64
1:D:265:CYS:SG	1:D:268:ILE:HG13	2.38	0.64
1:D:514:MET:HA	1:D:517:LYS:HD2	1.78	0.64
1:H:498:MET:HA	1:H:503:SER:HB3	1.77	0.64
1:B:351:SER:HA	1:B:389:LYS:HD2	1.79	0.64
1:G:648:LYS:HG3	1:H:489:LEU:HD21	1.78	0.64
1:H:420:ILE:HG21	1:H:578:HIS:H	1.63	0.64
1:L:189:ALA:HB3	1:L:202:VAL:HG13	1.80	0.64
1:B:236:LYS:HG3	1:B:237:LYS:H	1.61	0.64
1:E:351:SER:HA	1:E:389:LYS:HD2	1.80	0.64
1:F:86:LEU:HD23	1:F:87:ILE:HD12	1.79	0.64
1:J:643:GLN:HE21	1:J:647:GLN:HG3	1.63	0.64
1:K:514:MET:HA	1:K:517:LYS:HD2	1.79	0.64
1:L:185:LEU:HD12	1:L:193:PHE:HZ	1.63	0.64
1:A:13:GLY:H	1:A:14:PRO:CD	2.07	0.64
1:B:410:ILE:O	1:B:587:VAL:HG22	1.98	0.64
1:G:288:GLY:HA3	1:G:300:CYS:SG	2.38	0.64
1:H:114:CYS:SG	1:H:432:HIS:HB2	2.38	0.64
1:H:260:GLN:NE2	1:H:261:PRO:HA	2.11	0.64
1:I:265:CYS:SG	1:I:268:ILE:HG13	2.37	0.64
1:L:643:GLN:HE21	1:L:647:GLN:HG3	1.63	0.64
1:A:234:ILE:O	1:A:237:LYS:HB2	1.97	0.63
1:B:170:LYS:HA	1:B:177:LEU:HA	1.79	0.63
1:B:260:GLN:NE2	1:B:261:PRO:HA	2.11	0.63
1:B:29:VAL:HG22	1:B:44:LYS:HB2	1.80	0.63
1:C:324:ILE:HD12	1:C:324:ILE:H	1.63	0.63
1:F:25:GLY:H	1:F:28:ASN:HD22	1.46	0.63
1:J:265:CYS:SG	1:J:268:ILE:HG13	2.38	0.63
1:L:551:ARG:HB3	1:L:552:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:ASN:ND2	1:J:26:PHE:HA	2.13	0.63
1:H:463:THR:HG21	1:H:538:HIS:HD2	1.64	0.63
1:L:13:GLY:H	1:L:14:PRO:CD	2.11	0.63
1:A:141:ILE:HD12	1:A:200:ALA:HA	1.79	0.63
1:A:289:GLY:O	1:A:291:VAL:HG23	1.98	0.63
1:C:141:ILE:HD12	1:C:200:ALA:HA	1.79	0.63
1:E:189:ALA:HB3	1:E:202:VAL:HG13	1.81	0.63
1:G:324:ILE:H	1:G:324:ILE:HD12	1.63	0.63
1:J:354:LEU:HB3	1:J:384:VAL:HG12	1.81	0.63
1:J:351:SER:HA	1:J:389:LYS:HD2	1.81	0.63
1:K:351:SER:HA	1:K:389:LYS:HD2	1.81	0.63
1:C:643:GLN:HE21	1:C:647:GLN:HG3	1.61	0.63
1:G:222:LEU:HB2	1:G:230:TRP:HD1	1.61	0.63
1:I:189:ALA:HB3	1:I:202:VAL:HG13	1.81	0.63
1:J:88:HIS:CG	1:J:89:ASP:H	2.16	0.63
1:K:114:CYS:SG	1:K:432:HIS:HB2	2.37	0.63
1:B:74:VAL:HB	1:B:164:ILE:HG13	1.79	0.63
1:E:372:VAL:O	1:E:373:LEU:HD13	1.99	0.63
1:E:514:MET:HA	1:E:517:LYS:HD2	1.79	0.63
1:H:29:VAL:HG22	1:H:44:LYS:HB2	1.81	0.63
1:J:324:ILE:H	1:J:324:ILE:HD12	1.64	0.63
1:E:420:ILE:HG21	1:E:578:HIS:H	1.63	0.63
1:H:209:THR:HG22	1:H:220:PRO:HG3	1.81	0.63
1:B:562:GLN:HA	1:B:565:ILE:HD12	1.79	0.63
1:D:351:SER:HA	1:D:389:LYS:HD2	1.81	0.63
1:E:227:PRO:HA	1:E:230:TRP:HB2	1.80	0.63
1:G:29:VAL:HG21	2:G:701:5TL:CAE	2.28	0.63
1:H:189:ALA:HB3	1:H:202:VAL:HG13	1.81	0.63
1:J:463:THR:HG21	1:J:538:HIS:HD2	1.64	0.63
1:L:427:TRP:HZ3	1:L:567:LEU:HB3	1.63	0.63
1:G:189:ALA:HB3	1:G:202:VAL:HG13	1.80	0.63
1:H:431:VAL:HG21	1:H:568:TYR:HB2	1.81	0.63
1:A:139:LYS:HD2	1:A:172:VAL:HG21	1.80	0.63
1:C:502:ILE:HD12	1:D:654:LEU:HD11	1.78	0.63
1:H:48:LEU:HA	1:H:87:ILE:HD12	1.80	0.63
1:K:401:ARG:HH22	1:K:440:ASP:HB2	1.64	0.63
1:K:487:ILE:HA	1:K:646:ARG:HD2	1.79	0.63
1:A:469:LEU:HD12	1:A:625:VAL:HG13	1.80	0.62
1:D:25:GLY:H	1:D:28:ASN:HD22	1.47	0.62
1:E:222:LEU:HB2	1:E:230:TRP:HD1	1.64	0.62
1:F:77:CYS:HB2	1:F:94:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:351:SER:HA	1:L:389:LYS:HD2	1.81	0.62
1:A:396:GLY:N	1:A:397:PRO:HD3	2.10	0.62
1:G:143:ARG:NH2	1:G:144:ASP:HB2	2.15	0.62
1:G:25:GLY:H	1:G:28:ASN:HD22	1.46	0.62
1:H:473:SER:HB2	1:H:524:VAL:HA	1.80	0.62
1:I:185:LEU:HD13	1:I:186:GLN:N	2.13	0.62
1:K:281:ASN:O	1:K:287:ARG:HD3	1.99	0.62
1:K:25:GLY:H	1:K:28:ASN:HD22	1.48	0.62
1:L:143:ARG:NH2	1:L:144:ASP:HB2	2.14	0.62
1:L:170:LYS:HG2	1:L:177:LEU:HD23	1.81	0.62
1:A:351:SER:HA	1:A:389:LYS:HD2	1.80	0.62
1:C:212:PHE:CD2	1:C:220:PRO:HA	2.35	0.62
1:G:186:GLN:HE21	1:G:219:ARG:NH1	1.98	0.62
1:H:351:SER:HA	1:H:389:LYS:HD2	1.81	0.62
1:H:547:SER:HB3	1:H:548:PRO:HD2	1.80	0.62
1:K:13:GLY:N	1:K:14:PRO:HD3	2.14	0.62
1:K:29:VAL:HG22	1:K:44:LYS:HB2	1.81	0.62
1:D:170:LYS:HB3	1:D:177:LEU:HA	1.80	0.62
1:E:220:PRO:O	1:E:243:PHE:HA	2.00	0.62
1:G:141:ILE:HD12	1:G:200:ALA:HA	1.80	0.62
1:I:70:HIS:HB3	1:I:73:VAL:HG12	1.81	0.62
1:K:260:GLN:NE2	1:K:261:PRO:HA	2.09	0.62
1:A:220:PRO:O	1:A:243:PHE:HA	1.99	0.62
1:E:260:GLN:NE2	1:E:261:PRO:HA	2.10	0.62
1:E:29:VAL:HG22	1:E:44:LYS:HB2	1.81	0.62
1:E:324:ILE:HD12	1:E:324:ILE:H	1.65	0.62
1:E:501:GLY:HA2	1:F:658:CYS:HB3	1.81	0.62
1:H:420:ILE:HG21	1:H:578:HIS:N	2.14	0.62
1:I:220:PRO:O	1:I:243:PHE:HA	2.00	0.62
1:K:324:ILE:H	1:K:324:ILE:HD12	1.65	0.62
1:A:143:ARG:NH2	1:A:144:ASP:HB2	2.15	0.62
1:A:517:LYS:HD2	1:A:642:MET:HE1	1.80	0.62
1:D:98:CYS:HB3	1:D:152:LEU:O	1.99	0.62
1:D:298:PRO:O	1:D:302:VAL:HG23	2.00	0.62
1:F:143:ARG:NH2	1:F:144:ASP:HB2	2.14	0.62
1:J:25:GLY:H	1:J:28:ASN:HD22	1.47	0.62
1:L:73:VAL:HG12	1:L:74:VAL:HG23	1.80	0.62
1:E:25:GLY:H	1:E:28:ASN:HD22	1.48	0.62
1:F:21:LEU:HD12	2:F:701:5TL:CAG	2.29	0.62
1:H:298:PRO:O	1:H:302:VAL:HG23	2.00	0.62
1:I:334:LEU:HD11	1:I:364:PRO:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:CD2	1:B:220:PRO:HA	2.35	0.62
1:G:351:SER:HA	1:G:389:LYS:HD2	1.80	0.62
1:E:291:VAL:HA	1:E:298:PRO:HA	1.82	0.62
1:G:260:GLN:NE2	1:G:261:PRO:HA	2.09	0.62
1:H:25:GLY:H	1:H:28:ASN:HD22	1.47	0.62
1:J:85:ILE:HB	1:J:88:HIS:O	2.00	0.62
1:K:112:ASN:HB3	1:K:116:LEU:HD23	1.80	0.62
1:D:29:VAL:HG22	1:D:44:LYS:HB2	1.81	0.62
1:I:20:ARG:HG3	1:I:30:CYS:SG	2.40	0.62
1:J:29:VAL:HG22	1:J:44:LYS:HB2	1.81	0.62
1:C:595:GLN:CB	4:C:706:GLC:H3	2.30	0.61
1:G:185:LEU:HD12	1:G:193:PHE:HZ	1.65	0.61
1:H:324:ILE:H	1:H:324:ILE:HD12	1.64	0.61
1:K:221:PHE:HB2	1:K:230:TRP:CZ2	2.35	0.61
1:L:410:ILE:O	1:L:587:VAL:HG22	2.00	0.61
1:L:29:VAL:HG22	1:L:44:LYS:HB2	1.82	0.61
1:B:473:SER:HB2	1:B:524:VAL:HA	1.81	0.61
1:C:25:GLY:H	1:C:28:ASN:HD22	1.48	0.61
1:E:281:ASN:H	1:E:287:ARG:HD3	1.64	0.61
1:H:65:MET:HB3	1:H:76:ALA:HB2	1.80	0.61
1:C:395:GLU:H	1:C:395:GLU:CD	2.03	0.61
1:E:48:LEU:HA	1:E:87:ILE:HG21	1.81	0.61
1:F:260:GLN:NE2	1:F:261:PRO:HA	2.09	0.61
1:K:224:HIS:HE2	1:K:424:ARG:HD2	1.64	0.61
1:K:298:PRO:O	1:K:302:VAL:HG23	1.99	0.61
1:L:563:ARG:NH1	4:L:708:GLC:H2	2.08	0.61
1:B:143:ARG:NH2	1:B:144:ASP:HB2	2.14	0.61
1:C:29:VAL:HG22	1:C:44:LYS:HB2	1.82	0.61
1:D:215:ILE:HD13	1:D:264:LEU:HD11	1.83	0.61
1:I:25:GLY:H	1:I:28:ASN:HD22	1.49	0.61
1:A:25:GLY:H	1:A:28:ASN:HD22	1.47	0.61
1:E:265:CYS:SG	1:E:268:ILE:HG13	2.40	0.61
1:F:324:ILE:H	1:F:324:ILE:HD12	1.64	0.61
1:F:351:SER:HA	1:F:389:LYS:HD2	1.83	0.61
1:F:415:LYS:HA	1:F:584:THR:HB	1.83	0.61
1:I:29:VAL:HG22	1:I:44:LYS:HB2	1.81	0.61
1:A:431:VAL:HG21	1:A:568:TYR:HB2	1.83	0.61
1:E:392:THR:O	1:E:612:LEU:HD23	2.00	0.61
1:F:212:PHE:CD2	1:F:220:PRO:HA	2.35	0.61
1:I:227:PRO:HA	1:I:230:TRP:HB3	1.82	0.61
1:K:227:PRO:HA	1:K:230:TRP:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:265:CYS:SG	1:L:268:ILE:HG13	2.40	0.61
1:L:324:ILE:HD12	1:L:324:ILE:H	1.64	0.61
1:L:328:LEU:HD13	1:L:368:ALA:HB1	1.83	0.61
1:L:469:LEU:HD12	1:L:625:VAL:HG13	1.81	0.61
1:A:236:LYS:HG2	1:A:237:LYS:N	2.16	0.61
1:H:415:LYS:HA	1:H:584:THR:HB	1.83	0.61
1:I:427:TRP:HZ3	1:I:567:LEU:HB3	1.66	0.61
1:A:648:LYS:HG3	1:B:489:LEU:HD21	1.83	0.61
1:C:463:THR:HG21	1:C:538:HIS:HD2	1.66	0.61
1:K:396:GLY:N	1:K:397:PRO:HD3	2.16	0.61
1:K:427:TRP:HZ3	1:K:567:LEU:HB3	1.66	0.61
1:B:141:ILE:HG23	1:B:170:LYS:HB2	1.83	0.61
1:C:427:TRP:HZ3	1:C:567:LEU:HB3	1.66	0.61
1:F:265:CYS:SG	1:F:268:ILE:HG13	2.40	0.61
1:K:289:GLY:O	1:K:291:VAL:HG23	2.00	0.61
1:K:403:LEU:HB2	1:K:407:VAL:HB	1.83	0.61
1:K:98:CYS:HB3	1:K:152:LEU:O	2.00	0.61
1:L:222:LEU:HD22	1:L:244:ALA:O	2.00	0.61
1:D:294:THR:HG22	1:D:295:LEU:HD22	1.83	0.61
1:F:144:ASP:OD2	1:F:185:LEU:HD21	2.01	0.61
1:F:29:VAL:HG22	1:F:44:LYS:HB2	1.83	0.61
1:H:143:ARG:NH2	1:H:144:ASP:HB2	2.14	0.61
1:L:25:GLY:H	1:L:28:ASN:HD22	1.48	0.61
1:A:550:GLY:HA3	1:A:604:LEU:HD13	1.82	0.60
1:H:186:GLN:NE2	1:H:227:PRO:HD3	2.16	0.60
1:J:13:GLY:N	1:J:14:PRO:HD3	2.08	0.60
1:K:219:ARG:NH1	1:K:224:HIS:H	1.98	0.60
1:K:237:LYS:HE2	1:K:282:TRP:H	1.66	0.60
1:K:204:TYR:HB2	1:K:287:ARG:NH1	2.16	0.60
1:K:478:ALA:CB	1:L:475:GLN:HA	2.31	0.60
1:A:29:VAL:HG22	1:A:44:LYS:HB2	1.83	0.60
1:D:230:TRP:O	1:D:234:ILE:HG12	2.01	0.60
1:D:20:ARG:HG3	1:D:30:CYS:SG	2.42	0.60
1:E:234:ILE:HG22	1:E:254:PHE:HE1	1.66	0.60
1:E:392:THR:HG22	1:E:616:GLN:NE2	2.16	0.60
1:F:298:PRO:O	1:F:302:VAL:HG23	2.00	0.60
1:K:143:ARG:NH2	1:K:144:ASP:HB2	2.16	0.60
1:L:260:GLN:NE2	1:L:261:PRO:HA	2.10	0.60
1:A:291:VAL:HA	1:A:298:PRO:HA	1.84	0.60
1:B:265:CYS:O	1:B:269:VAL:HG23	2.01	0.60
1:L:72:ASN:HB2	1:L:131:GLY:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLY:H	1:B:28:ASN:HD22	1.49	0.60
1:B:354:LEU:HB2	1:B:362:LEU:HD13	1.84	0.60
1:C:143:ARG:NH2	1:C:144:ASP:HB2	2.15	0.60
1:D:143:ARG:NH2	1:D:144:ASP:HB2	2.15	0.60
1:E:143:ARG:NH2	1:E:144:ASP:HB2	2.16	0.60
1:E:43:ILE:HG13	1:E:94:ALA:HA	1.84	0.60
1:H:289:GLY:O	1:H:291:VAL:HG23	2.01	0.60
1:K:77:CYS:H	1:K:95:MET:HA	1.65	0.60
1:B:142:HIS:HA	1:B:169:ALA:CB	2.31	0.60
1:C:347:ILE:HD12	1:C:386:LEU:HD21	1.84	0.60
1:D:473:SER:HB2	1:D:524:VAL:HA	1.84	0.60
1:F:265:CYS:O	1:F:269:VAL:HG23	2.01	0.60
1:I:289:GLY:O	1:I:291:VAL:HG23	2.01	0.60
1:I:347:ILE:HD12	1:I:386:LEU:HD21	1.84	0.60
1:A:483:PHE:HZ	1:A:514:MET:HB3	1.65	0.60
1:B:319:THR:O	1:B:397:PRO:HD2	2.02	0.60
1:E:502:ILE:HD12	1:F:654:LEU:HD11	1.83	0.60
1:G:29:VAL:HG22	1:G:44:LYS:HB2	1.84	0.60
1:G:489:LEU:HD22	1:H:647:GLN:OE1	2.01	0.60
1:B:249:SER:HB3	1:D:185:LEU:H	1.67	0.60
1:I:403:LEU:HB2	1:I:407:VAL:HB	1.84	0.60
1:J:7:PRO:HG3	1:J:17:MET:SD	2.42	0.60
1:J:550:GLY:HA3	1:J:604:LEU:HD13	1.83	0.60
1:L:298:PRO:O	1:L:302:VAL:HG23	2.01	0.60
1:L:473:SER:HB2	1:L:524:VAL:HA	1.84	0.60
1:H:576:SER:OG	1:L:577:ASP:HA	2.01	0.60
1:B:86:LEU:HG	1:B:92:LEU:HD11	1.84	0.60
1:E:431:VAL:HG21	1:E:568:TYR:HB2	1.84	0.60
1:I:219:ARG:NH2	1:I:224:HIS:H	2.00	0.60
1:J:126:SER:HB2	1:J:308:LEU:CD1	2.32	0.60
1:B:543:GLU:HA	1:B:546:LYS:HE3	1.84	0.60
1:C:238:ASP:HB3	1:C:239:PRO:HD2	1.84	0.60
1:D:63:GLN:NE2	1:D:174:GLN:HE22	2.00	0.60
1:E:185:LEU:HD11	1:E:188:LEU:HB3	1.84	0.60
1:I:43:ILE:HG13	1:I:94:ALA:HA	1.83	0.60
1:J:219:ARG:HH22	1:J:224:HIS:H	1.50	0.60
1:L:354:LEU:HB3	1:L:384:VAL:CG1	2.31	0.60
1:B:356:SER:HB2	1:B:382:TYR:HE1	1.67	0.59
1:B:547:SER:HB3	1:B:548:PRO:HD2	1.82	0.59
1:C:265:CYS:O	1:C:269:VAL:HG23	2.02	0.59
1:C:431:VAL:HG21	1:C:568:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:GLY:N	1:F:397:PRO:HD3	2.16	0.59
1:I:143:ARG:NH2	1:I:144:ASP:HB2	2.16	0.59
1:I:265:CYS:O	1:I:269:VAL:HG23	2.02	0.59
1:J:240:LYS:HB3	1:J:277:GLN:HB3	1.83	0.59
1:K:265:CYS:SG	1:K:268:ILE:HG13	2.41	0.59
1:A:201:THR:HB	1:A:287:ARG:NH1	2.16	0.59
1:E:185:LEU:HD13	1:E:186:GLN:H	1.67	0.59
1:E:514:MET:HA	1:E:642:MET:HE1	1.84	0.59
1:E:473:SER:HB2	1:E:524:VAL:HA	1.84	0.59
1:L:424:ARG:NH1	1:L:572:LYS:HG2	2.16	0.59
1:A:260:GLN:NE2	1:A:261:PRO:HA	2.10	0.59
1:A:84:ASN:CG	1:A:85:ILE:H	2.06	0.59
1:B:237:LYS:HZ1	1:B:281:ASN:HA	1.65	0.59
1:C:142:HIS:ND1	1:C:169:ALA:HB2	2.17	0.59
1:D:6:ASP:N	1:D:7:PRO:HD2	2.17	0.59
1:D:46:CYS:SG	1:D:90:VAL:HG23	2.42	0.59
1:G:551:ARG:HB3	1:G:552:ARG:HH21	1.68	0.59
1:K:43:ILE:HG13	1:K:94:ALA:HA	1.84	0.59
1:K:463:THR:HG21	1:K:538:HIS:HD2	1.67	0.59
1:A:473:SER:HA	1:A:632:ILE:HG21	1.83	0.59
1:E:289:GLY:O	1:E:291:VAL:HG23	2.03	0.59
1:F:395:GLU:H	1:F:395:GLU:CD	2.05	0.59
1:G:186:GLN:NE2	1:G:219:ARG:NH1	2.50	0.59
1:G:415:LYS:HA	1:G:584:THR:HB	1.83	0.59
1:H:265:CYS:O	1:H:269:VAL:HG23	2.02	0.59
1:B:595:GLN:HG3	4:B:705:GLC:H62	1.84	0.59
1:E:222:LEU:HB2	1:E:230:TRP:CD1	2.37	0.59
1:F:410:ILE:HG23	1:F:583:SER:OG	2.03	0.59
1:I:392:THR:HG22	1:I:616:GLN:HE22	1.66	0.59
1:K:334:LEU:HD11	1:K:364:PRO:HA	1.82	0.59
1:B:576:SER:OG	1:F:577:ASP:HA	2.03	0.59
1:B:577:ASP:H	1:F:579:SER:CB	2.13	0.59
1:B:69:ASN:HA	1:B:75:LYS:HE3	1.84	0.59
1:D:347:ILE:HD12	1:D:386:LEU:HD21	1.84	0.59
1:E:20:ARG:HG3	1:E:30:CYS:SG	2.43	0.59
1:J:142:HIS:ND1	1:J:169:ALA:HB2	2.18	0.59
1:A:98:CYS:HA	1:A:153:GLN:NE2	2.17	0.59
1:A:347:ILE:HD12	1:A:386:LEU:HD21	1.85	0.59
1:C:403:LEU:HB2	1:C:407:VAL:HB	1.85	0.59
1:D:502:ILE:HG21	1:D:656:ILE:HD13	1.85	0.59
1:E:403:LEU:HB2	1:E:407:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284:PRO:HA	1:G:287:ARG:NH1	2.17	0.59
1:K:462:LEU:HD22	1:K:618:ILE:HG23	1.85	0.59
1:K:465:MET:HB3	1:K:625:VAL:HG11	1.85	0.59
1:C:548:PRO:HB2	1:C:552:ARG:HG3	1.84	0.59
1:D:265:CYS:O	1:D:269:VAL:HG23	2.02	0.59
1:D:289:GLY:O	1:D:291:VAL:HG23	2.01	0.59
1:F:141:ILE:HG23	1:F:170:LYS:HB2	1.84	0.59
1:G:212:PHE:CE2	1:G:220:PRO:HA	2.38	0.59
1:L:220:PRO:O	1:L:243:PHE:HA	2.03	0.59
1:C:489:LEU:HD11	1:D:648:LYS:HE3	1.85	0.59
1:E:401:ARG:HH22	1:E:440:ASP:HB2	1.66	0.59
1:E:393:VAL:HG13	1:E:609:SER:OG	2.03	0.59
1:G:347:ILE:HD12	1:G:386:LEU:HD21	1.85	0.59
1:G:473:SER:HA	1:G:632:ILE:HG21	1.83	0.59
1:J:347:ILE:HD12	1:J:386:LEU:HD21	1.84	0.59
1:L:171:ASP:O	1:L:176:GLU:HA	2.03	0.59
1:L:265:CYS:O	1:L:269:VAL:HG23	2.02	0.59
1:A:265:CYS:O	1:A:269:VAL:HG23	2.02	0.59
1:A:334:LEU:HD22	1:A:366:LYS:O	2.01	0.59
1:B:403:LEU:HB2	1:B:407:VAL:HB	1.85	0.59
1:C:424:ARG:HH11	1:C:572:LYS:HG2	1.68	0.59
1:D:403:LEU:HD23	1:D:403:LEU:H	1.67	0.59
1:G:316:LEU:HD22	1:G:383:MET:HE2	1.84	0.59
1:H:427:TRP:O	1:H:431:VAL:HG23	2.03	0.59
1:I:240:LYS:HD2	1:I:277:GLN:HB3	1.84	0.59
1:I:658:CYS:HB3	1:J:501:GLY:HA2	1.85	0.59
1:J:143:ARG:NH2	1:J:144:ASP:HB2	2.17	0.59
1:J:334:LEU:HD11	1:J:364:PRO:HA	1.85	0.59
1:K:417:GLN:HB3	1:K:581:SER:HB3	1.85	0.59
1:L:427:TRP:O	1:L:431:VAL:HG23	2.03	0.59
1:L:480:LEU:HD22	1:L:518:ALA:HB1	1.84	0.59
1:C:469:LEU:HD12	1:C:625:VAL:HG13	1.84	0.58
1:D:424:ARG:HH11	1:D:572:LYS:HG2	1.68	0.58
1:E:70:HIS:CD2	1:E:71:ALA:H	2.21	0.58
1:J:427:TRP:HZ3	1:J:567:LEU:HB3	1.68	0.58
1:J:43:ILE:HG13	1:J:94:ALA:HA	1.85	0.58
1:B:427:TRP:O	1:B:431:VAL:HG23	2.04	0.58
1:C:498:MET:HA	1:C:503:SER:HB3	1.84	0.58
1:H:314:HIS:HB2	1:H:383:MET:HG2	1.85	0.58
1:K:485:LYS:HG2	1:L:640:MET:HE1	1.85	0.58
1:B:207:PHE:O	1:B:211:VAL:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ILE:HG23	1:E:583:SER:OG	2.02	0.58
1:F:410:ILE:O	1:F:587:VAL:HG22	2.03	0.58
1:H:622:LEU:N	1:H:623:PRO:HD2	2.18	0.58
1:I:186:GLN:HG2	1:I:219:ARG:HD3	1.85	0.58
1:K:265:CYS:O	1:K:269:VAL:HG23	2.04	0.58
1:A:223:HIS:O	1:A:225:LEU:HD23	2.02	0.58
1:A:406:CYS:SG	1:A:407:VAL:HG23	2.44	0.58
1:B:281:ASN:HD22	1:B:282:TRP:N	2.02	0.58
1:B:424:ARG:NH1	1:B:572:LYS:HG2	2.18	0.58
1:A:577:ASP:N	1:C:579:SER:HB2	2.18	0.58
1:G:207:PHE:O	1:G:211:VAL:HG23	2.02	0.58
1:H:74:VAL:CG1	1:H:164:ILE:HA	2.33	0.58
1:H:401:ARG:HE	1:H:401:ARG:H	1.49	0.58
1:I:219:ARG:HH21	1:I:224:HIS:H	1.50	0.58
1:F:219:ARG:HE	1:F:224:HIS:N	1.98	0.58
1:F:289:GLY:O	1:F:291:VAL:HG23	2.03	0.58
1:G:265:CYS:O	1:G:269:VAL:HG23	2.02	0.58
1:H:354:LEU:HB2	1:H:362:LEU:HD13	1.86	0.58
1:D:288:GLY:HA3	1:D:300:CYS:SG	2.43	0.58
1:D:410:ILE:HG23	1:D:583:SER:OG	2.03	0.58
1:I:424:ARG:HH11	1:I:572:LYS:HG2	1.67	0.58
1:J:265:CYS:O	1:J:269:VAL:HG23	2.03	0.58
1:A:547:SER:HB2	1:A:548:PRO:HD2	1.86	0.58
1:A:98:CYS:HB3	1:A:152:LEU:O	2.02	0.58
1:B:234:ILE:HG23	1:B:254:PHE:HE1	1.68	0.58
1:D:412:GLN:CD	1:F:27:GLY:HA2	2.24	0.58
1:E:354:LEU:HB2	1:E:362:LEU:HD13	1.86	0.58
1:F:347:ILE:HD12	1:F:386:LEU:HD21	1.86	0.58
1:G:590:ILE:O	1:G:594:VAL:HG23	2.04	0.58
1:H:186:GLN:HE22	1:H:227:PRO:HD3	1.69	0.58
1:J:20:ARG:HG3	1:J:30:CYS:SG	2.44	0.58
1:I:648:LYS:HE3	1:J:489:LEU:HD11	1.86	0.58
1:K:70:HIS:O	1:K:73:VAL:HG12	2.04	0.58
1:D:43:ILE:HG13	1:D:94:ALA:HA	1.85	0.58
1:E:298:PRO:O	1:E:302:VAL:HG23	2.03	0.58
1:G:170:LYS:HG3	1:G:177:LEU:HA	1.86	0.58
1:H:74:VAL:HG11	1:H:164:ILE:HG13	1.85	0.58
1:J:46:CYS:SG	1:J:90:VAL:HG23	2.44	0.58
1:L:424:ARG:HH11	1:L:572:LYS:HG2	1.68	0.58
1:L:358:THR:O	1:L:453:LEU:HD13	2.03	0.58
1:L:590:ILE:O	1:L:594:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LYS:HG2	1:D:241:CYS:HB3	1.85	0.58
1:F:275:TRP:CZ2	1:F:304:MET:HE2	2.38	0.58
1:G:403:LEU:HB2	1:G:407:VAL:HB	1.85	0.58
1:L:72:ASN:HB2	1:L:131:GLY:HA3	1.85	0.58
1:B:595:GLN:HE21	5:B:706:PDX:C1	2.16	0.58
1:C:552:ARG:HE	1:C:552:ARG:N	2.02	0.58
1:C:590:ILE:O	1:C:594:VAL:HG23	2.03	0.58
1:D:506:LYS:H	1:D:506:LYS:HD3	1.69	0.58
1:G:473:SER:OG	1:G:524:VAL:HG13	2.03	0.58
1:H:597:GLN:O	1:H:601:LEU:HB2	2.04	0.58
1:I:396:GLY:HA2	1:I:398:PHE:CZ	2.39	0.58
1:J:506:LYS:H	1:J:506:LYS:HD3	1.69	0.58
1:L:373:LEU:HD23	1:L:373:LEU:H	1.69	0.58
1:K:497:GLN:HE22	1:L:654:LEU:CD2	2.17	0.58
1:B:191:GLU:OE2	1:B:284:PRO:HB3	2.03	0.57
1:B:236:LYS:HG3	1:B:237:LYS:N	2.19	0.57
1:E:77:CYS:H	1:E:95:MET:HA	1.68	0.57
1:F:427:TRP:O	1:F:431:VAL:HG23	2.04	0.57
1:G:622:LEU:N	1:G:623:PRO:HD2	2.19	0.57
1:H:237:LYS:HE2	1:H:282:TRP:H	1.69	0.57
1:I:112:ASN:CB	1:I:116:LEU:HD23	2.34	0.57
1:I:431:VAL:HG21	1:I:568:TYR:HB2	1.85	0.57
1:L:354:LEU:HB3	1:L:384:VAL:HG12	1.86	0.57
1:B:143:ARG:HG3	1:B:192:LEU:HD21	1.87	0.57
1:B:597:GLN:O	1:B:601:LEU:HB2	2.05	0.57
1:C:20:ARG:HG3	1:C:30:CYS:SG	2.44	0.57
1:F:622:LEU:N	1:F:623:PRO:HD2	2.20	0.57
1:F:43:ILE:HG13	1:F:94:ALA:HA	1.86	0.57
1:I:420:ILE:HG21	1:I:578:HIS:N	2.19	0.57
1:J:237:LYS:HD2	1:J:238:ASP:O	2.04	0.57
1:J:122:LEU:HD11	1:J:268:ILE:HD13	1.85	0.57
1:K:212:PHE:CD2	1:K:220:PRO:HA	2.39	0.57
1:K:431:VAL:HG21	1:K:568:TYR:HB2	1.87	0.57
1:A:373:LEU:HB2	1:A:378:GLY:CA	2.34	0.57
1:A:403:LEU:HB2	1:A:407:VAL:HB	1.86	0.57
1:B:142:HIS:ND1	1:B:169:ALA:HB2	2.19	0.57
1:C:219:ARG:NH2	1:C:223:HIS:HB2	2.15	0.57
1:D:417:GLN:HB3	1:D:581:SER:HB2	1.86	0.57
1:F:358:THR:O	1:F:453:LEU:HD13	2.04	0.57
1:H:403:LEU:HB2	1:H:407:VAL:HB	1.86	0.57
1:J:260:GLN:NE2	1:J:261:PRO:HA	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:403:LEU:HB2	1:J:407:VAL:HB	1.86	0.57
1:K:227:PRO:HA	1:K:230:TRP:HB3	1.84	0.57
1:L:347:ILE:HD12	1:L:386:LEU:HD21	1.86	0.57
1:L:403:LEU:HB2	1:L:407:VAL:HB	1.87	0.57
1:A:622:LEU:N	1:A:623:PRO:HD2	2.19	0.57
1:A:74:VAL:CG1	1:A:164:ILE:HA	2.34	0.57
1:D:313:VAL:HG22	1:D:372:VAL:HG12	1.87	0.57
1:D:403:LEU:HB2	1:D:407:VAL:HB	1.86	0.57
1:J:509:LYS:O	1:J:513:GLU:HG2	2.05	0.57
1:L:79:VAL:HG21	1:L:83:LEU:HD13	1.86	0.57
1:A:590:ILE:O	1:A:594:VAL:HG23	2.05	0.57
1:C:230:TRP:O	1:C:234:ILE:HG12	2.04	0.57
1:D:102:ASP:HB3	2:D:701:5TL:CAN	2.34	0.57
1:F:590:ILE:O	1:F:594:VAL:HG23	2.04	0.57
1:G:43:ILE:HG13	1:G:94:ALA:HA	1.85	0.57
1:H:224:HIS:O	1:H:225:LEU:HD22	2.04	0.57
1:J:333:SER:HA	1:J:368:ALA:H	1.69	0.57
1:J:7:PRO:O	1:J:8:GLU:HB3	2.05	0.57
1:A:13:GLY:N	1:A:14:PRO:HD3	2.11	0.57
1:B:20:ARG:HG3	1:B:30:CYS:SG	2.44	0.57
1:B:319:THR:HG22	1:B:394:TYR:CE1	2.39	0.57
1:C:219:ARG:HH21	1:C:223:HIS:CB	2.15	0.57
1:C:509:LYS:O	1:C:513:GLU:HG2	2.05	0.57
1:D:597:GLN:O	1:D:601:LEU:HB2	2.03	0.57
1:E:506:LYS:HD3	1:E:506:LYS:H	1.70	0.57
1:F:118:GLU:HG2	1:F:379:CYS:SG	2.45	0.57
1:F:71:ALA:C	1:F:73:VAL:H	2.07	0.57
1:H:207:PHE:O	1:H:211:VAL:HG23	2.04	0.57
1:H:424:ARG:HH11	1:H:572:LYS:HG2	1.67	0.57
1:G:648:LYS:HE3	1:H:489:LEU:HD11	1.87	0.57
1:J:597:GLN:O	1:J:601:LEU:HB2	2.03	0.57
1:K:354:LEU:HB2	1:K:362:LEU:HD13	1.87	0.57
1:K:427:TRP:O	1:K:431:VAL:HG23	2.04	0.57
1:L:506:LYS:H	1:L:506:LYS:HD3	1.70	0.57
1:A:117:LYS:O	1:A:121:ILE:HG13	2.05	0.57
1:C:209:THR:HG22	1:C:220:PRO:HG3	1.85	0.57
1:E:139:LYS:HD2	1:E:172:VAL:HG11	1.87	0.57
1:H:509:LYS:O	1:H:513:GLU:HG2	2.05	0.57
1:I:110:PRO:O	1:I:113:CYS:HB3	2.04	0.57
1:K:501:GLY:HA2	1:L:658:CYS:HB3	1.87	0.57
1:B:542:MET:HA	1:B:545:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LEU:N	1:B:623:PRO:HD2	2.20	0.57
1:E:265:CYS:O	1:E:269:VAL:HG23	2.05	0.57
1:F:403:LEU:HB2	1:F:407:VAL:HB	1.87	0.57
1:F:410:ILE:HD12	1:F:583:SER:OG	2.04	0.57
1:G:552:ARG:HE	1:G:552:ARG:N	2.02	0.57
1:I:231:HIS:HB3	1:I:282:TRP:HH2	1.68	0.57
1:J:143:ARG:HG3	1:J:192:LEU:HD21	1.87	0.57
1:K:551:ARG:HB3	1:K:552:ARG:HH21	1.70	0.57
1:L:622:LEU:N	1:L:623:PRO:HD2	2.20	0.57
1:B:401:ARG:HD2	1:B:401:ARG:H	1.68	0.57
1:D:427:TRP:O	1:D:431:VAL:HG23	2.04	0.57
1:D:552:ARG:N	1:D:552:ARG:HE	2.03	0.57
1:E:143:ARG:HG3	1:E:192:LEU:HD21	1.86	0.57
1:G:86:LEU:HD12	1:G:87:ILE:HG13	1.86	0.57
1:I:509:LYS:O	1:I:513:GLU:HG2	2.05	0.57
1:J:267:LEU:HD12	1:J:312:ILE:HG23	1.85	0.57
1:J:87:ILE:O	1:J:88:HIS:HB2	2.05	0.57
1:L:354:LEU:HB2	1:L:362:LEU:HD13	1.87	0.57
1:L:320:SER:C	1:L:398:PHE:HB3	2.25	0.57
1:L:410:ILE:HD12	1:L:583:SER:OG	2.05	0.57
1:C:43:ILE:HG13	1:C:94:ALA:HA	1.86	0.57
1:E:427:TRP:O	1:E:431:VAL:HG23	2.05	0.57
1:G:506:LYS:H	1:G:506:LYS:HD3	1.70	0.57
1:G:483:PHE:HZ	1:G:514:MET:HB3	1.69	0.57
1:G:655:LYS:HE3	1:H:497:GLN:OE1	2.05	0.57
1:H:143:ARG:HG3	1:H:192:LEU:HD21	1.87	0.57
1:H:543:GLU:HA	1:H:546:LYS:NZ	2.20	0.57
4:L:705:GLC:H62	5:L:706:PDX:C5	2.34	0.57
3:A:705:5LS:C6	4:A:706:GLC:H5	2.35	0.56
1:C:222:LEU:HB2	1:C:230:TRP:CD1	2.40	0.56
1:C:221:PHE:HB2	1:C:230:TRP:HE1	1.70	0.56
1:D:235:LYS:HA	1:D:282:TRP:CH2	2.40	0.56
1:D:86:LEU:HD23	1:D:91:PRO:HA	1.87	0.56
1:F:506:LYS:H	1:F:506:LYS:HD3	1.70	0.56
1:G:403:LEU:HD23	1:G:403:LEU:H	1.70	0.56
1:H:303:LEU:O	1:H:307:ILE:HG13	2.05	0.56
1:J:552:ARG:N	1:J:552:ARG:HE	2.04	0.56
1:A:354:LEU:HB2	1:A:362:LEU:HD13	1.86	0.56
1:A:502:ILE:HD13	1:A:656:ILE:HD12	1.87	0.56
1:C:427:TRP:O	1:C:431:VAL:HG23	2.05	0.56
1:F:320:SER:HA	1:F:398:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:PRO:HA	1:G:230:TRP:CB	2.36	0.56
1:J:622:LEU:N	1:J:623:PRO:HD2	2.21	0.56
1:K:506:LYS:H	1:K:506:LYS:HD3	1.70	0.56
1:K:622:LEU:N	1:K:623:PRO:HD2	2.19	0.56
1:A:91:PRO:O	1:A:92:LEU:HD12	2.05	0.56
1:C:303:LEU:O	1:C:307:ILE:HG13	2.06	0.56
1:D:143:ARG:HG3	1:D:192:LEU:HD21	1.87	0.56
1:D:207:PHE:O	1:D:211:VAL:HG23	2.05	0.56
1:D:622:LEU:N	1:D:623:PRO:HD2	2.21	0.56
1:E:480:LEU:HD22	1:E:518:ALA:HB1	1.86	0.56
1:F:159:ILE:HG12	1:F:377:ARG:HH12	1.69	0.56
1:G:406:CYS:SG	1:G:407:VAL:HG23	2.46	0.56
1:G:427:TRP:HZ3	1:G:567:LEU:HB3	1.70	0.56
1:G:597:GLN:O	1:G:601:LEU:HB2	2.05	0.56
1:J:207:PHE:O	1:J:211:VAL:HG23	2.05	0.56
1:L:20:ARG:HG3	1:L:30:CYS:SG	2.45	0.56
1:L:237:LYS:HE2	1:L:282:TRP:H	1.69	0.56
1:A:427:TRP:HZ3	1:A:567:LEU:HB3	1.71	0.56
1:A:514:MET:HA	1:A:642:MET:HE1	1.86	0.56
1:B:250:GLY:HA3	1:D:226:GLN:HG2	1.87	0.56
1:D:226:GLN:O	1:D:230:TRP:HB2	2.05	0.56
1:E:347:ILE:HD12	1:E:386:LEU:HD21	1.86	0.56
1:E:395:GLU:HG3	1:E:397:PRO:HD3	1.87	0.56
1:E:401:ARG:HG3	1:E:433:TYR:CE1	2.41	0.56
1:F:105:LYS:HD2	4:F:703:GLC:H61	1.88	0.56
1:G:392:THR:HG22	1:G:616:GLN:HE22	1.70	0.56
1:G:427:TRP:O	1:G:431:VAL:HG23	2.05	0.56
1:J:354:LEU:HB2	1:J:362:LEU:HD13	1.88	0.56
1:K:207:PHE:O	1:K:211:VAL:HG23	2.05	0.56
1:K:347:ILE:HD12	1:K:386:LEU:HD21	1.87	0.56
1:K:509:LYS:O	1:K:513:GLU:HG2	2.05	0.56
1:A:141:ILE:HG13	1:A:203:ASP:OD1	2.06	0.56
1:A:506:LYS:H	1:A:506:LYS:HD3	1.70	0.56
1:C:142:HIS:HA	1:C:169:ALA:CB	2.35	0.56
1:D:237:LYS:HE3	1:D:281:ASN:HA	1.88	0.56
1:E:318:MET:CE	1:E:447:GLY:HA3	2.35	0.56
1:H:427:TRP:CZ3	1:H:567:LEU:HB3	2.40	0.56
1:J:79:VAL:HG11	1:J:83:LEU:HD22	1.88	0.56
1:A:415:LYS:HA	1:A:584:THR:HB	1.86	0.56
1:D:509:LYS:O	1:D:513:GLU:HG2	2.06	0.56
1:D:589:ILE:CD1	1:D:589:ILE:H	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ASN:ND2	1:E:85:ILE:H	2.04	0.56
1:F:240:LYS:HD3	1:F:277:GLN:HB3	1.86	0.56
1:F:74:VAL:HA	1:F:96:GLU:OE1	2.05	0.56
1:G:222:LEU:N	1:G:230:TRP:HE1	2.01	0.56
1:H:43:ILE:HG13	1:H:94:ALA:HA	1.86	0.56
1:I:590:ILE:O	1:I:594:VAL:HG23	2.04	0.56
1:I:502:ILE:HG23	1:J:658:CYS:SG	2.46	0.56
1:K:396:GLY:H	1:K:397:PRO:HD3	1.70	0.56
1:E:278:LEU:O	1:E:287:ARG:HG3	2.06	0.56
1:E:445:PHE:CE2	1:E:551:ARG:HD2	2.41	0.56
1:A:427:TRP:O	1:A:431:VAL:HG23	2.05	0.56
1:B:509:LYS:O	1:B:513:GLU:HG2	2.06	0.56
1:B:590:ILE:O	1:B:594:VAL:HG23	2.06	0.56
1:C:212:PHE:CE2	1:C:220:PRO:HA	2.41	0.56
1:E:267:LEU:HD12	1:E:312:ILE:HG23	1.86	0.56
1:F:354:LEU:HB2	1:F:362:LEU:HD13	1.88	0.56
1:G:498:MET:HA	1:G:503:SER:HB3	1.86	0.56
1:G:480:LEU:HD22	1:G:518:ALA:HB1	1.87	0.56
1:G:77:CYS:O	1:G:94:ALA:HB3	2.06	0.56
1:H:412:GLN:NE2	1:J:20:ARG:HG2	2.20	0.56
1:L:289:GLY:O	1:L:291:VAL:HG23	2.06	0.56
1:L:334:LEU:HD11	1:L:364:PRO:HA	1.86	0.56
1:L:43:ILE:HG13	1:L:94:ALA:HA	1.87	0.56
1:L:552:ARG:N	1:L:552:ARG:HE	2.02	0.56
1:A:212:PHE:CE2	1:A:220:PRO:HA	2.41	0.56
1:C:415:LYS:HA	1:C:584:THR:HB	1.88	0.56
1:E:552:ARG:HE	1:E:552:ARG:N	2.02	0.56
1:G:97:TYR:HA	2:G:701:5TL:NAW	2.20	0.56
1:H:639:VAL:HA	1:H:642:MET:HG3	1.87	0.56
1:J:298:PRO:O	1:J:302:VAL:HG23	2.06	0.56
1:D:544:LEU:HD11	1:D:610:LYS:HB3	1.88	0.56
1:E:478:ALA:CB	1:F:475:GLN:HA	2.36	0.56
1:G:231:HIS:N	1:G:231:HIS:ND1	2.53	0.56
1:G:262:ASN:ND2	1:G:264:LEU:H	2.04	0.56
1:H:623:PRO:O	1:H:627:VAL:HG23	2.05	0.56
1:I:143:ARG:HG3	1:I:192:LEU:HD21	1.88	0.56
1:I:552:ARG:HE	1:I:552:ARG:N	2.03	0.56
1:K:143:ARG:HG3	1:K:192:LEU:HD21	1.88	0.56
1:A:262:ASN:ND2	1:A:264:LEU:H	2.04	0.56
1:B:43:ILE:HG13	1:B:94:ALA:HA	1.86	0.56
1:D:546:LYS:HA	6:D:710:5TJ:S4	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ILE:O	1:D:587:VAL:HG22	2.06	0.56
1:F:480:LEU:HD22	1:F:518:ALA:HB1	1.88	0.56
1:F:639:VAL:HA	1:F:642:MET:HG3	1.88	0.56
1:G:222:LEU:HD22	1:G:230:TRP:CD1	2.38	0.56
1:I:506:LYS:H	1:I:506:LYS:HD3	1.69	0.56
1:I:575:PRO:HB3	1:K:574:ARG:HH12	1.69	0.56
1:I:622:LEU:N	1:I:623:PRO:HD2	2.21	0.56
1:J:227:PRO:HA	1:J:230:TRP:CB	2.29	0.56
1:K:20:ARG:HG3	1:K:30:CYS:SG	2.46	0.56
1:L:143:ARG:HG3	1:L:192:LEU:HD21	1.86	0.56
1:A:597:GLN:O	1:A:601:LEU:HB2	2.06	0.55
1:B:303:LEU:O	1:B:307:ILE:HG13	2.06	0.55
1:C:622:LEU:N	1:C:623:PRO:HD2	2.20	0.55
1:D:354:LEU:HB2	1:D:362:LEU:HD13	1.89	0.55
1:D:411:VAL:HG12	1:D:590:ILE:HG21	1.88	0.55
1:E:98:CYS:HB3	1:E:152:LEU:O	2.05	0.55
1:E:396:GLY:N	1:E:397:PRO:HD3	2.16	0.55
1:F:143:ARG:HG3	1:F:192:LEU:HD21	1.87	0.55
1:F:597:GLN:O	1:F:601:LEU:HB2	2.06	0.55
1:G:170:LYS:CG	1:G:177:LEU:HG	2.36	0.55
1:G:354:LEU:HB2	1:G:362:LEU:HD13	1.88	0.55
1:G:551:ARG:O	1:G:551:ARG:HG3	2.06	0.55
1:H:20:ARG:HG3	1:H:30:CYS:SG	2.46	0.55
1:I:354:LEU:HB2	1:I:362:LEU:HD13	1.88	0.55
1:J:284:PRO:HG2	1:J:285:GLN:H	1.70	0.55
1:J:363:ASP:HB3	1:J:370:GLN:HE22	1.70	0.55
1:J:427:TRP:O	1:J:431:VAL:HG23	2.05	0.55
1:K:262:ASN:ND2	1:K:264:LEU:H	2.04	0.55
1:L:396:GLY:N	1:L:397:PRO:HD3	2.21	0.55
1:A:70:HIS:CD2	1:A:72:ASN:HB3	2.42	0.55
1:B:298:PRO:O	1:B:302:VAL:HG23	2.06	0.55
1:C:354:LEU:HB2	1:C:362:LEU:HD13	1.88	0.55
1:D:401:ARG:HH22	1:D:436:GLY:C	2.09	0.55
1:E:462:LEU:HD22	1:E:618:ILE:HG23	1.88	0.55
1:F:509:LYS:O	1:F:513:GLU:HG2	2.06	0.55
1:G:46:CYS:HA	1:G:58:TRP:CH2	2.41	0.55
1:H:347:ILE:HD12	1:H:386:LEU:HD21	1.86	0.55
1:L:509:LYS:O	1:L:513:GLU:HG2	2.06	0.55
1:A:552:ARG:HE	1:A:552:ARG:N	2.04	0.55
1:B:249:SER:O	1:D:227:PRO:HG2	2.06	0.55
1:C:98:CYS:HA	1:C:153:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:LEU:O	1:E:307:ILE:HG13	2.07	0.55
1:E:316:LEU:HB2	1:E:383:MET:CE	2.36	0.55
1:G:21:LEU:HD12	2:G:701:5TL:CAJ	2.37	0.55
1:H:69:ASN:ND2	1:H:75:LYS:HE2	2.21	0.55
1:J:188:LEU:HD21	1:J:192:LEU:HD22	1.88	0.55
1:K:303:LEU:O	1:K:307:ILE:HG13	2.07	0.55
1:L:223:HIS:O	1:L:225:LEU:HG	2.07	0.55
1:A:185:LEU:O	1:A:186:GLN:HG2	2.06	0.55
1:A:207:PHE:O	1:A:211:VAL:HG23	2.06	0.55
1:B:219:ARG:H	1:B:219:ARG:HH11	1.53	0.55
1:C:191:GLU:CD	1:C:284:PRO:HB3	2.26	0.55
1:C:396:GLY:HA2	1:C:398:PHE:CE2	2.42	0.55
1:E:406:CYS:SG	1:E:407:VAL:HG23	2.47	0.55
1:E:489:LEU:HD21	1:F:648:LYS:HG3	1.88	0.55
1:A:574:ARG:NH1	1:E:575:PRO:HB3	2.20	0.55
1:E:622:LEU:N	1:E:623:PRO:HD2	2.20	0.55
1:G:98:CYS:HA	1:G:153:GLN:NE2	2.20	0.55
1:H:141:ILE:HG13	1:H:203:ASP:OD1	2.06	0.55
1:H:410:ILE:HG23	1:H:583:SER:OG	2.07	0.55
1:I:294:THR:HG22	1:I:295:LEU:HD12	1.89	0.55
1:J:589:ILE:H	1:J:589:ILE:CD1	2.20	0.55
1:K:410:ILE:HG23	1:K:583:SER:OG	2.05	0.55
1:A:236:LYS:HZ2	1:A:237:LYS:H	1.55	0.55
1:B:240:LYS:O	1:B:277:GLN:HG2	2.06	0.55
1:B:577:ASP:HA	1:D:576:SER:OG	2.06	0.55
1:C:506:LYS:HD3	1:C:506:LYS:H	1.70	0.55
1:D:427:TRP:CZ3	1:D:567:LEU:HB3	2.39	0.55
1:E:639:VAL:HA	1:E:642:MET:HG3	1.88	0.55
1:G:141:ILE:HG13	1:G:203:ASP:OD1	2.07	0.55
1:G:509:LYS:O	1:G:513:GLU:HG2	2.06	0.55
1:H:46:CYS:SG	1:H:90:VAL:HB	2.47	0.55
1:J:469:LEU:HD12	1:J:625:VAL:HG13	1.88	0.55
1:L:315:ILE:HD12	1:L:384:VAL:HB	1.89	0.55
1:L:502:ILE:HD13	1:L:656:ILE:HD12	1.89	0.55
1:A:43:ILE:HG13	1:A:94:ALA:HA	1.87	0.55
1:B:347:ILE:HD12	1:B:386:LEU:HD21	1.86	0.55
1:C:143:ARG:HG3	1:C:192:LEU:HD21	1.88	0.55
1:E:46:CYS:HA	1:E:58:TRP:CH2	2.41	0.55
1:G:289:GLY:O	1:G:291:VAL:HG23	2.06	0.55
1:J:123:SER:HB2	1:J:377:ARG:HD3	1.88	0.55
1:A:17:MET:HB3	1:A:32:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLY:N	1:C:14:PRO:HD3	2.21	0.55
1:F:20:ARG:HG3	1:F:30:CYS:SG	2.47	0.55
1:G:278:LEU:HD23	1:G:288:GLY:HA2	1.88	0.55
1:G:303:LEU:O	1:G:307:ILE:HG13	2.06	0.55
1:J:212:PHE:CE2	1:J:220:PRO:HA	2.40	0.55
1:L:589:ILE:N	1:L:589:ILE:HD12	2.20	0.55
1:L:639:VAL:HA	1:L:642:MET:HG3	1.89	0.55
1:A:143:ARG:HG3	1:A:192:LEU:HD21	1.88	0.55
1:A:70:HIS:NE2	1:A:72:ASN:HB3	2.22	0.55
1:B:426:VAL:HG23	1:B:427:TRP:HD1	1.71	0.55
1:C:141:ILE:HG13	1:C:203:ASP:OD1	2.07	0.55
1:C:77:CYS:O	1:C:94:ALA:HB3	2.07	0.55
1:D:186:GLN:HE21	1:D:219:ARG:HE	1.54	0.55
1:D:589:ILE:HD12	1:D:589:ILE:N	2.20	0.55
1:F:362:LEU:HG	1:F:363:ASP:H	1.72	0.55
1:E:502:ILE:HG13	1:F:658:CYS:SG	2.47	0.55
1:G:222:LEU:HB3	1:G:225:LEU:HB2	1.89	0.55
1:G:275:TRP:CZ2	1:G:304:MET:HE2	2.42	0.55
1:L:238:ASP:HB3	1:L:239:PRO:HD2	1.89	0.55
1:L:362:LEU:HG	1:L:363:ASP:H	1.72	0.55
1:L:597:GLN:O	1:L:601:LEU:HB2	2.06	0.55
1:D:550:GLY:HA3	1:D:604:LEU:HD13	1.89	0.55
1:I:417:GLN:HB3	1:I:581:SER:HB3	1.88	0.55
1:I:639:VAL:HA	1:I:642:MET:HG3	1.89	0.55
1:I:49:GLU:HA	1:I:88:HIS:HB2	1.88	0.55
1:J:116:LEU:HD12	1:J:116:LEU:H	1.72	0.55
1:K:117:LYS:O	1:K:121:ILE:HG13	2.07	0.55
1:K:141:ILE:HG13	1:K:203:ASP:OD1	2.06	0.55
1:L:75:LYS:O	1:L:95:MET:HA	2.07	0.55
1:B:506:LYS:H	1:B:506:LYS:HD3	1.70	0.55
1:E:470:ILE:O	1:E:474:GLN:HG2	2.07	0.55
1:F:18:ARG:HH21	1:F:33:GLN:NE2	2.05	0.55
1:J:46:CYS:HA	1:J:58:TRP:CH2	2.42	0.55
1:J:590:ILE:O	1:J:594:VAL:HG23	2.06	0.55
1:L:473:SER:OG	1:L:524:VAL:HG13	2.07	0.55
1:A:47:ARG:O	1:A:87:ILE:HB	2.07	0.54
1:B:401:ARG:HG2	1:B:433:TYR:HE1	1.72	0.54
1:C:207:PHE:O	1:C:211:VAL:HG23	2.06	0.54
1:D:240:LYS:HB3	1:D:277:GLN:HB3	1.88	0.54
1:E:424:ARG:NH1	1:E:572:LYS:HG2	2.22	0.54
1:E:509:LYS:O	1:E:513:GLU:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:GLY:HA2	2:F:701:5TL:CAQ	2.37	0.54
1:I:227:PRO:HG2	1:K:249:SER:O	2.07	0.54
1:A:303:LEU:O	1:A:307:ILE:HG13	2.07	0.54
1:A:46:CYS:HA	1:A:58:TRP:CH2	2.42	0.54
1:C:363:ASP:HB3	1:C:370:GLN:HE22	1.71	0.54
1:E:401:ARG:HG3	1:E:433:TYR:HE1	1.73	0.54
1:E:597:GLN:O	1:E:601:LEU:HB2	2.07	0.54
1:F:141:ILE:HG13	1:F:203:ASP:OD1	2.07	0.54
1:F:240:LYS:HB3	1:F:277:GLN:HB3	1.88	0.54
1:F:62:ILE:HG22	1:F:93:LEU:HD13	1.90	0.54
1:G:281:ASN:HB3	1:G:287:ARG:HG2	1.89	0.54
1:G:639:VAL:HA	1:G:642:MET:HG3	1.89	0.54
1:H:506:LYS:HD3	1:H:506:LYS:H	1.70	0.54
1:I:219:ARG:NE	1:I:223:HIS:HA	2.19	0.54
1:I:597:GLN:O	1:I:601:LEU:HB2	2.08	0.54
1:K:406:CYS:SG	1:K:407:VAL:HG23	2.47	0.54
1:L:79:VAL:HG11	1:L:83:LEU:CD1	2.37	0.54
1:A:107:LEU:HD23	1:A:116:LEU:HD11	1.88	0.54
1:A:470:ILE:O	1:A:474:GLN:HG2	2.07	0.54
1:A:574:ARG:HD2	1:A:577:ASP:OD2	2.08	0.54
1:B:552:ARG:HE	1:B:552:ARG:N	2.04	0.54
1:B:639:VAL:HA	1:B:642:MET:HG3	1.88	0.54
1:B:84:ASN:ND2	1:B:86:LEU:H	2.04	0.54
1:D:188:LEU:HD21	1:D:192:LEU:HD22	1.89	0.54
1:E:318:MET:HE1	1:E:444:LEU:O	2.06	0.54
1:G:13:GLY:N	1:G:14:PRO:HD3	2.22	0.54
1:G:20:ARG:HG3	1:G:30:CYS:SG	2.47	0.54
1:G:362:LEU:HG	1:G:363:ASP:H	1.72	0.54
1:G:574:ARG:NH1	1:K:575:PRO:HB3	2.23	0.54
1:H:590:ILE:O	1:H:594:VAL:HG23	2.07	0.54
1:J:275:TRP:CZ2	1:J:304:MET:HE2	2.42	0.54
1:C:50:LEU:HD13	1:C:90:VAL:HG21	1.90	0.54
1:C:639:VAL:HA	1:C:642:MET:HG3	1.90	0.54
1:E:141:ILE:HG13	1:E:203:ASP:OD1	2.07	0.54
1:G:212:PHE:CD2	1:G:220:PRO:HA	2.43	0.54
1:G:17:MET:HB3	1:G:32:TYR:CE1	2.42	0.54
1:I:55:ARG:HH21	1:I:88:HIS:CE1	2.25	0.54
1:K:392:THR:HG22	1:K:616:GLN:HE22	1.73	0.54
1:A:489:LEU:HD11	1:B:648:LYS:HE3	1.90	0.54
1:C:387:PHE:CZ	1:C:451:ALA:HB2	2.41	0.54
1:D:639:VAL:HA	1:D:642:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:GLY:HA3	1:E:215:ILE:O	2.07	0.54
1:F:220:PRO:O	1:F:243:PHE:HA	2.06	0.54
1:H:406:CYS:SG	1:H:407:VAL:HG23	2.48	0.54
1:H:412:GLN:HE22	1:J:20:ARG:HG2	1.73	0.54
1:I:303:LEU:O	1:I:307:ILE:HG13	2.08	0.54
1:J:249:SER:HB3	1:L:185:LEU:H	1.73	0.54
1:J:623:PRO:O	1:J:627:VAL:HG23	2.07	0.54
1:L:141:ILE:HG13	1:L:203:ASP:OD1	2.08	0.54
1:A:509:LYS:O	1:A:513:GLU:HG2	2.06	0.54
1:B:188:LEU:HD21	1:B:192:LEU:HD22	1.90	0.54
1:C:17:MET:HB3	1:C:32:TYR:CE1	2.43	0.54
1:D:17:MET:HB3	1:D:32:TYR:CE1	2.43	0.54
1:E:207:PHE:O	1:E:211:VAL:HG23	2.08	0.54
1:H:222:LEU:HB2	1:H:230:TRP:CD1	2.42	0.54
1:H:233:LYS:HE2	1:H:252:VAL:HG11	1.90	0.54
1:J:589:ILE:HD12	1:J:589:ILE:N	2.21	0.54
1:K:420:ILE:HG21	1:K:578:HIS:H	1.72	0.54
1:K:73:VAL:HG22	1:K:74:VAL:H	1.72	0.54
1:L:420:ILE:HG21	1:L:578:HIS:H	1.72	0.54
1:L:589:ILE:CD1	1:L:589:ILE:H	2.20	0.54
1:C:597:GLN:O	1:C:601:LEU:HB2	2.08	0.54
1:E:291:VAL:HG22	1:E:298:PRO:HB3	1.90	0.54
1:F:470:ILE:O	1:F:474:GLN:HG2	2.08	0.54
1:G:550:GLY:HA3	1:G:604:LEU:HD13	1.90	0.54
1:H:188:LEU:HD21	1:H:192:LEU:HD22	1.90	0.54
1:K:224:HIS:NE2	1:K:424:ARG:HD2	2.22	0.54
1:K:470:ILE:O	1:K:474:GLN:HG2	2.08	0.54
1:L:278:LEU:O	1:L:287:ARG:HG3	2.08	0.54
1:L:427:TRP:CZ3	1:L:567:LEU:HB3	2.41	0.54
1:C:589:ILE:HD12	1:C:589:ILE:N	2.21	0.54
1:E:187:TYR:OH	1:E:219:ARG:HD3	2.08	0.54
1:F:589:ILE:HD12	1:F:589:ILE:N	2.21	0.54
1:J:359:GLY:HA3	1:J:453:LEU:HB2	1.90	0.54
1:K:17:MET:HB3	1:K:32:TYR:CE1	2.43	0.54
1:K:423:LEU:HA	1:K:426:VAL:CG2	2.38	0.54
1:K:465:MET:CB	1:K:625:VAL:HG11	2.38	0.54
1:L:207:PHE:O	1:L:211:VAL:HG23	2.07	0.54
1:L:46:CYS:HA	1:L:58:TRP:CH2	2.43	0.54
1:A:74:VAL:HB	1:A:164:ILE:HG13	1.89	0.54
1:C:237:LYS:NZ	1:C:281:ASN:HA	2.22	0.54
1:D:470:ILE:O	1:D:474:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:TRP:HZ3	1:E:567:LEU:HB3	1.72	0.54
1:F:473:SER:HB2	1:F:524:VAL:HA	1.90	0.54
1:F:552:ARG:HE	1:F:552:ARG:N	2.04	0.54
1:F:427:TRP:HZ2	1:F:583:SER:HA	1.73	0.54
1:F:589:ILE:CD1	1:F:589:ILE:H	2.20	0.54
1:F:86:LEU:HD23	1:F:87:ILE:CD1	2.38	0.54
1:I:395:GLU:HG2	1:I:396:GLY:H	1.73	0.54
1:I:420:ILE:HG21	1:I:578:HIS:H	1.72	0.54
1:I:50:LEU:HD12	1:I:50:LEU:H	1.73	0.54
1:J:639:VAL:HA	1:J:642:MET:HG3	1.90	0.54
1:K:204:TYR:HB2	1:K:287:ARG:HH12	1.72	0.54
1:K:46:CYS:HA	1:K:58:TRP:CH2	2.42	0.54
1:A:204:TYR:HB2	1:A:287:ARG:NH1	2.23	0.54
1:A:362:LEU:HG	1:A:363:ASP:H	1.73	0.54
1:A:654:LEU:HD11	1:B:502:ILE:HD11	1.89	0.54
1:B:46:CYS:HA	1:B:58:TRP:CH2	2.42	0.54
1:D:141:ILE:HG13	1:D:203:ASP:OD1	2.08	0.54
1:G:143:ARG:HG3	1:G:192:LEU:HD21	1.89	0.54
1:I:17:MET:HB3	1:I:32:TYR:CE1	2.43	0.54
1:J:141:ILE:HG13	1:J:203:ASP:OD1	2.08	0.54
3:J:704:5LS:C6	4:J:705:GLC:H5	2.37	0.54
1:K:597:GLN:O	1:K:601:LEU:HB2	2.08	0.54
1:K:639:VAL:HA	1:K:642:MET:HG3	1.89	0.54
1:K:6:ASP:N	1:K:7:PRO:HD2	2.23	0.54
1:L:488:GLN:HB3	1:L:515:GLU:OE2	2.07	0.54
1:B:587:VAL:O	1:B:591:VAL:HG23	2.08	0.53
1:B:68:LEU:HD21	1:B:140:ILE:HD12	1.90	0.53
1:C:406:CYS:SG	1:C:407:VAL:HG23	2.47	0.53
1:E:420:ILE:HG21	1:E:578:HIS:N	2.22	0.53
1:F:7:PRO:HG3	1:F:17:MET:HE1	1.89	0.53
1:F:303:LEU:O	1:F:307:ILE:HG13	2.08	0.53
1:G:184:THR:OG1	1:I:248:MET:HB3	2.07	0.53
1:G:186:GLN:NE2	1:G:219:ARG:HH11	2.06	0.53
1:H:267:LEU:HD13	1:H:327:LEU:HB2	1.90	0.53
1:I:70:HIS:CG	1:I:71:ALA:H	2.25	0.53
1:J:18:ARG:HH21	1:J:33:GLN:NE2	2.04	0.53
1:J:17:MET:HB3	1:J:32:TYR:CE1	2.43	0.53
1:L:373:LEU:HD23	1:L:373:LEU:N	2.23	0.53
1:B:141:ILE:O	1:B:169:ALA:HB1	2.09	0.53
1:D:18:ARG:HH21	1:D:33:GLN:NE2	2.05	0.53
1:D:362:LEU:HG	1:D:363:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:HD12	1:D:50:LEU:H	1.74	0.53
1:F:46:CYS:HA	1:F:58:TRP:CH2	2.43	0.53
1:H:362:LEU:HG	1:H:363:ASP:H	1.73	0.53
1:I:406:CYS:SG	1:I:407:VAL:HG23	2.48	0.53
1:I:426:VAL:HG23	1:I:427:TRP:HD1	1.72	0.53
1:I:427:TRP:O	1:I:431:VAL:HG23	2.08	0.53
1:I:589:ILE:H	1:I:589:ILE:CD1	2.21	0.53
1:K:98:CYS:HA	1:K:153:GLN:NE2	2.23	0.53
1:K:589:ILE:H	1:K:589:ILE:CD1	2.21	0.53
1:L:470:ILE:O	1:L:474:GLN:HG2	2.09	0.53
1:B:18:ARG:HH21	1:B:33:GLN:NE2	2.06	0.53
1:B:26:PHE:HA	1:F:408:ASN:ND2	2.24	0.53
1:D:275:TRP:CZ2	1:D:304:MET:HE2	2.44	0.53
1:D:502:ILE:HG21	1:D:656:ILE:CD1	2.38	0.53
1:F:17:MET:HB3	1:F:32:TYR:CE1	2.43	0.53
1:F:201:THR:C	1:F:287:ARG:HH21	2.11	0.53
1:F:334:LEU:HD11	1:F:364:PRO:HA	1.90	0.53
1:G:589:ILE:N	1:G:589:ILE:HD12	2.20	0.53
1:J:240:LYS:O	1:J:277:GLN:HG2	2.08	0.53
1:J:551:ARG:HB3	1:J:552:ARG:HH21	1.74	0.53
1:K:623:PRO:O	1:K:627:VAL:HG23	2.08	0.53
1:K:46:CYS:N	1:K:86:LEU:HD23	2.22	0.53
1:L:158:LYS:HD2	1:L:376:VAL:HG13	1.89	0.53
1:A:655:LYS:HA	1:A:658:CYS:SG	2.49	0.53
1:B:176:GLU:HB2	1:B:177:LEU:HD12	1.90	0.53
1:B:406:CYS:SG	1:B:407:VAL:HG23	2.48	0.53
1:C:29:VAL:HG21	2:C:701:5TL:CAE	2.38	0.53
1:E:262:ASN:ND2	1:E:264:LEU:H	2.07	0.53
1:H:552:ARG:N	1:H:552:ARG:HE	2.06	0.53
1:I:589:ILE:HD12	1:I:589:ILE:N	2.22	0.53
1:K:222:LEU:HB2	1:K:230:TRP:CD1	2.44	0.53
1:K:426:VAL:HG23	1:K:427:TRP:HD1	1.72	0.53
1:L:17:MET:HB3	1:L:32:TYR:CE1	2.43	0.53
1:A:412:GLN:CD	1:E:27:GLY:HA2	2.29	0.53
1:A:589:ILE:HD12	1:A:589:ILE:N	2.21	0.53
1:C:589:ILE:CD1	1:C:589:ILE:H	2.21	0.53
1:D:98:CYS:HA	1:D:153:GLN:NE2	2.23	0.53
1:D:185:LEU:HD13	1:D:186:GLN:H	1.72	0.53
1:E:234:ILE:HG22	1:E:254:PHE:CE1	2.44	0.53
1:E:426:VAL:HG23	1:E:427:TRP:HD1	1.72	0.53
1:F:102:ASP:OD1	2:F:701:5TL:CAN	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:HIS:ND1	1:F:169:ALA:HB2	2.23	0.53
1:H:413:ASP:OD1	1:H:416:ILE:HB	2.08	0.53
1:H:600:VAL:HA	1:H:603:GLU:HB3	1.91	0.53
1:J:600:VAL:HA	1:J:603:GLU:HB3	1.90	0.53
1:K:480:LEU:HD22	1:K:518:ALA:HB1	1.91	0.53
1:K:552:ARG:HE	1:K:552:ARG:N	2.06	0.53
1:K:79:VAL:HG21	1:K:83:LEU:HD13	1.90	0.53
1:A:20:ARG:HG3	1:A:30:CYS:SG	2.48	0.53
1:D:180:GLU:HG2	1:D:195:ASN:ND2	2.24	0.53
1:F:207:PHE:O	1:F:211:VAL:HG23	2.08	0.53
1:H:426:VAL:HG23	1:H:427:TRP:HD1	1.73	0.53
1:I:48:LEU:HA	1:I:87:ILE:HG21	1.89	0.53
1:I:551:ARG:HB3	1:I:552:ARG:HH21	1.73	0.53
1:J:98:CYS:HB3	1:J:152:LEU:O	2.08	0.53
1:K:401:ARG:HH22	1:K:440:ASP:CB	2.22	0.53
1:L:406:CYS:SG	1:L:407:VAL:HG23	2.48	0.53
1:A:222:LEU:HD13	1:A:244:ALA:O	2.09	0.53
1:C:50:LEU:HD12	1:C:50:LEU:H	1.74	0.53
1:D:590:ILE:O	1:D:594:VAL:HG23	2.08	0.53
1:D:655:LYS:HA	1:D:658:CYS:SG	2.49	0.53
1:E:334:LEU:HD11	1:E:364:PRO:HA	1.89	0.53
1:E:423:LEU:HA	1:E:426:VAL:CG2	2.39	0.53
1:E:6:ASP:N	1:E:7:PRO:HD2	2.24	0.53
1:G:139:LYS:HD2	1:G:172:VAL:HG21	1.91	0.53
1:G:413:ASP:OD1	1:G:416:ILE:HB	2.09	0.53
1:G:470:ILE:O	1:G:474:GLN:HG2	2.08	0.53
1:H:18:ARG:HH21	1:H:33:GLN:NE2	2.06	0.53
1:H:275:TRP:CZ2	1:H:304:MET:HE2	2.43	0.53
1:H:50:LEU:HD13	1:H:90:VAL:HG21	1.90	0.53
1:I:170:LYS:HG2	1:I:177:LEU:HG	1.91	0.53
1:I:401:ARG:NH2	1:I:440:ASP:HB2	2.24	0.53
1:J:303:LEU:O	1:J:307:ILE:HG13	2.09	0.53
1:J:415:LYS:HA	1:J:584:THR:HB	1.90	0.53
1:K:415:LYS:HA	1:K:584:THR:HB	1.89	0.53
1:A:227:PRO:CA	1:A:230:TRP:HB3	2.27	0.53
1:B:219:ARG:CZ	1:B:224:HIS:H	2.22	0.53
1:C:473:SER:HB2	1:C:524:VAL:HA	1.89	0.53
1:C:410:ILE:HG23	1:C:583:SER:OG	2.09	0.53
1:D:600:VAL:HA	1:D:603:GLU:HB3	1.90	0.53
1:E:549:TYR:H	1:E:552:ARG:HD2	1.74	0.53
1:F:267:LEU:HD12	1:F:312:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:ARG:HH21	1:I:224:HIS:N	2.07	0.53
1:J:655:LYS:HA	1:J:658:CYS:SG	2.49	0.53
1:A:29:VAL:HG21	2:A:701:5TL:CAE	2.39	0.53
1:B:50:LEU:HD12	1:B:50:LEU:H	1.74	0.53
1:G:600:VAL:HA	1:G:603:GLU:HB3	1.91	0.53
1:H:589:ILE:HD12	1:H:589:ILE:N	2.20	0.53
1:I:362:LEU:HG	1:I:363:ASP:H	1.73	0.53
1:J:334:LEU:HD22	1:J:366:LYS:O	2.08	0.53
1:J:487:ILE:HG12	1:J:515:GLU:HB2	1.90	0.53
1:J:50:LEU:H	1:J:50:LEU:HD12	1.74	0.53
1:K:376:VAL:HG13	1:K:377:ARG:H	1.74	0.53
1:B:413:ASP:OD1	1:B:416:ILE:HB	2.08	0.53
1:B:600:VAL:HA	1:B:603:GLU:HB3	1.91	0.53
1:D:513:GLU:O	1:D:517:LYS:HG3	2.09	0.53
1:E:362:LEU:HG	1:E:363:ASP:H	1.73	0.53
1:E:50:LEU:HD12	1:E:50:LEU:H	1.73	0.53
1:G:50:LEU:HD12	1:G:50:LEU:H	1.74	0.53
1:G:547:SER:OG	1:G:548:PRO:HD2	2.09	0.53
1:G:68:LEU:C	1:G:69:ASN:HD22	2.12	0.53
1:I:470:ILE:O	1:I:474:GLN:HG2	2.09	0.53
1:K:50:LEU:H	1:K:50:LEU:HD12	1.73	0.53
1:L:221:PHE:HB2	1:L:230:TRP:HE1	1.74	0.53
1:A:413:ASP:OD1	1:A:416:ILE:HB	2.10	0.52
1:D:46:CYS:HA	1:D:58:TRP:CH2	2.44	0.52
1:D:623:PRO:O	1:D:627:VAL:HG23	2.09	0.52
1:E:219:ARG:NH2	1:E:224:HIS:HB2	2.24	0.52
1:G:185:LEU:H	1:I:249:SER:HB3	1.75	0.52
1:J:362:LEU:HG	1:J:363:ASP:H	1.73	0.52
1:J:420:ILE:HG21	1:J:578:HIS:N	2.23	0.52
1:K:600:VAL:HA	1:K:603:GLU:HB3	1.91	0.52
1:L:141:ILE:CG2	1:L:170:LYS:HB2	2.37	0.52
1:A:488:GLN:HB3	1:A:515:GLU:OE2	2.10	0.52
1:C:222:LEU:H	1:C:230:TRP:HE1	1.55	0.52
1:C:362:LEU:HG	1:C:363:ASP:H	1.73	0.52
1:D:303:LEU:O	1:D:307:ILE:HG13	2.09	0.52
1:E:188:LEU:HD21	1:E:192:LEU:HD22	1.91	0.52
1:H:46:CYS:HA	1:H:58:TRP:CH2	2.43	0.52
1:J:470:ILE:O	1:J:474:GLN:HG2	2.10	0.52
1:K:362:LEU:HG	1:K:363:ASP:H	1.73	0.52
1:L:188:LEU:HD21	1:L:192:LEU:HD22	1.91	0.52
1:A:426:VAL:HG23	1:A:427:TRP:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD21	1:B:648:LYS:HG3	1.90	0.52
1:A:639:VAL:HA	1:A:642:MET:HG3	1.92	0.52
1:B:589:ILE:HD12	1:B:589:ILE:N	2.20	0.52
1:B:465:MET:HB3	1:B:625:VAL:HG11	1.91	0.52
1:H:212:PHE:CD2	1:H:220:PRO:HA	2.45	0.52
1:H:410:ILE:O	1:H:587:VAL:HG22	2.09	0.52
1:H:587:VAL:O	1:H:591:VAL:HG23	2.10	0.52
1:I:222:LEU:HB2	1:I:230:TRP:CD1	2.44	0.52
1:J:408:ASN:ND2	1:L:26:PHE:HA	2.25	0.52
1:J:513:GLU:O	1:J:517:LYS:HG3	2.09	0.52
1:K:489:LEU:HD11	1:L:648:LYS:HE3	1.91	0.52
1:A:20:ARG:C	1:A:21:LEU:HD22	2.30	0.52
1:A:513:GLU:O	1:A:517:LYS:HG3	2.08	0.52
1:A:623:PRO:O	1:A:627:VAL:HG23	2.10	0.52
1:B:234:ILE:HD12	1:B:234:ILE:N	2.24	0.52
1:C:227:PRO:HA	1:C:230:TRP:CB	2.33	0.52
1:C:74:VAL:HG21	1:C:95:MET:CE	2.34	0.52
1:E:590:ILE:O	1:E:594:VAL:HG23	2.09	0.52
1:H:50:LEU:H	1:H:50:LEU:HD12	1.74	0.52
1:J:587:VAL:O	1:J:591:VAL:HG23	2.09	0.52
1:L:117:LYS:O	1:L:121:ILE:HG13	2.10	0.52
1:A:377:ARG:HE	1:A:377:ARG:HA	1.75	0.52
1:A:50:LEU:H	1:A:50:LEU:HD12	1.74	0.52
1:D:46:CYS:HB2	1:D:87:ILE:HB	1.92	0.52
1:E:17:MET:HB3	1:E:32:TYR:CE1	2.45	0.52
1:E:513:GLU:O	1:E:517:LYS:HG3	2.10	0.52
1:E:600:VAL:HA	1:E:603:GLU:HB3	1.92	0.52
1:G:73:VAL:HG22	1:G:74:VAL:N	2.22	0.52
1:H:513:GLU:O	1:H:517:LYS:HG3	2.09	0.52
1:I:21:LEU:HD12	2:I:701:5TL:CAJ	2.39	0.52
1:K:185:LEU:HD13	1:K:186:GLN:N	2.20	0.52
1:K:590:ILE:O	1:K:594:VAL:HG23	2.08	0.52
1:L:420:ILE:HD11	1:L:571:LEU:HG	1.92	0.52
1:A:17:MET:HB3	1:A:32:TYR:CD1	2.45	0.52
1:B:141:ILE:HG13	1:B:203:ASP:OD1	2.09	0.52
1:B:185:LEU:HD13	1:B:186:GLN:H	1.75	0.52
1:F:275:TRP:HZ2	1:F:304:MET:HE2	1.75	0.52
1:F:513:GLU:O	1:F:517:LYS:HG3	2.10	0.52
1:F:655:LYS:HA	1:F:658:CYS:SG	2.50	0.52
1:D:416:ILE:HD13	2:F:701:5TL:O4	2.10	0.52
1:G:431:VAL:HG21	1:G:568:TYR:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:MET:HB3	1:H:32:TYR:CE1	2.44	0.52
1:H:373:LEU:N	1:H:373:LEU:HD22	2.25	0.52
1:H:574:ARG:NH1	1:H:575:PRO:HD2	2.24	0.52
1:I:207:PHE:O	1:I:211:VAL:HG23	2.09	0.52
1:I:234:ILE:HG22	1:I:254:PHE:HE1	1.75	0.52
1:I:550:GLY:HA3	1:I:604:LEU:HD13	1.92	0.52
1:L:328:LEU:HD11	1:L:337:LEU:HD22	1.91	0.52
1:B:427:TRP:CZ3	1:B:567:LEU:HB3	2.42	0.52
1:D:118:GLU:HB2	1:D:263:SER:O	2.09	0.52
1:D:222:LEU:HB2	1:D:230:TRP:NE1	2.24	0.52
1:D:240:LYS:O	1:D:277:GLN:HG2	2.10	0.52
1:D:426:VAL:HG23	1:D:427:TRP:HD1	1.74	0.52
1:H:376:VAL:HG23	1:H:377:ARG:H	1.75	0.52
1:I:141:ILE:HG13	1:I:203:ASP:OD1	2.10	0.52
1:I:46:CYS:HA	1:I:58:TRP:CH2	2.44	0.52
1:L:240:LYS:HB3	1:L:277:GLN:HB3	1.92	0.52
1:A:480:LEU:CD2	1:A:518:ALA:HB1	2.40	0.52
1:A:654:LEU:CD2	1:B:497:GLN:HE22	2.23	0.52
1:B:431:VAL:HG21	1:B:568:TYR:HB2	1.92	0.52
1:C:284:PRO:HA	1:C:287:ARG:NH2	2.24	0.52
1:C:470:ILE:O	1:C:474:GLN:HG2	2.10	0.52
1:D:281:ASN:O	1:D:282:TRP:HB2	2.09	0.52
1:D:8:GLU:HB2	1:D:87:ILE:HG12	1.91	0.52
1:G:383:MET:HG2	1:G:384:VAL:N	2.25	0.52
1:G:98:CYS:HB3	1:G:152:LEU:O	2.09	0.52
1:I:469:LEU:HD12	1:I:625:VAL:HG13	1.92	0.52
1:B:17:MET:HB3	1:B:32:TYR:CE1	2.44	0.52
1:B:362:LEU:HG	1:B:363:ASP:H	1.75	0.52
1:D:114:CYS:HB2	1:D:432:HIS:CD2	2.45	0.52
1:D:328:LEU:HD11	1:D:337:LEU:HD22	1.92	0.52
1:E:589:ILE:H	1:E:589:ILE:CD1	2.23	0.52
1:G:185:LEU:HD21	1:G:188:LEU:HB2	1.91	0.52
1:I:284:PRO:HA	1:I:287:ARG:NH2	2.24	0.52
1:J:236:LYS:HD3	1:J:237:LYS:N	2.25	0.52
1:K:513:GLU:O	1:K:517:LYS:HG3	2.10	0.52
1:L:177:LEU:HD11	1:L:198:TYR:CE2	2.45	0.52
1:B:84:ASN:CG	1:B:85:ILE:H	2.14	0.52
1:C:262:ASN:ND2	1:C:264:LEU:H	2.08	0.52
1:C:460:ALA:O	1:C:464:LYS:HG3	2.10	0.52
1:D:248:MET:O	1:F:184:THR:HG23	2.10	0.52
1:F:186:GLN:NE2	1:F:227:PRO:HD3	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:VAL:HG23	1:G:427:TRP:HD1	1.74	0.52
1:G:513:GLU:O	1:G:517:LYS:HG3	2.09	0.52
1:G:523:GLU:HB2	1:G:632:ILE:HG12	1.92	0.52
1:I:298:PRO:O	1:I:302:VAL:HG23	2.10	0.52
1:I:489:LEU:HD11	1:J:648:LYS:HE3	1.92	0.52
1:I:62:ILE:HG22	1:I:93:LEU:HD13	1.91	0.52
1:L:513:GLU:O	1:L:517:LYS:HG3	2.11	0.52
1:A:222:LEU:HB2	1:A:230:TRP:CD1	2.37	0.51
1:C:188:LEU:HD21	1:C:192:LEU:HD22	1.92	0.51
1:C:291:VAL:HG12	1:C:298:PRO:HA	1.92	0.51
1:C:417:GLN:HB3	1:C:581:SER:HB2	1.92	0.51
1:D:283:ASP:HB3	1:D:286:GLN:HB2	1.91	0.51
1:E:212:PHE:CE2	1:E:220:PRO:HA	2.45	0.51
1:F:328:LEU:HD11	1:F:337:LEU:HD22	1.92	0.51
1:G:18:ARG:HH21	1:G:33:GLN:NE2	2.04	0.51
1:G:20:ARG:C	1:G:21:LEU:HD22	2.31	0.51
1:H:366:LYS:HB2	1:H:370:GLN:HG2	1.92	0.51
1:H:412:GLN:HB3	1:J:21:LEU:O	2.10	0.51
1:K:18:ARG:HH21	1:K:33:GLN:NE2	2.05	0.51
1:K:88:HIS:O	1:K:90:VAL:HG12	2.10	0.51
1:A:188:LEU:HD21	1:A:192:LEU:HD22	1.91	0.51
1:A:600:VAL:HA	1:A:603:GLU:HB3	1.92	0.51
1:B:29:VAL:HG21	2:B:701:5TL:CAF	2.40	0.51
1:E:655:LYS:HA	1:E:658:CYS:SG	2.51	0.51
1:J:426:VAL:HG23	1:J:427:TRP:HD1	1.75	0.51
1:J:358:THR:O	1:J:453:LEU:HD13	2.11	0.51
1:J:420:ILE:HG21	1:J:578:HIS:H	1.75	0.51
1:K:473:SER:HB2	1:K:524:VAL:HA	1.92	0.51
1:L:320:SER:O	1:L:398:PHE:HB3	2.10	0.51
1:A:408:ASN:HD21	1:E:26:PHE:HD1	1.57	0.51
1:C:222:LEU:HB3	1:C:225:LEU:HB2	1.93	0.51
1:D:316:LEU:HB2	1:D:383:MET:SD	2.50	0.51
1:F:240:LYS:O	1:F:277:GLN:HG2	2.11	0.51
1:F:413:ASP:OD1	1:F:416:ILE:HB	2.11	0.51
1:H:222:LEU:HB2	1:H:230:TRP:HD1	1.76	0.51
1:K:188:LEU:HD21	1:K:192:LEU:HD22	1.92	0.51
1:K:413:ASP:OD1	1:K:416:ILE:HB	2.10	0.51
1:K:589:ILE:HD12	1:K:589:ILE:N	2.22	0.51
1:L:413:ASP:OD1	1:L:416:ILE:HB	2.11	0.51
1:K:497:GLN:OE1	1:L:655:LYS:HE3	2.09	0.51
1:D:275:TRP:HZ2	1:D:304:MET:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:MET:HB3	1:G:32:TYR:CD1	2.46	0.51
1:G:33:GLN:HA	1:G:40:LYS:HA	1.92	0.51
1:I:262:ASN:ND2	1:I:264:LEU:H	2.09	0.51
1:J:413:ASP:OD1	1:J:416:ILE:HB	2.10	0.51
1:J:473:SER:CB	1:J:527:ILE:HD11	2.41	0.51
1:K:278:LEU:HD23	1:K:288:GLY:HA2	1.92	0.51
1:K:477:LYS:HE3	1:K:524:VAL:HG11	1.93	0.51
1:A:396:GLY:H	1:A:397:PRO:CD	2.12	0.51
1:C:48:LEU:HA	1:C:87:ILE:CG2	2.39	0.51
1:D:220:PRO:O	1:D:243:PHE:HA	2.09	0.51
1:D:587:VAL:O	1:D:591:VAL:HG23	2.10	0.51
1:E:18:ARG:HH21	1:E:33:GLN:NE2	2.06	0.51
1:E:84:ASN:HD22	1:E:86:LEU:H	1.56	0.51
1:G:650:ILE:HG21	1:H:650:ILE:HG21	1.92	0.51
1:I:221:PHE:HB2	1:I:230:TRP:NE1	2.22	0.51
1:J:97:TYR:HA	2:J:701:5TL:OAO	2.10	0.51
1:K:230:TRP:O	1:K:234:ILE:HG13	2.10	0.51
1:K:291:VAL:HA	1:K:298:PRO:HA	1.93	0.51
1:L:219:ARG:HE	1:L:223:HIS:HA	1.76	0.51
1:A:219:ARG:HH21	1:A:223:HIS:HB2	1.75	0.51
1:B:410:ILE:HG23	1:B:583:SER:OG	2.11	0.51
1:C:426:VAL:HG23	1:C:427:TRP:HD1	1.75	0.51
1:C:600:VAL:HA	1:C:603:GLU:HB3	1.92	0.51
1:C:98:CYS:HB3	1:C:152:LEU:O	2.11	0.51
1:D:74:VAL:CG1	1:D:164:ILE:HA	2.40	0.51
1:D:63:GLN:HE22	1:D:174:GLN:NE2	2.05	0.51
1:E:413:ASP:OD1	1:E:416:ILE:HB	2.11	0.51
1:F:288:GLY:HA3	1:F:300:CYS:SG	2.50	0.51
1:F:587:VAL:O	1:F:591:VAL:HG23	2.10	0.51
1:I:18:ARG:HH21	1:I:33:GLN:NE2	2.06	0.51
1:I:513:GLU:O	1:I:517:LYS:HG3	2.10	0.51
1:I:600:VAL:HA	1:I:603:GLU:HB3	1.92	0.51
1:J:328:LEU:HD11	1:J:337:LEU:HD22	1.93	0.51
1:K:62:ILE:HG22	1:K:93:LEU:HD13	1.92	0.51
1:B:513:GLU:O	1:B:517:LYS:HG3	2.10	0.51
1:C:18:ARG:HH21	1:C:33:GLN:NE2	2.06	0.51
1:C:328:LEU:HD13	1:C:368:ALA:HB1	1.92	0.51
1:E:227:PRO:HA	1:E:230:TRP:HB3	1.93	0.51
1:G:239:PRO:O	1:G:240:LYS:HB2	2.09	0.51
1:G:392:THR:O	1:G:612:LEU:HD23	2.11	0.51
1:H:133:ARG:CZ	1:H:297:GLN:HE22	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:589:ILE:CD1	1:H:589:ILE:H	2.19	0.51
1:I:586:MET:O	1:I:590:ILE:HG13	2.11	0.51
1:I:655:LYS:HA	1:I:658:CYS:SG	2.51	0.51
1:K:294:THR:HB	1:K:295:LEU:HD12	1.93	0.51
1:K:487:ILE:CA	1:K:646:ARG:HD2	2.41	0.51
1:L:600:VAL:HA	1:L:603:GLU:HB3	1.91	0.51
1:A:574:ARG:HH12	1:E:575:PRO:HB3	1.76	0.51
1:A:410:ILE:HG23	1:A:583:SER:OG	2.11	0.51
1:C:46:CYS:HA	1:C:58:TRP:CH2	2.44	0.51
1:C:70:HIS:CD2	1:C:72:ASN:H	2.28	0.51
1:D:112:ASN:HB3	1:D:116:LEU:HD23	1.93	0.51
1:E:284:PRO:HG2	1:E:285:GLN:HE21	1.76	0.51
1:E:460:ALA:O	1:E:464:LYS:HG3	2.11	0.51
1:I:20:ARG:C	1:I:21:LEU:HD22	2.31	0.51
1:I:423:LEU:HA	1:I:426:VAL:CG2	2.39	0.51
1:L:215:ILE:HD13	1:L:264:LEU:HD11	1.91	0.51
1:L:463:THR:HG21	1:L:538:HIS:HD2	1.76	0.51
1:A:33:GLN:HA	1:A:40:LYS:HA	1.93	0.51
1:A:654:LEU:HD21	1:B:497:GLN:HE22	1.75	0.51
1:B:401:ARG:HG2	1:B:433:TYR:CE1	2.46	0.51
1:B:62:ILE:HG22	1:B:93:LEU:HD13	1.93	0.51
1:B:9:PHE:CZ	1:B:82:GLU:HB3	2.46	0.51
1:D:262:ASN:ND2	1:D:264:LEU:H	2.09	0.51
1:D:544:LEU:HD21	1:D:610:LYS:HD2	1.93	0.51
1:E:182:VAL:HG12	1:E:183:GLY:H	1.75	0.51
1:F:98:CYS:HB3	1:F:152:LEU:O	2.10	0.51
1:G:410:ILE:O	1:G:587:VAL:HG22	2.11	0.51
1:G:589:ILE:CD1	1:G:589:ILE:H	2.19	0.51
1:H:328:LEU:HD11	1:H:337:LEU:HD22	1.92	0.51
1:J:581:SER:O	1:J:582:ASP:HB2	2.11	0.51
1:L:587:VAL:O	1:L:591:VAL:HG23	2.11	0.51
1:D:463:THR:HG21	1:D:538:HIS:CD2	2.45	0.51
1:E:21:LEU:HD12	2:E:701:5TL:CAJ	2.41	0.51
1:G:219:ARG:HH22	1:G:224:HIS:N	2.09	0.51
1:G:45:SER:OG	1:G:86:LEU:HD11	2.11	0.51
1:H:411:VAL:HG12	1:H:590:ILE:HG21	1.93	0.51
1:H:62:ILE:HG22	1:H:93:LEU:HD13	1.93	0.51
1:I:188:LEU:HD21	1:I:192:LEU:HD22	1.93	0.51
1:I:33:GLN:HA	1:I:40:LYS:HA	1.92	0.51
1:K:226:GLN:O	1:K:230:TRP:HB2	2.11	0.51
1:L:143:ARG:HB3	1:L:170:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:LYS:HG3	1:D:489:LEU:HD21	1.92	0.50
1:F:406:CYS:SG	1:F:407:VAL:HG23	2.50	0.50
1:F:76:ALA:HB1	1:F:93:LEU:HD11	1.94	0.50
1:G:574:ARG:HB2	1:G:574:ARG:NH1	2.26	0.50
1:I:186:GLN:CG	1:I:219:ARG:HD3	2.41	0.50
1:K:158:LYS:HB3	1:K:376:VAL:HG23	1.93	0.50
1:K:320:SER:C	1:K:398:PHE:HB3	2.31	0.50
1:L:177:LEU:HD11	1:L:198:TYR:HE2	1.76	0.50
1:L:29:VAL:HG21	2:L:701:5TL:CAF	2.41	0.50
1:L:62:ILE:HG22	1:L:93:LEU:HD13	1.93	0.50
1:A:574:ARG:NH1	1:A:574:ARG:HB2	2.26	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HG21	1.93	0.50
1:C:17:MET:HB3	1:C:32:TYR:CD1	2.46	0.50
1:E:11:ALA:O	1:E:14:PRO:HD3	2.10	0.50
1:E:487:ILE:CA	1:E:646:ARG:HD2	2.40	0.50
1:F:192:LEU:H	1:F:192:LEU:HD12	1.76	0.50
1:F:289:GLY:O	1:F:291:VAL:N	2.45	0.50
1:G:219:ARG:HH22	1:G:224:HIS:H	1.60	0.50
1:K:328:LEU:HD11	1:K:337:LEU:HD22	1.93	0.50
1:L:191:GLU:OE2	1:L:287:ARG:NH2	2.44	0.50
1:L:50:LEU:HD12	1:L:50:LEU:H	1.75	0.50
1:B:275:TRP:CZ2	1:B:304:MET:HE2	2.45	0.50
1:B:470:ILE:O	1:B:474:GLN:HG2	2.10	0.50
1:D:423:LEU:HA	1:D:426:VAL:CG2	2.40	0.50
1:G:294:THR:HB	1:G:295:LEU:HD12	1.92	0.50
1:G:7:PRO:HG3	1:G:32:TYR:OH	2.11	0.50
1:H:655:LYS:HA	1:H:658:CYS:SG	2.51	0.50
1:K:376:VAL:HG13	1:K:377:ARG:N	2.26	0.50
1:K:318:MET:HE1	1:K:444:LEU:O	2.11	0.50
1:K:502:ILE:HD13	1:K:656:ILE:HD12	1.93	0.50
1:A:149:ASN:O	1:A:164:ILE:HG22	2.12	0.50
1:A:18:ARG:HH21	1:A:33:GLN:NE2	2.06	0.50
1:B:73:VAL:HG22	1:B:74:VAL:H	1.76	0.50
1:C:328:LEU:HD11	1:C:337:LEU:HD22	1.93	0.50
1:C:427:TRP:CZ3	1:C:567:LEU:HB3	2.46	0.50
1:F:188:LEU:HD21	1:F:192:LEU:HD22	1.93	0.50
1:F:284:PRO:HG2	1:F:285:GLN:H	1.77	0.50
1:F:50:LEU:H	1:F:50:LEU:HD12	1.75	0.50
1:G:222:LEU:CD2	1:G:230:TRP:HA	2.41	0.50
1:I:141:ILE:HG23	1:I:170:LYS:HB2	1.94	0.50
1:K:574:ARG:NH1	1:K:575:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ILE:HA	1:A:423:LEU:HB2	1.94	0.50
1:B:215:ILE:HD13	1:B:264:LEU:HD11	1.93	0.50
1:B:328:LEU:HD11	1:B:337:LEU:HD22	1.93	0.50
1:B:460:ALA:O	1:B:464:LYS:HG3	2.12	0.50
1:D:413:ASP:OD1	1:D:416:ILE:HB	2.11	0.50
1:E:485:LYS:HG2	1:F:640:MET:HE1	1.94	0.50
1:E:497:GLN:HE22	1:F:654:LEU:CD2	2.24	0.50
1:G:469:LEU:HD12	1:G:625:VAL:HG13	1.93	0.50
1:G:655:LYS:HA	1:G:658:CYS:SG	2.52	0.50
1:H:27:GLY:HA2	1:L:412:GLN:CD	2.31	0.50
1:I:77:CYS:H	1:I:95:MET:HA	1.75	0.50
1:K:76:ALA:HA	1:K:95:MET:HA	1.92	0.50
1:A:185:LEU:HD12	1:A:193:PHE:HZ	1.76	0.50
1:A:410:ILE:O	1:A:587:VAL:HG22	2.12	0.50
1:B:212:PHE:CE2	1:B:220:PRO:HA	2.47	0.50
1:B:589:ILE:CD1	1:B:589:ILE:H	2.20	0.50
1:C:507:MET:CE	1:C:653:LEU:HD22	2.40	0.50
1:E:547:SER:OG	1:E:548:PRO:HD2	2.12	0.50
1:F:523:GLU:HB2	1:F:632:ILE:HG12	1.93	0.50
1:F:547:SER:HB3	1:F:548:PRO:HD2	1.92	0.50
1:G:46:CYS:SG	1:G:90:VAL:HB	2.52	0.50
1:H:17:MET:HB3	1:H:32:TYR:CD1	2.47	0.50
1:J:88:HIS:CG	1:J:89:ASP:N	2.80	0.50
1:K:17:MET:HB3	1:K:32:TYR:CD1	2.46	0.50
1:K:232:GLU:HA	1:K:235:LYS:HE2	1.92	0.50
1:L:17:MET:HB3	1:L:32:TYR:CD1	2.46	0.50
1:A:561:GLU:O	1:A:565:ILE:HG13	2.12	0.50
1:B:238:ASP:HB3	1:B:239:PRO:HD2	1.92	0.50
1:C:318:MET:HE1	1:C:447:GLY:HA3	1.94	0.50
1:C:513:GLU:O	1:C:517:LYS:HG3	2.11	0.50
1:D:460:ALA:O	1:D:464:LYS:HG3	2.11	0.50
1:E:587:VAL:O	1:E:591:VAL:HG23	2.11	0.50
1:G:199:THR:HG21	1:G:285:GLN:NE2	2.22	0.50
1:G:234:ILE:O	1:G:237:LYS:HB2	2.12	0.50
1:G:62:ILE:HG22	1:G:93:LEU:HD13	1.94	0.50
1:I:212:PHE:CE2	1:I:220:PRO:HA	2.47	0.50
1:I:29:VAL:HG21	2:I:701:5TL:CAF	2.42	0.50
1:I:328:LEU:HD11	1:I:337:LEU:HD22	1.94	0.50
1:A:113:CYS:SG	1:A:428:ALA:HB1	2.52	0.50
1:A:655:LYS:HE3	1:B:497:GLN:OE1	2.12	0.50
1:C:33:GLN:HA	1:C:40:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ILE:HD11	1:C:571:LEU:HG	1.93	0.50
1:C:658:CYS:HB3	1:D:501:GLY:HA2	1.94	0.50
1:E:62:ILE:HG22	1:E:93:LEU:HD13	1.93	0.50
1:F:33:GLN:HA	1:F:40:LYS:HA	1.93	0.50
1:H:396:GLY:C	1:H:398:PHE:H	2.15	0.50
1:H:542:MET:HA	1:H:545:GLN:HE21	1.76	0.50
1:J:289:GLY:O	1:J:291:VAL:HG23	2.10	0.50
1:J:418:LEU:HB2	1:J:423:LEU:HD21	1.94	0.50
1:J:86:LEU:HD11	1:J:92:LEU:HG	1.94	0.50
1:I:184:THR:OG1	1:K:248:MET:HB3	2.11	0.50
1:L:33:GLN:HA	1:L:40:LYS:HA	1.93	0.50
1:A:395:GLU:HG3	1:A:396:GLY:N	2.27	0.50
1:A:589:ILE:H	1:A:589:ILE:CD1	2.20	0.50
1:B:655:LYS:HA	1:B:658:CYS:SG	2.51	0.50
1:C:65:MET:SD	1:C:166:LEU:HD23	2.51	0.50
1:C:62:ILE:HG22	1:C:93:LEU:HD13	1.94	0.50
1:D:548:PRO:HG2	1:D:607:HIS:NE2	2.27	0.50
1:E:316:LEU:HB2	1:E:383:MET:HE2	1.94	0.50
1:E:589:ILE:N	1:E:589:ILE:HD12	2.24	0.50
1:F:423:LEU:HA	1:F:426:VAL:CG2	2.41	0.50
1:F:600:VAL:HA	1:F:603:GLU:HB3	1.93	0.50
1:G:188:LEU:HD21	1:G:192:LEU:HD22	1.93	0.50
1:H:574:ARG:O	1:H:576:SER:N	2.45	0.50
1:I:320:SER:C	1:I:398:PHE:HB3	2.33	0.50
1:I:576:SER:OG	1:K:580:TYR:HB2	2.12	0.50
1:I:623:PRO:O	1:I:627:VAL:HG23	2.11	0.50
4:J:705:GLC:C6	5:J:706:PDX:H5	2.42	0.50
1:L:18:ARG:HH21	1:L:33:GLN:NE2	2.05	0.50
1:L:303:LEU:O	1:L:307:ILE:HG13	2.12	0.50
1:L:73:VAL:O	1:L:162:LYS:HB3	2.12	0.50
1:A:170:LYS:HG3	1:A:177:LEU:HA	1.94	0.49
1:A:328:LEU:HD11	1:A:337:LEU:HD22	1.94	0.49
1:A:487:ILE:CG1	1:A:515:GLU:HB2	2.41	0.49
1:A:62:ILE:HG22	1:A:93:LEU:HD13	1.94	0.49
1:C:473:SER:CB	1:C:527:ILE:HD11	2.42	0.49
1:E:415:LYS:HA	1:E:584:THR:HB	1.93	0.49
1:G:222:LEU:CD2	1:G:230:TRP:HD1	2.23	0.49
1:H:31:LEU:HG	1:H:97:TYR:CE2	2.47	0.49
1:H:420:ILE:HD11	1:H:571:LEU:HG	1.94	0.49
1:I:17:MET:HB3	1:I:32:TYR:CD1	2.47	0.49
1:I:192:LEU:H	1:I:192:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:460:ALA:O	1:I:464:LYS:HG3	2.12	0.49
1:J:215:ILE:HG21	1:J:258:LEU:HD21	1.94	0.49
1:J:460:ALA:O	1:J:464:LYS:HG3	2.12	0.49
1:K:460:ALA:O	1:K:464:LYS:HG3	2.12	0.49
1:L:655:LYS:HA	1:L:658:CYS:SG	2.52	0.49
1:B:73:VAL:HG22	1:B:74:VAL:N	2.27	0.49
1:C:20:ARG:C	1:C:21:LEU:HD22	2.33	0.49
1:D:396:GLY:HA2	1:D:398:PHE:CE2	2.47	0.49
1:E:485:LYS:O	1:E:489:LEU:HB2	2.12	0.49
1:G:220:PRO:HG2	1:G:221:PHE:HD2	1.76	0.49
1:H:470:ILE:O	1:H:474:GLN:HG2	2.10	0.49
1:J:251:GLU:HA	1:L:228:PHE:CD1	2.47	0.49
1:J:485:LYS:O	1:J:489:LEU:HB2	2.12	0.49
1:B:262:ASN:ND2	1:B:264:LEU:H	2.10	0.49
1:B:392:THR:HG22	1:B:616:GLN:NE2	2.26	0.49
1:B:401:ARG:HH11	1:B:437:LEU:HD23	1.77	0.49
1:D:62:ILE:HG22	1:D:93:LEU:HD13	1.93	0.49
1:F:262:ASN:ND2	1:F:264:LEU:H	2.10	0.49
1:F:574:ARG:HB2	1:F:574:ARG:NH1	2.26	0.49
1:G:146:LYS:NZ	1:G:182:VAL:HG11	2.28	0.49
1:J:283:ASP:O	1:J:287:ARG:HG3	2.13	0.49
1:K:587:VAL:O	1:K:591:VAL:HG23	2.12	0.49
1:L:395:GLU:HG3	1:L:397:PRO:HD3	1.94	0.49
1:B:401:ARG:HD2	1:B:401:ARG:N	2.27	0.49
1:B:574:ARG:HB2	1:B:574:ARG:NH1	2.26	0.49
1:C:85:ILE:HB	1:C:90:VAL:H	1.78	0.49
1:E:20:ARG:C	1:E:21:LEU:HD22	2.32	0.49
1:F:320:SER:C	1:F:398:PHE:HB3	2.33	0.49
1:G:401:ARG:HH22	1:G:436:GLY:C	2.16	0.49
1:H:222:LEU:HD22	1:H:244:ALA:O	2.12	0.49
1:I:29:VAL:HG22	1:I:44:LYS:CB	2.42	0.49
1:J:387:PHE:CZ	1:J:451:ALA:HB2	2.47	0.49
1:L:395:GLU:CG	1:L:396:GLY:H	2.26	0.49
5:B:703:PDX:O3X	5:B:703:PDX:H2	2.12	0.49
1:C:655:LYS:HA	1:C:658:CYS:SG	2.52	0.49
1:D:221:PHE:HB2	1:D:230:TRP:HZ2	1.76	0.49
1:D:406:CYS:SG	1:D:407:VAL:HG23	2.51	0.49
1:C:647:GLN:OE1	1:D:489:LEU:HD22	2.13	0.49
1:D:580:TYR:HB2	1:F:576:SER:OG	2.13	0.49
1:E:141:ILE:HG23	1:E:170:LYS:HB2	1.94	0.49
1:F:112:ASN:HB3	1:F:116:LEU:CD2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:LYS:CE	1:F:281:ASN:HA	2.41	0.49
1:F:473:SER:OG	1:F:524:VAL:HG13	2.13	0.49
1:H:574:ARG:HB2	1:H:574:ARG:NH1	2.27	0.49
1:I:222:LEU:HB2	1:I:230:TRP:HD1	1.77	0.49
1:I:563:ARG:HH12	4:I:706:GLC:H2	1.78	0.49
1:J:133:ARG:NE	1:J:297:GLN:HE22	2.10	0.49
1:J:33:GLN:HA	1:J:40:LYS:HA	1.93	0.49
1:J:574:ARG:NH1	1:J:575:PRO:HD2	2.26	0.49
1:K:185:LEU:O	1:K:186:GLN:HB2	2.12	0.49
1:K:485:LYS:O	1:K:489:LEU:HB2	2.12	0.49
1:A:395:GLU:OE2	1:A:397:PRO:HG3	2.12	0.49
1:D:354:LEU:HB3	1:D:384:VAL:CG1	2.43	0.49
1:E:33:GLN:HA	1:E:40:LYS:HA	1.94	0.49
1:F:356:SER:HB2	1:F:382:TYR:CE1	2.47	0.49
1:G:60:HIS:O	1:G:63:GLN:HB3	2.12	0.49
1:H:460:ALA:O	1:H:464:LYS:HG3	2.12	0.49
1:J:315:ILE:HD12	1:J:384:VAL:HB	1.95	0.49
1:J:74:VAL:O	1:J:74:VAL:HG13	2.13	0.49
1:K:289:GLY:N	1:K:290:PRO:CD	2.76	0.49
1:L:574:ARG:HB2	1:L:574:ARG:NH1	2.27	0.49
1:L:79:VAL:HG11	1:L:83:LEU:HD13	1.95	0.49
1:A:418:LEU:HB2	1:A:423:LEU:HD21	1.93	0.49
1:C:29:VAL:HG22	1:C:44:LYS:CB	2.42	0.49
1:D:222:LEU:HB3	1:D:225:LEU:HB2	1.95	0.49
1:F:222:LEU:HD23	1:F:225:LEU:HG	1.95	0.49
1:H:33:GLN:HA	1:H:40:LYS:HA	1.94	0.49
1:G:489:LEU:HD13	1:H:643:GLN:HG3	1.95	0.49
1:I:547:SER:HB3	1:I:548:PRO:HD2	1.95	0.49
1:J:7:PRO:C	1:J:9:PHE:H	2.16	0.49
1:K:574:ARG:HD2	1:K:577:ASP:OD1	2.12	0.49
1:L:423:LEU:HA	1:L:426:VAL:CG2	2.41	0.49
1:C:395:GLU:HG2	1:C:397:PRO:CD	2.35	0.49
1:C:423:LEU:HA	1:C:426:VAL:CG2	2.40	0.49
1:C:74:VAL:CG2	1:C:95:MET:HB2	2.43	0.49
1:D:17:MET:HB3	1:D:32:TYR:CD1	2.47	0.49
1:E:98:CYS:HA	1:E:153:GLN:NE2	2.27	0.49
1:F:17:MET:HB3	1:F:32:TYR:CD1	2.47	0.49
1:F:43:ILE:N	1:F:43:ILE:HD12	2.28	0.49
1:G:234:ILE:HG22	1:G:254:PHE:HE1	1.78	0.49
1:H:192:LEU:H	1:H:192:LEU:HD12	1.76	0.49
1:H:549:TYR:N	1:H:552:ARG:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:424:ARG:HH11	1:K:572:LYS:HG2	1.78	0.49
1:A:48:LEU:O	1:A:50:LEU:HD12	2.13	0.49
1:A:658:CYS:SG	1:B:501:GLY:HA2	2.53	0.49
1:B:219:ARG:NH1	1:B:224:HIS:H	2.11	0.49
1:C:334:LEU:HD11	1:C:364:PRO:HA	1.95	0.49
1:C:413:ASP:OD1	1:C:416:ILE:HB	2.12	0.49
1:C:653:LEU:HG	1:C:656:ILE:HD11	1.95	0.49
1:C:82:GLU:H	1:C:82:GLU:CD	2.15	0.49
1:D:33:GLN:HA	1:D:40:LYS:HA	1.93	0.49
1:E:29:VAL:HG22	1:E:44:LYS:CB	2.42	0.49
1:E:47:ARG:O	1:E:87:ILE:HB	2.13	0.49
1:G:48:LEU:O	1:G:50:LEU:HD12	2.13	0.49
1:I:413:ASP:OD1	1:I:416:ILE:HB	2.12	0.49
1:J:392:THR:O	1:J:612:LEU:HD23	2.13	0.49
1:K:319:THR:HG22	1:K:394:TYR:CE1	2.48	0.49
1:L:316:LEU:HB2	1:L:383:MET:SD	2.52	0.49
1:A:166:LEU:N	1:A:166:LEU:HD22	2.27	0.49
1:A:485:LYS:O	1:A:489:LEU:HB2	2.12	0.49
1:A:513:GLU:HB3	1:A:517:LYS:HE3	1.95	0.49
1:A:523:GLU:OE1	1:A:526:VAL:HG21	2.12	0.49
1:B:17:MET:HB3	1:B:32:TYR:CD1	2.48	0.49
1:B:33:GLN:HA	1:B:40:LYS:HA	1.94	0.49
1:B:29:VAL:HG22	1:B:44:LYS:CB	2.42	0.49
1:C:574:ARG:NH1	1:C:574:ARG:HB2	2.27	0.49
1:D:227:PRO:HA	1:D:230:TRP:CB	2.41	0.49
1:D:199:THR:HG21	1:D:284:PRO:HB2	1.95	0.49
1:D:469:LEU:HD12	1:D:625:VAL:HG13	1.95	0.49
1:G:328:LEU:HD11	1:G:337:LEU:HD22	1.95	0.49
1:G:418:LEU:HB2	1:G:423:LEU:HD21	1.93	0.49
1:G:44:LYS:HB3	1:G:93:LEU:HB3	1.95	0.49
1:H:477:LYS:HE3	1:H:524:VAL:HG11	1.94	0.49
1:I:372:VAL:HG13	1:I:372:VAL:O	2.13	0.49
1:J:62:ILE:HG22	1:J:93:LEU:HD13	1.94	0.49
1:K:33:GLN:HA	1:K:40:LYS:HA	1.94	0.49
1:K:654:LEU:HD11	1:L:502:ILE:HD12	1.94	0.49
1:A:373:LEU:HB2	1:A:378:GLY:HA2	1.95	0.48
1:A:427:TRP:HZ2	1:A:583:SER:HA	1.78	0.48
1:B:142:HIS:HA	1:B:169:ALA:HB2	1.94	0.48
1:B:219:ARG:NH2	1:B:224:HIS:H	2.10	0.48
1:D:574:ARG:NH1	1:D:575:PRO:HD2	2.27	0.48
1:E:201:THR:HA	1:E:204:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:523:GLU:OE1	1:E:526:VAL:HG21	2.13	0.48
1:F:186:GLN:CG	1:F:219:ARG:HD3	2.42	0.48
1:F:426:VAL:HG23	1:F:427:TRP:HD1	1.77	0.48
1:G:236:LYS:CG	1:G:237:LYS:N	2.76	0.48
1:G:653:LEU:HG	1:G:656:ILE:HD11	1.95	0.48
1:H:262:ASN:ND2	1:H:264:LEU:H	2.11	0.48
1:H:268:ILE:O	1:H:272:MET:HB2	2.13	0.48
1:H:240:LYS:HB3	1:H:277:GLN:HB3	1.94	0.48
1:H:424:ARG:HD3	1:H:572:LYS:HE2	1.94	0.48
1:I:205:TRP:HB2	1:I:287:ARG:NH1	2.28	0.48
1:I:463:THR:HG21	1:I:538:HIS:HD2	1.79	0.48
1:I:587:VAL:HA	1:I:590:ILE:HD12	1.95	0.48
1:J:262:ASN:ND2	1:J:264:LEU:H	2.11	0.48
1:J:29:VAL:HG22	1:J:44:LYS:CB	2.42	0.48
1:J:31:LEU:HG	1:J:97:TYR:CE2	2.48	0.48
1:J:574:ARG:HB2	1:J:574:ARG:NH1	2.27	0.48
1:K:452:MET:SD	1:K:611:LEU:HD22	2.53	0.48
1:K:31:LEU:HG	1:K:97:TYR:CE2	2.48	0.48
1:L:13:GLY:N	1:L:14:PRO:CD	2.70	0.48
1:B:31:LEU:HG	1:B:97:TYR:CE2	2.48	0.48
1:B:70:HIS:HB3	1:B:73:VAL:HG12	1.96	0.48
1:E:117:LYS:O	1:E:121:ILE:HG13	2.13	0.48
1:E:224:HIS:O	1:E:225:LEU:HD22	2.12	0.48
1:E:328:LEU:HD11	1:E:337:LEU:HD22	1.95	0.48
1:E:489:LEU:HD22	1:F:647:GLN:OE1	2.12	0.48
1:F:513:GLU:HB3	1:F:517:LYS:HE3	1.95	0.48
1:F:427:TRP:HZ3	1:F:567:LEU:HB3	1.77	0.48
1:G:298:PRO:O	1:G:302:VAL:HG23	2.13	0.48
1:G:460:ALA:O	1:G:464:LYS:HG3	2.14	0.48
1:H:192:LEU:N	1:H:192:LEU:HD12	2.28	0.48
1:H:237:LYS:HE2	1:H:281:ASN:HA	1.95	0.48
1:I:209:THR:HG22	1:I:220:PRO:HG3	1.95	0.48
1:J:275:TRP:HZ2	1:J:304:MET:HE2	1.78	0.48
1:K:79:VAL:HG11	1:K:83:LEU:CD1	2.39	0.48
1:L:410:ILE:HG23	1:L:583:SER:OG	2.13	0.48
1:A:186:GLN:HE21	1:A:227:PRO:HD3	1.78	0.48
1:A:221:PHE:HB2	1:A:230:TRP:NE1	2.25	0.48
1:A:278:LEU:HD23	1:A:288:GLY:HA2	1.95	0.48
1:A:223:HIS:NE2	1:A:425:LYS:HE3	2.28	0.48
1:A:473:SER:O	1:A:524:VAL:HG22	2.12	0.48
1:B:103:LEU:HD22	1:B:150:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ARG:HH12	3:B:707:5LS:C3	2.26	0.48
1:D:31:LEU:HG	1:D:97:TYR:CE2	2.49	0.48
1:D:29:VAL:HG22	1:D:44:LYS:CB	2.43	0.48
1:D:485:LYS:O	1:D:489:LEU:HB2	2.13	0.48
1:E:17:MET:HB3	1:E:32:TYR:CD1	2.48	0.48
1:F:192:LEU:HD12	1:F:192:LEU:N	2.28	0.48
1:J:367:PRO:O	1:J:370:GLN:HG2	2.11	0.48
1:K:45:SER:HA	1:K:86:LEU:CD2	2.43	0.48
1:L:262:ASN:ND2	1:L:264:LEU:H	2.11	0.48
1:A:60:HIS:O	1:A:63:GLN:HB3	2.13	0.48
1:C:192:LEU:H	1:C:192:LEU:HD12	1.78	0.48
1:E:563:ARG:NH1	4:E:706:GLC:H2	2.24	0.48
1:G:283:ASP:O	1:G:287:ARG:HG3	2.13	0.48
1:I:574:ARG:HB2	1:I:574:ARG:NH1	2.27	0.48
1:J:13:GLY:N	1:J:14:PRO:CD	2.68	0.48
1:J:201:THR:HA	1:J:204:TYR:CD1	2.49	0.48
1:J:292:ASP:OD2	1:J:294:THR:HB	2.14	0.48
1:J:523:GLU:OE1	1:J:526:VAL:HG21	2.14	0.48
1:K:182:VAL:HG12	1:K:183:GLY:H	1.78	0.48
1:K:185:LEU:HD12	1:K:193:PHE:HZ	1.78	0.48
1:K:574:ARG:HB2	1:K:574:ARG:NH1	2.27	0.48
1:L:219:ARG:HG2	1:L:220:PRO:HD2	1.96	0.48
1:L:426:VAL:HG23	1:L:427:TRP:HD1	1.77	0.48
1:L:485:LYS:O	1:L:489:LEU:HB2	2.12	0.48
1:L:31:LEU:HG	1:L:97:TYR:CE2	2.48	0.48
1:A:31:LEU:HG	1:A:97:TYR:CE2	2.49	0.48
1:A:460:ALA:O	1:A:464:LYS:HG3	2.14	0.48
1:B:430:ALA:O	1:B:434:VAL:HG23	2.14	0.48
1:C:285:GLN:HA	1:C:285:GLN:OE1	2.14	0.48
1:D:201:THR:HA	1:D:204:TYR:CD1	2.49	0.48
1:E:513:GLU:HB3	1:E:517:LYS:HE3	1.96	0.48
1:E:81:GLU:HG2	1:E:82:GLU:OE1	2.14	0.48
1:F:485:LYS:O	1:F:489:LEU:HB2	2.12	0.48
1:G:485:LYS:O	1:G:489:LEU:HB2	2.13	0.48
1:G:410:ILE:HG23	1:G:583:SER:OG	2.14	0.48
1:H:363:ASP:OD1	1:H:365:ARG:HB2	2.12	0.48
1:H:47:ARG:O	1:H:87:ILE:HD12	2.13	0.48
1:J:406:CYS:SG	1:J:407:VAL:HG23	2.52	0.48
1:J:473:SER:HB3	1:J:632:ILE:HD13	1.95	0.48
1:J:483:PHE:HZ	1:J:514:MET:HB3	1.78	0.48
1:K:420:ILE:HG21	1:K:578:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:586:MET:O	1:K:590:ILE:HG13	2.14	0.48
1:A:334:LEU:HD11	1:A:364:PRO:HA	1.94	0.48
1:A:97:TYR:HA	2:A:701:5TL:OAO	2.14	0.48
1:C:177:LEU:N	1:C:177:LEU:HD12	2.29	0.48
1:C:418:LEU:HB2	1:C:423:LEU:HD21	1.96	0.48
1:D:513:GLU:HB3	1:D:517:LYS:HE3	1.94	0.48
1:G:31:LEU:HG	1:G:97:TYR:CE2	2.49	0.48
1:H:615:LYS:O	1:H:619:ILE:HG13	2.14	0.48
1:I:410:ILE:HG23	1:I:583:SER:OG	2.13	0.48
1:J:17:MET:HB3	1:J:32:TYR:CD1	2.48	0.48
1:J:473:SER:HB3	1:J:527:ILE:HD11	1.96	0.48
3:H:705:5LS:C6	4:J:702:GLC:H5	2.43	0.48
4:J:705:GLC:H62	5:J:706:PDX:H5	1.95	0.48
1:L:142:HIS:ND1	1:L:169:ALA:HB2	2.29	0.48
1:L:513:GLU:HB3	1:L:517:LYS:HE3	1.96	0.48
1:L:549:TYR:HD2	1:L:552:ARG:NH1	2.11	0.48
1:A:143:ARG:HG2	1:A:143:ARG:HH21	1.78	0.48
1:B:222:LEU:HB2	1:B:230:TRP:NE1	2.28	0.48
1:B:242:ILE:HG22	1:B:280:LEU:HD12	1.95	0.48
1:A:648:LYS:HE3	1:B:489:LEU:HD11	1.96	0.48
1:C:178:CYS:HB2	1:C:179:THR:H	1.57	0.48
1:C:318:MET:HE1	1:C:444:LEU:O	2.14	0.48
1:C:420:ILE:HG21	1:C:578:HIS:N	2.28	0.48
1:C:410:ILE:HD12	1:C:583:SER:OG	2.13	0.48
1:C:31:LEU:HG	1:C:97:TYR:CE2	2.49	0.48
1:D:615:LYS:O	1:D:619:ILE:HG13	2.14	0.48
1:E:143:ARG:HG2	1:E:143:ARG:HH21	1.78	0.48
1:E:158:LYS:HB3	1:E:376:VAL:CG1	2.44	0.48
1:E:648:LYS:HE3	1:F:489:LEU:HD11	1.94	0.48
1:F:86:LEU:HD11	1:F:92:LEU:CD1	2.44	0.48
1:H:420:ILE:HA	1:H:423:LEU:HB2	1.96	0.48
1:I:192:LEU:HD12	1:I:192:LEU:N	2.29	0.48
1:I:424:ARG:HD3	1:I:572:LYS:HE2	1.95	0.48
1:I:653:LEU:HG	1:I:656:ILE:HD11	1.95	0.48
1:K:20:ARG:C	1:K:21:LEU:HD22	2.33	0.48
1:K:48:LEU:O	1:K:50:LEU:HD12	2.14	0.48
1:K:655:LYS:HA	1:K:658:CYS:SG	2.54	0.48
1:L:170:LYS:HA	1:L:177:LEU:HA	1.95	0.48
1:L:192:LEU:HD12	1:L:192:LEU:H	1.78	0.48
1:L:29:VAL:HG22	1:L:44:LYS:CB	2.44	0.48
1:L:653:LEU:HG	1:L:656:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD13	1:B:186:GLN:N	2.29	0.48
1:B:20:ARG:C	1:B:21:LEU:HD22	2.34	0.48
1:B:574:ARG:O	1:B:576:SER:N	2.46	0.48
1:B:615:LYS:O	1:B:619:ILE:HG13	2.14	0.48
1:C:141:ILE:O	1:C:169:ALA:HB1	2.14	0.48
1:C:201:THR:HA	1:C:204:TYR:CD1	2.49	0.48
1:D:60:HIS:O	1:D:63:GLN:HB3	2.14	0.48
1:E:43:ILE:HD12	1:E:43:ILE:N	2.29	0.48
1:G:523:GLU:OE1	1:G:526:VAL:HG21	2.13	0.48
1:G:651:TRP:CZ2	1:H:490:ASP:HB3	2.48	0.48
1:H:278:LEU:CD2	1:H:299:ARG:HB3	2.44	0.48
1:H:418:LEU:HB2	1:H:423:LEU:HD21	1.96	0.48
1:H:401:ARG:HH12	1:H:440:ASP:HB2	1.77	0.48
1:H:29:VAL:HG22	1:H:44:LYS:CB	2.43	0.48
1:I:117:LYS:O	1:I:121:ILE:HG13	2.14	0.48
1:I:227:PRO:HG3	1:K:249:SER:HB2	1.95	0.48
1:J:221:PHE:HB2	1:J:230:TRP:CZ2	2.48	0.48
1:K:227:PRO:HA	1:K:230:TRP:HB2	1.95	0.48
1:B:465:MET:CB	1:B:625:VAL:HG11	2.43	0.48
1:C:485:LYS:O	1:C:489:LEU:HB2	2.14	0.48
1:C:44:LYS:HB3	1:C:93:LEU:HB3	1.96	0.48
1:F:31:LEU:HG	1:F:97:TYR:CE2	2.49	0.48
1:G:166:LEU:N	1:G:166:LEU:HD22	2.28	0.48
1:G:494:TYR:HE1	1:G:503:SER:HA	1.79	0.48
1:G:623:PRO:O	1:G:627:VAL:HG23	2.14	0.48
1:H:523:GLU:OE1	1:H:526:VAL:HG21	2.14	0.48
1:I:513:GLU:HB3	1:I:517:LYS:HE3	1.96	0.48
1:I:60:HIS:O	1:I:63:GLN:HB3	2.14	0.48
1:K:29:VAL:HG22	1:K:44:LYS:CB	2.42	0.48
1:K:587:VAL:HA	1:K:590:ILE:HD12	1.96	0.48
1:K:60:HIS:O	1:K:63:GLN:HB3	2.13	0.48
1:C:267:LEU:HD13	1:C:327:LEU:HB2	1.94	0.48
1:D:653:LEU:HG	1:D:656:ILE:HD11	1.96	0.48
1:E:72:ASN:OD1	1:E:127:ASP:HA	2.14	0.48
1:E:224:HIS:C	1:E:225:LEU:HD22	2.34	0.48
1:F:14:PRO:O	1:F:35:ARG:HG2	2.14	0.48
1:F:448:GLN:OE1	1:F:549:TYR:HB3	2.14	0.48
1:H:513:GLU:HB3	1:H:517:LYS:HE3	1.95	0.48
1:I:485:LYS:O	1:I:489:LEU:HB2	2.14	0.48
1:I:44:LYS:HB3	1:I:93:LEU:HB3	1.96	0.48
1:J:480:LEU:HD22	1:J:518:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:653:LEU:HG	1:J:656:ILE:HD11	1.96	0.48
1:J:70:HIS:HB3	1:J:73:VAL:HG23	1.95	0.48
1:L:219:ARG:HG3	1:L:219:ARG:HH11	1.79	0.48
1:L:240:LYS:O	1:L:277:GLN:HG2	2.14	0.48
1:K:648:LYS:HE3	1:L:489:LEU:HD11	1.95	0.48
1:B:384:VAL:HG12	1:B:385:TYR:N	2.29	0.47
1:B:420:ILE:HA	1:B:423:LEU:HB2	1.96	0.47
1:B:418:LEU:HB2	1:B:423:LEU:HD21	1.96	0.47
1:B:523:GLU:OE1	1:B:526:VAL:HG21	2.14	0.47
1:F:122:LEU:HD12	1:F:379:CYS:SG	2.53	0.47
1:F:586:MET:O	1:F:590:ILE:HG13	2.14	0.47
1:G:334:LEU:HD11	1:G:364:PRO:HA	1.95	0.47
1:G:420:ILE:HA	1:G:423:LEU:HB2	1.96	0.47
1:I:418:LEU:HB2	1:I:423:LEU:HD21	1.96	0.47
1:A:401:ARG:NH2	1:A:437:LEU:HD23	2.28	0.47
1:A:70:HIS:C	1:A:72:ASN:H	2.18	0.47
1:B:143:ARG:HH21	1:B:143:ARG:HG2	1.79	0.47
1:B:192:LEU:H	1:B:192:LEU:HD12	1.78	0.47
1:B:290:PRO:HB2	1:B:299:ARG:CB	2.36	0.47
1:B:411:VAL:HG12	1:B:590:ILE:HG21	1.96	0.47
1:D:166:LEU:N	1:D:166:LEU:HD22	2.29	0.47
1:D:192:LEU:HD12	1:D:192:LEU:H	1.77	0.47
1:E:574:ARG:NH1	1:E:574:ARG:HB2	2.28	0.47
1:F:363:ASP:HB3	1:F:370:GLN:HE22	1.79	0.47
1:G:513:GLU:HB3	1:G:517:LYS:HE3	1.96	0.47
1:G:587:VAL:O	1:G:591:VAL:HG23	2.12	0.47
1:H:242:ILE:HG22	1:H:280:LEU:HD12	1.96	0.47
1:I:387:PHE:CZ	1:I:451:ALA:HB2	2.49	0.47
1:I:587:VAL:O	1:I:591:VAL:HG23	2.13	0.47
1:J:166:LEU:N	1:J:166:LEU:HD22	2.29	0.47
1:J:392:THR:HG22	1:J:616:GLN:HE22	1.79	0.47
1:J:598:ASP:O	1:J:602:LYS:HG2	2.14	0.47
1:K:143:ARG:HG2	1:K:143:ARG:HH21	1.78	0.47
1:L:315:ILE:CD1	1:L:384:VAL:HB	2.45	0.47
1:C:60:HIS:O	1:C:63:GLN:HB3	2.14	0.47
1:D:418:LEU:HB2	1:D:423:LEU:HD21	1.97	0.47
1:D:523:GLU:OE1	1:D:526:VAL:HG21	2.14	0.47
1:D:574:ARG:NH1	1:D:574:ARG:HB2	2.28	0.47
1:D:598:ASP:O	1:D:602:LYS:HG2	2.14	0.47
1:D:633:LYS:HA	1:D:636:ASP:HB3	1.96	0.47
1:E:430:ALA:O	1:E:434:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:LYS:HD3	1:E:534:ILE:HG21	1.96	0.47
1:F:460:ALA:O	1:F:464:LYS:HG3	2.14	0.47
1:G:201:THR:C	1:G:287:ARG:HH21	2.17	0.47
1:G:561:GLU:O	1:G:565:ILE:HG13	2.15	0.47
1:H:635:ALA:HA	1:H:638:THR:OG1	2.14	0.47
1:H:60:HIS:O	1:H:63:GLN:HB3	2.14	0.47
1:H:83:LEU:O	1:H:84:ASN:HB3	2.14	0.47
1:I:31:LEU:HG	1:I:97:TYR:CE2	2.49	0.47
1:I:537:LEU:O	1:I:541:ILE:HG13	2.14	0.47
1:J:20:ARG:C	1:J:21:LEU:HD22	2.35	0.47
1:J:427:TRP:CZ3	1:J:567:LEU:HB3	2.47	0.47
1:K:43:ILE:HD12	1:K:43:ILE:N	2.29	0.47
1:L:396:GLY:HA2	1:L:398:PHE:CE2	2.49	0.47
1:L:417:GLN:HB3	1:L:581:SER:HB2	1.95	0.47
1:L:635:ALA:HA	1:L:638:THR:OG1	2.15	0.47
1:A:643:GLN:HG3	1:B:489:LEU:HD13	1.97	0.47
1:B:268:ILE:O	1:B:272:MET:HB2	2.15	0.47
1:B:623:PRO:O	1:B:627:VAL:HG23	2.14	0.47
1:C:420:ILE:HA	1:C:423:LEU:HB2	1.96	0.47
1:C:466:LYS:HD3	1:C:534:ILE:HD13	1.96	0.47
1:C:473:SER:HB3	1:C:632:ILE:HD13	1.96	0.47
1:D:541:ILE:CD1	1:D:618:ILE:HD11	2.44	0.47
1:E:418:LEU:HB2	1:E:423:LEU:HD21	1.96	0.47
1:E:48:LEU:O	1:E:50:LEU:HD12	2.15	0.47
1:F:356:SER:HB2	1:F:382:TYR:HE1	1.79	0.47
1:F:623:PRO:O	1:F:627:VAL:HG23	2.15	0.47
1:G:199:THR:CG2	1:G:285:GLN:HE22	2.22	0.47
1:H:201:THR:HA	1:H:204:TYR:CD1	2.49	0.47
1:J:116:LEU:O	1:J:121:ILE:HD11	2.14	0.47
1:J:192:LEU:HD12	1:J:192:LEU:H	1.78	0.47
1:J:77:CYS:H	1:J:95:MET:HA	1.80	0.47
1:K:523:GLU:OE1	1:K:526:VAL:HG21	2.14	0.47
1:K:85:ILE:HD12	1:K:89:ASP:HA	1.97	0.47
1:A:44:LYS:HB3	1:A:93:LEU:HB3	1.97	0.47
1:A:51:SER:HB2	1:A:54:ASN:OD1	2.14	0.47
1:A:84:ASN:ND2	1:A:85:ILE:H	2.13	0.47
1:B:317:ASN:ND2	1:B:319:THR:HG23	2.30	0.47
1:B:14:PRO:O	1:B:35:ARG:HG2	2.14	0.47
1:B:477:LYS:HE3	1:B:524:VAL:HG11	1.95	0.47
4:C:706:GLC:H61	4:C:706:GLC:O3	2.14	0.47
1:D:199:THR:CG2	1:D:284:PRO:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:635:ALA:HA	1:D:638:THR:OG1	2.14	0.47
1:D:68:LEU:HD21	1:D:140:ILE:HD12	1.96	0.47
1:E:239:PRO:O	1:E:240:LYS:HB2	2.15	0.47
1:F:201:THR:HA	1:F:204:TYR:CD1	2.49	0.47
1:F:75:LYS:HD2	1:F:76:ALA:N	2.30	0.47
1:G:396:GLY:N	1:G:397:PRO:CD	2.77	0.47
1:I:72:ASN:ND2	1:I:130:SER:HB3	2.29	0.47
1:J:121:ILE:HG21	1:J:264:LEU:HD21	1.96	0.47
1:J:657:ALA:HA	1:J:660:GLN:HG3	1.97	0.47
1:K:408:ASN:HA	1:K:411:VAL:HG22	1.97	0.47
1:K:48:LEU:HA	1:K:87:ILE:HG21	1.97	0.47
1:K:502:ILE:CD1	1:K:656:ILE:HD12	2.45	0.47
1:L:387:PHE:CZ	1:L:451:ALA:HB2	2.50	0.47
1:L:48:LEU:HA	1:L:87:ILE:CD1	2.44	0.47
1:A:236:LYS:NZ	1:A:237:LYS:H	2.12	0.47
1:A:320:SER:CA	1:A:398:PHE:HB3	2.41	0.47
1:A:653:LEU:HG	1:A:656:ILE:HD11	1.96	0.47
1:B:106:LEU:HD11	1:B:152:LEU:HG	1.96	0.47
1:D:420:ILE:HG21	1:D:578:HIS:N	2.24	0.47
1:F:551:ARG:HB3	1:F:552:ARG:HH21	1.80	0.47
1:F:635:ALA:HA	1:F:638:THR:OG1	2.15	0.47
1:H:487:ILE:HG23	1:H:488:GLN:N	2.30	0.47
1:H:74:VAL:HG21	1:H:95:MET:HE3	1.97	0.47
1:I:201:THR:HA	1:I:204:TYR:CD1	2.50	0.47
1:J:116:LEU:HD12	1:J:116:LEU:N	2.30	0.47
1:K:166:LEU:N	1:K:166:LEU:HD22	2.30	0.47
1:L:267:LEU:HD12	1:L:312:ILE:HG23	1.95	0.47
1:L:418:LEU:HB2	1:L:423:LEU:HD21	1.96	0.47
1:L:86:LEU:CD1	1:L:87:ILE:HG13	2.45	0.47
1:B:170:LYS:NZ	1:B:192:LEU:HD11	2.29	0.47
1:B:222:LEU:HD22	1:B:244:ALA:O	2.15	0.47
1:B:240:LYS:HB3	1:B:277:GLN:CB	2.43	0.47
1:C:316:LEU:HB2	1:C:383:MET:CE	2.45	0.47
1:D:74:VAL:HG21	1:D:164:ILE:HG13	1.97	0.47
1:D:268:ILE:O	1:D:272:MET:HB2	2.15	0.47
1:D:563:ARG:HH22	3:D:705:5LS:C6	2.27	0.47
1:E:373:LEU:HD22	1:E:373:LEU:N	2.29	0.47
1:E:60:HIS:O	1:E:63:GLN:HB3	2.14	0.47
1:F:182:VAL:HB	1:F:185:LEU:HD23	1.96	0.47
1:G:408:ASN:HA	1:G:411:VAL:HG22	1.95	0.47
1:G:420:ILE:HG21	1:G:578:HIS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ILE:N	1:H:43:ILE:HD12	2.29	0.47
1:H:485:LYS:O	1:H:489:LEU:HB2	2.14	0.47
1:H:543:GLU:HA	1:H:546:LYS:HZ3	1.79	0.47
1:H:633:LYS:HA	1:H:636:ASP:HB3	1.97	0.47
1:J:319:THR:HG22	1:J:394:TYR:CE1	2.49	0.47
1:K:201:THR:HA	1:K:204:TYR:CD1	2.50	0.47
1:K:420:ILE:HA	1:K:423:LEU:HB2	1.97	0.47
1:K:387:PHE:CZ	1:K:451:ALA:HB2	2.49	0.47
1:K:51:SER:HB2	1:K:54:ASN:OD1	2.15	0.47
1:L:201:THR:HA	1:L:204:TYR:CD1	2.49	0.47
1:L:60:HIS:O	1:L:63:GLN:HB3	2.13	0.47
1:C:365:ARG:HD2	1:C:365:ARG:N	2.30	0.47
1:C:537:LEU:O	1:C:541:ILE:HG13	2.15	0.47
1:D:77:CYS:H	1:D:95:MET:HA	1.80	0.47
1:E:31:LEU:HG	1:E:97:TYR:CE2	2.50	0.47
1:E:323:ILE:N	1:E:323:ILE:HD12	2.30	0.47
1:E:574:ARG:NH1	1:E:575:PRO:HD2	2.30	0.47
1:F:281:ASN:OD1	1:F:286:GLN:HB3	2.15	0.47
1:G:143:ARG:HG2	1:G:143:ARG:HH21	1.80	0.47
1:H:117:LYS:O	1:H:121:ILE:HG13	2.15	0.47
1:H:44:LYS:HB3	1:H:93:LEU:HB3	1.96	0.47
1:K:7:PRO:HG3	1:K:17:MET:SD	2.54	0.47
1:L:523:GLU:HB2	1:L:632:ILE:HG12	1.97	0.47
1:L:623:PRO:O	1:L:627:VAL:HG23	2.15	0.47
1:B:103:LEU:HB3	1:B:147:PRO:O	2.15	0.47
1:C:513:GLU:HB3	1:C:517:LYS:HE3	1.97	0.47
1:D:20:ARG:C	1:D:21:LEU:HD22	2.36	0.47
1:D:473:SER:HB3	1:D:632:ILE:HD13	1.95	0.47
1:D:74:VAL:HG11	1:D:164:ILE:HA	1.96	0.47
1:E:548:PRO:HG2	1:E:607:HIS:NE2	2.30	0.47
1:F:219:ARG:NE	1:F:224:HIS:H	2.02	0.47
1:F:653:LEU:HG	1:F:656:ILE:HD11	1.96	0.47
1:G:576:SER:HB2	1:I:577:ASP:HA	1.97	0.47
1:H:51:SER:HB2	1:H:54:ASN:OD1	2.15	0.47
1:H:45:SER:OG	1:H:86:LEU:HD11	2.14	0.47
1:I:501:GLY:HA2	1:J:658:CYS:HB3	1.97	0.47
1:I:633:LYS:HA	1:I:636:ASP:HB3	1.97	0.47
1:J:615:LYS:O	1:J:619:ILE:HG13	2.15	0.47
1:J:44:LYS:HB3	1:J:93:LEU:HB3	1.97	0.47
1:K:192:LEU:H	1:K:192:LEU:HD12	1.80	0.47
1:K:401:ARG:HG2	1:K:433:TYR:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:513:GLU:HB3	1:K:517:LYS:HE3	1.97	0.47
1:L:192:LEU:HD12	1:L:192:LEU:N	2.30	0.47
1:H:227:PRO:HG3	1:L:249:SER:HB2	1.97	0.47
1:B:192:LEU:HD12	1:B:192:LEU:N	2.30	0.47
1:B:635:ALA:HA	1:B:638:THR:OG1	2.15	0.47
1:C:317:ASN:ND2	1:C:319:THR:HG23	2.30	0.47
1:C:424:ARG:HD3	1:C:572:LYS:HE2	1.97	0.47
1:C:587:VAL:O	1:C:591:VAL:HG23	2.14	0.47
1:C:633:LYS:HA	1:C:636:ASP:HB3	1.97	0.47
1:D:51:SER:HB2	1:D:54:ASN:OD1	2.15	0.47
1:E:408:ASN:HA	1:E:411:VAL:HG22	1.97	0.47
1:E:420:ILE:HA	1:E:423:LEU:HB2	1.97	0.47
1:E:88:HIS:O	1:E:90:VAL:N	2.47	0.47
1:F:418:LEU:HB2	1:F:423:LEU:HD21	1.96	0.47
1:F:523:GLU:OE1	1:F:526:VAL:HG21	2.15	0.47
1:H:401:ARG:H	1:H:401:ARG:NE	2.12	0.47
1:I:404:SER:HB2	1:I:406:CYS:SG	2.54	0.47
1:I:43:ILE:N	1:I:43:ILE:HD12	2.29	0.47
1:J:420:ILE:HA	1:J:423:LEU:HB2	1.96	0.47
1:K:541:ILE:HD11	1:K:618:ILE:HD11	1.97	0.47
1:K:73:VAL:HG22	1:K:74:VAL:N	2.30	0.47
1:L:586:MET:O	1:L:590:ILE:HG13	2.15	0.47
1:A:29:VAL:HG22	1:A:44:LYS:CB	2.44	0.47
1:A:586:MET:O	1:A:590:ILE:HG13	2.15	0.47
1:B:219:ARG:HB2	1:B:219:ARG:HH11	1.80	0.47
1:B:44:LYS:HB3	1:B:93:LEU:HB3	1.97	0.47
1:C:404:SER:HB2	1:C:406:CYS:SG	2.54	0.47
1:D:387:PHE:CZ	1:D:451:ALA:HB2	2.49	0.47
1:G:219:ARG:HH12	1:G:224:HIS:H	1.62	0.47
1:I:430:ALA:O	1:I:434:VAL:HG23	2.14	0.47
1:J:513:GLU:HB3	1:J:517:LYS:HE3	1.95	0.47
1:J:633:LYS:HA	1:J:636:ASP:HB3	1.97	0.47
1:J:60:HIS:O	1:J:63:GLN:HB3	2.15	0.47
1:J:88:HIS:HD2	1:J:90:VAL:HG22	1.80	0.47
1:K:396:GLY:HA2	1:K:398:PHE:CE2	2.50	0.47
1:K:452:MET:O	1:K:456:LEU:HG	2.15	0.47
1:L:44:LYS:HB3	1:L:93:LEU:HB3	1.97	0.47
1:A:587:VAL:O	1:A:591:VAL:HG23	2.14	0.46
1:B:408:ASN:ND2	1:D:26:PHE:HA	2.29	0.46
1:C:192:LEU:N	1:C:192:LEU:HD12	2.30	0.46
1:D:14:PRO:O	1:D:35:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HD12	1:D:192:LEU:N	2.30	0.46
1:F:240:LYS:HA	1:F:240:LYS:NZ	2.30	0.46
1:F:29:VAL:HG22	1:F:44:LYS:CB	2.45	0.46
1:G:201:THR:HA	1:G:204:TYR:CD1	2.51	0.46
1:G:404:SER:HB2	1:G:406:CYS:SG	2.55	0.46
1:H:166:LEU:N	1:H:166:LEU:HD22	2.29	0.46
1:H:215:ILE:HD13	1:H:264:LEU:HD11	1.97	0.46
1:I:236:LYS:HG2	1:I:237:LYS:N	2.30	0.46
1:I:615:LYS:O	1:I:619:ILE:HG13	2.15	0.46
1:I:487:ILE:HA	1:I:646:ARG:HD2	1.97	0.46
1:I:98:CYS:HA	1:I:153:GLN:NE2	2.29	0.46
1:J:219:ARG:NH2	1:J:224:HIS:H	2.13	0.46
1:J:408:ASN:HA	1:J:411:VAL:HG22	1.97	0.46
4:J:705:GLC:H61	5:J:706:PDX:C3	2.39	0.46
1:K:502:ILE:HG12	1:K:656:ILE:HD12	1.96	0.46
1:L:20:ARG:C	1:L:21:LEU:HD22	2.35	0.46
1:L:268:ILE:O	1:L:272:MET:HB2	2.14	0.46
1:B:103:LEU:HB2	1:B:150:ILE:HB	1.96	0.46
1:B:401:ARG:NH1	1:B:437:LEU:HD23	2.29	0.46
1:B:595:GLN:CB	4:B:705:GLC:H62	2.45	0.46
1:B:60:HIS:O	1:B:63:GLN:HB3	2.15	0.46
1:C:523:GLU:OE1	1:C:526:VAL:HG21	2.14	0.46
1:C:635:ALA:HA	1:C:638:THR:OG1	2.15	0.46
1:E:633:LYS:HA	1:E:636:ASP:HB3	1.97	0.46
1:F:70:HIS:O	1:F:71:ALA:HB3	2.15	0.46
1:G:514:MET:CA	1:G:642:MET:HE1	2.43	0.46
1:G:560:LEU:O	1:G:563:ARG:HB2	2.15	0.46
1:H:430:ALA:O	1:H:434:VAL:HG23	2.15	0.46
1:I:560:LEU:O	1:I:563:ARG:HB2	2.16	0.46
1:I:635:ALA:HA	1:I:638:THR:OG1	2.15	0.46
1:I:657:ALA:HA	1:I:660:GLN:HG3	1.97	0.46
1:A:275:TRP:CZ2	1:A:304:MET:HE2	2.50	0.46
1:B:117:LYS:N	1:B:117:LYS:HE2	2.31	0.46
1:B:485:LYS:O	1:B:489:LEU:HB2	2.14	0.46
1:D:294:THR:C	1:D:295:LEU:HD22	2.35	0.46
1:D:657:ALA:HA	1:D:660:GLN:HG3	1.97	0.46
1:E:166:LEU:HD22	1:E:166:LEU:N	2.31	0.46
1:G:70:HIS:O	1:G:73:VAL:HG12	2.14	0.46
1:I:523:GLU:OE1	1:I:526:VAL:HG21	2.14	0.46
1:J:268:ILE:O	1:J:272:MET:HB2	2.15	0.46
1:J:51:SER:HB2	1:J:54:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:418:LEU:HB2	1:K:423:LEU:HD21	1.97	0.46
1:L:323:ILE:HD12	1:L:323:ILE:N	2.31	0.46
1:L:316:LEU:HB2	1:L:383:MET:CE	2.46	0.46
1:A:284:PRO:HG2	1:A:285:GLN:H	1.80	0.46
1:B:513:GLU:HB3	1:B:517:LYS:HE3	1.98	0.46
1:B:653:LEU:HG	1:B:656:ILE:HD11	1.96	0.46
1:C:445:PHE:HE1	1:C:549:TYR:HB3	1.81	0.46
1:C:586:MET:O	1:C:590:ILE:HG13	2.16	0.46
1:D:249:SER:HB3	1:F:184:THR:CA	2.45	0.46
1:E:497:GLN:HE22	1:F:654:LEU:HD21	1.81	0.46
1:E:51:SER:HB2	1:E:54:ASN:OD1	2.15	0.46
1:E:635:ALA:HA	1:E:638:THR:OG1	2.15	0.46
1:F:268:ILE:O	1:F:272:MET:HB2	2.14	0.46
1:G:295:LEU:C	1:G:297:GLN:H	2.19	0.46
1:G:51:SER:HB2	1:G:54:ASN:OD1	2.14	0.46
1:G:621:LEU:O	1:G:625:VAL:HG23	2.16	0.46
1:J:238:ASP:CB	1:J:239:PRO:HD2	2.45	0.46
1:L:523:GLU:OE1	1:L:526:VAL:HG21	2.16	0.46
1:L:424:ARG:HD3	1:L:572:LYS:HE2	1.97	0.46
1:A:473:SER:HB2	1:A:524:VAL:HG22	1.97	0.46
1:A:507:MET:HE3	1:A:653:LEU:HD22	1.96	0.46
1:B:281:ASN:HD22	1:B:282:TRP:H	1.63	0.46
1:B:657:ALA:HA	1:B:660:GLN:HG3	1.98	0.46
1:C:142:HIS:HA	1:C:169:ALA:HB2	1.98	0.46
1:E:463:THR:HA	1:E:534:ILE:HD11	1.97	0.46
1:E:477:LYS:HE3	1:E:524:VAL:HG11	1.98	0.46
1:F:60:HIS:O	1:F:63:GLN:HB3	2.14	0.46
1:F:44:LYS:HB3	1:F:93:LEU:HB3	1.98	0.46
1:G:423:LEU:HA	1:G:426:VAL:CG2	2.41	0.46
1:H:143:ARG:HG2	1:H:143:ARG:HH21	1.81	0.46
1:H:48:LEU:HA	1:H:87:ILE:CD1	2.45	0.46
1:H:537:LEU:O	1:H:541:ILE:HG13	2.15	0.46
1:I:445:PHE:CE2	1:I:551:ARG:HD2	2.51	0.46
1:J:537:LEU:O	1:J:541:ILE:HG13	2.16	0.46
1:J:586:MET:O	1:J:590:ILE:HG13	2.15	0.46
1:L:43:ILE:HD12	1:L:43:ILE:N	2.31	0.46
1:C:267:LEU:HD12	1:C:312:ILE:HG23	1.97	0.46
1:C:49:GLU:HA	1:C:88:HIS:HB2	1.98	0.46
1:E:192:LEU:H	1:E:192:LEU:HD12	1.81	0.46
1:F:141:ILE:CG2	1:F:170:LYS:HB2	2.46	0.46
1:F:396:GLY:HA2	1:F:398:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:LEU:HD12	1:G:407:VAL:HG12	1.98	0.46
1:G:43:ILE:HD12	1:G:43:ILE:N	2.30	0.46
1:G:29:VAL:HG22	1:G:44:LYS:CB	2.44	0.46
1:G:487:ILE:HG23	1:G:488:GLN:N	2.31	0.46
1:G:579:SER:HB3	1:K:577:ASP:N	2.28	0.46
1:H:74:VAL:O	1:H:74:VAL:HG13	2.15	0.46
1:I:396:GLY:HA2	1:I:398:PHE:CE2	2.50	0.46
1:I:420:ILE:HA	1:I:423:LEU:HB2	1.97	0.46
1:J:219:ARG:NE	1:J:219:ARG:H	2.14	0.46
1:K:363:ASP:OD1	1:K:365:ARG:HB2	2.15	0.46
1:B:117:LYS:O	1:B:121:ILE:HG13	2.16	0.46
1:B:201:THR:HA	1:B:204:TYR:CD1	2.51	0.46
1:C:205:TRP:HE3	1:C:287:ARG:HH12	1.62	0.46
1:C:48:LEU:O	1:C:50:LEU:HD12	2.16	0.46
1:A:576:SER:OG	1:C:577:ASP:HA	2.15	0.46
1:D:274:ASN:HA	1:D:277:GLN:NE2	2.31	0.46
1:A:249:SER:HB2	1:E:227:PRO:HG3	1.98	0.46
1:E:586:MET:O	1:E:590:ILE:HG13	2.16	0.46
1:F:487:ILE:HG12	1:F:515:GLU:HB2	1.98	0.46
1:F:592:HIS:CD2	4:F:706:GLC:H2	2.51	0.46
1:G:13:GLY:H	1:G:14:PRO:HD3	1.81	0.46
1:G:320:SER:HA	1:G:398:PHE:HB3	1.97	0.46
1:H:27:GLY:O	1:H:45:SER:HB3	2.16	0.46
1:H:657:ALA:HA	1:H:660:GLN:HG3	1.98	0.46
1:I:143:ARG:H	1:I:143:ARG:CD	2.29	0.46
1:I:183:GLY:O	1:I:185:LEU:N	2.49	0.46
1:I:408:ASN:HA	1:I:411:VAL:HG22	1.97	0.46
1:J:192:LEU:N	1:J:192:LEU:HD12	2.31	0.46
1:A:166:LEU:C	1:A:168:TYR:H	2.19	0.46
1:A:182:VAL:HG12	1:A:183:GLY:N	2.28	0.46
1:A:201:THR:HA	1:A:204:TYR:CD1	2.51	0.46
1:A:323:ILE:N	1:A:323:ILE:HD12	2.31	0.46
1:A:633:LYS:HA	1:A:636:ASP:HB3	1.97	0.46
1:B:170:LYS:HG2	1:B:177:LEU:HG	1.98	0.46
1:B:222:LEU:HB2	1:B:230:TRP:CD1	2.51	0.46
1:B:231:HIS:C	1:B:233:LYS:H	2.19	0.46
1:B:408:ASN:HA	1:B:411:VAL:HG22	1.97	0.46
1:C:507:MET:HE3	1:C:653:LEU:HD22	1.96	0.46
1:C:95:MET:HE2	1:C:164:ILE:HD11	1.97	0.46
1:D:72:ASN:O	1:D:162:LYS:HA	2.16	0.46
1:D:81:GLU:CD	1:D:81:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LEU:HD22	1:F:166:LEU:N	2.30	0.46
1:F:51:SER:HB2	1:F:54:ASN:OD1	2.15	0.46
1:G:192:LEU:HD12	1:G:192:LEU:N	2.31	0.46
1:G:192:LEU:HD12	1:G:192:LEU:H	1.80	0.46
1:G:323:ILE:HD12	1:G:323:ILE:N	2.31	0.46
1:G:537:LEU:O	1:G:541:ILE:HG13	2.16	0.46
1:G:77:CYS:SG	1:G:78:ASP:N	2.88	0.46
1:I:274:ASN:HA	1:I:277:GLN:NE2	2.31	0.46
1:I:401:ARG:HH21	1:I:440:ASP:HB2	1.80	0.46
1:J:477:LYS:HE3	1:J:524:VAL:HG11	1.97	0.46
1:J:635:ALA:HA	1:J:638:THR:OG1	2.16	0.46
1:K:268:ILE:O	1:K:272:MET:HB2	2.16	0.46
1:A:204:TYR:HH	1:A:301:PHE:HE2	1.63	0.46
1:A:281:ASN:HB3	1:A:287:ARG:HG3	1.98	0.46
1:A:598:ASP:O	1:A:602:LYS:HG2	2.15	0.46
1:A:651:TRP:HZ2	1:B:490:ASP:HB3	1.81	0.46
1:B:51:SER:HB2	1:B:54:ASN:OD1	2.16	0.46
1:B:537:LEU:O	1:B:541:ILE:HG13	2.16	0.46
1:B:598:ASP:O	1:B:602:LYS:HG2	2.15	0.46
1:B:633:LYS:HA	1:B:636:ASP:HB3	1.98	0.46
1:C:274:ASN:HA	1:C:277:GLN:NE2	2.31	0.46
1:C:615:LYS:O	1:C:619:ILE:HG13	2.15	0.46
1:D:323:ILE:N	1:D:323:ILE:HD12	2.31	0.46
1:E:279:MET:O	1:E:287:ARG:HD2	2.15	0.46
1:E:74:VAL:HG21	1:E:95:MET:CE	2.45	0.46
1:F:80:PRO:HB3	1:F:92:LEU:H	1.80	0.46
1:G:219:ARG:HH12	1:G:224:HIS:N	2.14	0.46
1:G:420:ILE:HG21	1:G:578:HIS:H	1.81	0.46
1:H:408:ASN:HA	1:H:411:VAL:HG22	1.98	0.46
1:H:480:LEU:HD22	1:H:518:ALA:HB1	1.97	0.46
1:H:549:TYR:H	1:H:552:ARG:HD2	1.80	0.46
1:I:420:ILE:HD11	1:I:571:LEU:HG	1.98	0.46
1:L:51:SER:HB2	1:L:54:ASN:OD1	2.16	0.46
1:L:615:LYS:O	1:L:619:ILE:HG13	2.16	0.46
1:B:27:GLY:O	1:B:45:SER:HB3	2.16	0.46
1:B:487:ILE:HG23	1:B:488:GLN:N	2.31	0.46
1:C:143:ARG:HG2	1:C:143:ARG:HH21	1.80	0.46
1:C:598:ASP:O	1:C:602:LYS:HG2	2.16	0.46
1:C:393:VAL:HG13	1:C:609:SER:OG	2.16	0.46
1:C:616:GLN:O	1:C:620:ASP:HB2	2.15	0.46
1:C:623:PRO:O	1:C:627:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ALA:HA	1:C:660:GLN:HG3	1.98	0.46
1:D:359:GLY:HA3	1:D:453:LEU:HB2	1.98	0.46
1:D:44:LYS:HB3	1:D:93:LEU:HB3	1.98	0.46
1:E:623:PRO:O	1:E:627:VAL:HG23	2.15	0.46
1:E:465:MET:HB3	1:E:625:VAL:HG11	1.97	0.46
1:E:44:LYS:HB3	1:E:93:LEU:HB3	1.98	0.46
1:F:20:ARG:C	1:F:21:LEU:HD22	2.36	0.46
1:F:395:GLU:HG2	1:F:396:GLY:N	2.24	0.46
1:F:430:ALA:O	1:F:434:VAL:HG23	2.16	0.46
1:F:615:LYS:O	1:F:619:ILE:HG13	2.16	0.46
1:G:489:LEU:HD13	1:H:643:GLN:CG	2.45	0.46
1:G:598:ASP:O	1:G:602:LYS:HG2	2.16	0.46
1:H:274:ASN:HA	1:H:277:GLN:NE2	2.31	0.46
1:I:143:ARG:HH21	1:I:143:ARG:HG2	1.80	0.46
1:I:403:LEU:HD12	1:I:407:VAL:HG12	1.98	0.46
1:I:427:TRP:CZ3	1:I:567:LEU:HB3	2.49	0.46
1:I:473:SER:HB2	1:I:524:VAL:HA	1.97	0.46
1:I:501:GLY:HA3	1:J:655:LYS:HE2	1.98	0.46
1:K:466:LYS:HD3	1:K:534:ILE:HG21	1.98	0.46
1:K:537:LEU:O	1:K:541:ILE:HG13	2.15	0.46
1:L:212:PHE:CD2	1:L:220:PRO:HA	2.51	0.46
1:A:616:GLN:O	1:A:620:ASP:HB2	2.16	0.45
1:B:142:HIS:HA	1:B:169:ALA:HB1	1.98	0.45
1:B:293:LEU:H	1:B:293:LEU:HD22	1.80	0.45
1:C:408:ASN:HA	1:C:411:VAL:HG22	1.97	0.45
1:C:51:SER:HB2	1:C:54:ASN:OD1	2.15	0.45
1:D:408:ASN:HA	1:D:411:VAL:HG22	1.98	0.45
1:E:140:ILE:HG12	1:E:171:ASP:OD2	2.15	0.45
1:E:615:LYS:O	1:E:619:ILE:HG13	2.15	0.45
1:E:653:LEU:HG	1:E:656:ILE:HD11	1.97	0.45
1:F:420:ILE:HA	1:F:423:LEU:HB2	1.97	0.45
1:G:616:GLN:O	1:G:620:ASP:HB2	2.16	0.45
1:H:139:LYS:HB3	1:H:172:VAL:HG11	1.97	0.45
1:H:20:ARG:C	1:H:21:LEU:HD22	2.36	0.45
1:H:220:PRO:O	1:H:243:PHE:HA	2.17	0.45
1:H:26:PHE:HA	1:L:408:ASN:ND2	2.31	0.45
1:I:21:LEU:HD12	2:I:701:5TL:CAL	2.46	0.45
1:I:227:PRO:HA	1:I:230:TRP:CB	2.46	0.45
1:I:275:TRP:CZ2	1:I:304:MET:HE2	2.51	0.45
1:I:598:ASP:O	1:I:602:LYS:HG2	2.16	0.45
1:J:267:LEU:HD13	1:J:327:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:ASN:HD21	1:J:26:PHE:HA	1.78	0.45
1:K:149:ASN:O	1:K:164:ILE:HG22	2.16	0.45
1:K:190:PRO:HA	1:K:193:PHE:CD1	2.52	0.45
1:L:420:ILE:HA	1:L:423:LEU:HB2	1.97	0.45
1:L:65:MET:HB3	1:L:76:ALA:CB	2.41	0.45
1:A:651:TRP:CZ2	1:B:490:ASP:HB3	2.51	0.45
1:D:209:THR:N	1:D:280:LEU:HD21	2.32	0.45
1:D:430:ALA:O	1:D:434:VAL:HG23	2.16	0.45
1:D:586:MET:O	1:D:590:ILE:HG13	2.16	0.45
1:D:8:GLU:O	1:D:9:PHE:HB2	2.16	0.45
1:E:452:MET:O	1:E:456:LEU:HG	2.16	0.45
1:E:587:VAL:HA	1:E:590:ILE:HD12	1.98	0.45
1:E:621:LEU:O	1:E:625:VAL:HG23	2.16	0.45
1:F:427:TRP:CZ2	1:F:583:SER:HA	2.51	0.45
1:G:219:ARG:HH12	1:G:224:HIS:HA	1.81	0.45
1:G:237:LYS:CE	1:G:282:TRP:H	2.29	0.45
1:G:586:MET:O	1:G:590:ILE:HG13	2.15	0.45
1:G:635:ALA:HA	1:G:638:THR:OG1	2.15	0.45
1:H:273:GLU:O	1:H:277:GLN:HG3	2.16	0.45
1:H:317:ASN:ND2	1:H:319:THR:HG23	2.32	0.45
1:I:466:LYS:HD3	1:I:534:ILE:HD13	1.98	0.45
1:J:48:LEU:O	1:J:50:LEU:HD12	2.16	0.45
1:L:185:LEU:HD11	1:L:188:LEU:CB	2.30	0.45
1:L:238:ASP:CB	1:L:239:PRO:HD2	2.46	0.45
1:L:537:LEU:O	1:L:541:ILE:HG13	2.15	0.45
1:A:487:ILE:HG23	1:A:488:GLN:N	2.31	0.45
1:B:37:LEU:HB3	1:B:38:ASP:H	1.67	0.45
1:B:423:LEU:HA	1:B:426:VAL:CG2	2.42	0.45
1:C:292:ASP:O	1:C:296:LYS:HA	2.17	0.45
1:C:43:ILE:N	1:C:43:ILE:HD12	2.31	0.45
1:D:283:ASP:OD2	1:D:284:PRO:HD2	2.17	0.45
1:D:537:LEU:O	1:D:541:ILE:HG13	2.17	0.45
1:E:144:ASP:OD1	1:E:182:VAL:HG11	2.16	0.45
1:A:579:SER:HB2	1:E:578:HIS:ND1	2.31	0.45
1:F:101:GLY:HA2	2:F:701:5TL:CAR	2.46	0.45
1:F:143:ARG:HG2	1:F:143:ARG:HH21	1.81	0.45
1:G:149:ASN:O	1:G:164:ILE:HG22	2.16	0.45
1:H:29:VAL:HG21	2:H:701:5TL:CAF	2.47	0.45
1:H:586:MET:O	1:H:590:ILE:HG13	2.16	0.45
1:H:587:VAL:HA	1:H:590:ILE:HD12	1.98	0.45
1:I:268:ILE:O	1:I:272:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:LEU:HB3	1:I:84:ASN:H	1.59	0.45
1:J:273:GLU:O	1:J:277:GLN:HG3	2.17	0.45
1:J:423:LEU:HA	1:J:426:VAL:CG2	2.42	0.45
1:K:502:ILE:HD12	1:L:654:LEU:CD1	2.41	0.45
1:L:430:ALA:O	1:L:434:VAL:HG23	2.16	0.45
1:L:411:VAL:HG12	1:L:590:ILE:HG21	1.97	0.45
1:L:657:ALA:HA	1:L:660:GLN:HG3	1.98	0.45
1:A:27:GLY:HA2	1:C:412:GLN:NE2	2.31	0.45
1:A:587:VAL:HA	1:A:590:ILE:HD12	1.97	0.45
1:B:143:ARG:H	1:B:143:ARG:CD	2.30	0.45
1:B:324:ILE:N	1:B:324:ILE:HD12	2.30	0.45
1:C:166:LEU:N	1:C:166:LEU:HD22	2.32	0.45
1:C:410:ILE:O	1:C:587:VAL:HG22	2.16	0.45
1:D:237:LYS:CG	1:D:241:CYS:HB3	2.46	0.45
1:E:215:ILE:HD13	1:E:264:LEU:HD11	1.97	0.45
1:E:616:GLN:O	1:E:620:ASP:HB2	2.16	0.45
1:F:238:ASP:CB	1:F:239:PRO:HD2	2.45	0.45
1:F:633:LYS:HA	1:F:636:ASP:HB3	1.97	0.45
1:G:204:TYR:HH	1:G:301:PHE:HE2	1.61	0.45
1:G:222:LEU:HD12	1:G:244:ALA:O	2.16	0.45
1:G:417:GLN:HB3	1:G:581:SER:HB3	1.98	0.45
1:H:212:PHE:CE2	1:H:220:PRO:HA	2.52	0.45
1:H:563:ARG:HH12	4:H:703:GLC:H2	1.80	0.45
1:H:616:GLN:O	1:H:620:ASP:HB2	2.17	0.45
1:I:230:TRP:O	1:I:234:ILE:HG12	2.16	0.45
1:I:392:THR:O	1:I:612:LEU:HD23	2.17	0.45
1:J:240:LYS:HD3	1:J:281:ASN:OD1	2.17	0.45
1:J:37:LEU:HB3	1:J:38:ASP:H	1.67	0.45
1:K:445:PHE:HA	1:K:604:LEU:HD21	1.98	0.45
1:K:633:LYS:HA	1:K:636:ASP:HB3	1.98	0.45
1:K:657:ALA:HA	1:K:660:GLN:HG3	1.99	0.45
1:L:459:ASN:HD21	1:L:538:HIS:CD2	2.34	0.45
1:A:540:GLU:O	1:A:544:LEU:HG	2.16	0.45
1:A:621:LEU:O	1:A:625:VAL:HG23	2.17	0.45
1:B:34:HIS:CE1	1:B:37:LEU:HD23	2.52	0.45
1:B:373:LEU:N	1:B:373:LEU:HD22	2.31	0.45
1:B:420:ILE:HD11	1:B:571:LEU:HG	1.98	0.45
1:D:143:ARG:HH21	1:D:143:ARG:HG2	1.81	0.45
1:D:548:PRO:CB	1:D:552:ARG:HG3	2.46	0.45
1:G:231:HIS:O	1:G:235:LYS:N	2.49	0.45
1:G:587:VAL:HA	1:G:590:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:LEU:HD21	1:I:140:ILE:HD12	1.98	0.45
1:J:279:MET:O	1:J:287:ARG:HD2	2.16	0.45
1:K:238:ASP:OD2	1:K:239:PRO:HD2	2.16	0.45
1:K:273:GLU:O	1:K:277:GLN:HG3	2.17	0.45
1:K:551:ARG:HG2	1:K:551:ARG:O	2.17	0.45
1:L:212:PHE:CE2	1:L:220:PRO:HA	2.52	0.45
1:L:27:GLY:O	1:L:45:SER:HB3	2.17	0.45
1:L:427:TRP:HZ2	1:L:583:SER:HA	1.81	0.45
1:L:616:GLN:O	1:L:620:ASP:HB2	2.16	0.45
1:A:74:VAL:HG11	1:A:164:ILE:HA	1.98	0.45
1:A:354:LEU:HB3	1:A:384:VAL:HG11	1.99	0.45
1:A:373:LEU:N	1:A:373:LEU:HD22	2.32	0.45
1:A:408:ASN:HA	1:A:411:VAL:HG22	1.98	0.45
1:A:657:ALA:HA	1:A:660:GLN:HG3	1.99	0.45
1:C:107:LEU:HD23	1:C:116:LEU:HD11	1.99	0.45
1:E:225:LEU:O	1:E:226:GLN:C	2.55	0.45
1:E:87:ILE:O	1:E:88:HIS:HB3	2.16	0.45
1:G:657:ALA:HA	1:G:660:GLN:HG3	1.99	0.45
1:H:34:HIS:CE1	1:H:37:LEU:HD23	2.52	0.45
1:H:549:TYR:HB2	1:H:552:ARG:CZ	2.47	0.45
1:H:560:LEU:O	1:H:563:ARG:HB2	2.16	0.45
1:H:79:VAL:CG1	1:H:83:LEU:HD11	2.46	0.45
1:I:395:GLU:HG2	1:I:396:GLY:N	2.31	0.45
1:J:314:HIS:ND1	1:J:380:ASP:HA	2.32	0.45
1:J:412:GLN:NE2	1:L:27:GLY:HA2	2.32	0.45
1:K:115:GLY:HA3	1:K:215:ILE:O	2.15	0.45
1:K:403:LEU:HD12	1:K:407:VAL:HG12	1.99	0.45
1:K:615:LYS:O	1:K:619:ILE:HG13	2.16	0.45
1:H:185:LEU:HB3	1:L:249:SER:HB3	1.99	0.45
1:A:190:PRO:HA	1:A:193:PHE:CD1	2.52	0.45
1:A:615:LYS:O	1:A:619:ILE:HG13	2.16	0.45
1:B:415:LYS:HD3	1:B:584:THR:HG21	1.98	0.45
1:C:268:ILE:O	1:C:272:MET:HB2	2.16	0.45
1:C:430:ALA:O	1:C:434:VAL:HG23	2.16	0.45
1:D:404:SER:HB2	1:D:406:CYS:SG	2.56	0.45
1:D:477:LYS:HE3	1:D:524:VAL:HG11	1.98	0.45
1:D:544:LEU:HD21	1:D:610:LYS:CD	2.46	0.45
1:E:537:LEU:O	1:E:541:ILE:HG13	2.15	0.45
1:F:8:GLU:HB2	1:F:45:SER:OG	2.16	0.45
1:F:657:ALA:HA	1:F:660:GLN:HG3	1.99	0.45
1:G:142:HIS:HA	1:G:169:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:PRO:HG2	1:G:221:PHE:CD2	2.52	0.45
1:G:236:LYS:HG2	1:G:237:LYS:H	1.82	0.45
1:G:408:ASN:HD21	1:K:26:PHE:HD1	1.63	0.45
1:H:323:ILE:N	1:H:323:ILE:HD12	2.32	0.45
1:I:65:MET:SD	1:I:166:LEU:HD23	2.56	0.45
1:I:275:TRP:CH2	1:I:279:MET:HG3	2.52	0.45
1:I:48:LEU:O	1:I:50:LEU:HD12	2.16	0.45
1:L:460:ALA:O	1:L:464:LYS:HG3	2.16	0.45
1:L:560:LEU:HB3	1:L:593:THR:HG22	1.97	0.45
1:L:587:VAL:HA	1:L:590:ILE:HD12	1.98	0.45
1:L:589:ILE:O	1:L:593:THR:HG23	2.16	0.45
1:L:89:ASP:O	1:L:90:VAL:HG13	2.17	0.45
1:A:430:ALA:O	1:A:434:VAL:HG23	2.16	0.45
1:A:537:LEU:O	1:A:541:ILE:HG13	2.16	0.45
1:A:459:ASN:HD21	1:A:538:HIS:CD2	2.34	0.45
1:B:364:PRO:C	1:B:366:LYS:H	2.20	0.45
1:C:323:ILE:N	1:C:323:ILE:HD12	2.31	0.45
1:C:50:LEU:HD22	1:C:90:VAL:HG11	1.99	0.45
1:C:57:ARG:O	1:C:60:HIS:HB3	2.17	0.45
9:C:708:5TM:O6	9:C:708:5TM:C1	2.65	0.45
1:C:89:ASP:O	1:C:90:VAL:HG13	2.17	0.45
1:D:37:LEU:HB3	1:D:38:ASP:H	1.67	0.45
1:E:318:MET:HE1	1:E:447:GLY:HA3	1.98	0.45
1:E:657:ALA:HA	1:E:660:GLN:HG3	1.99	0.45
1:F:72:ASN:O	1:F:162:LYS:HA	2.17	0.45
1:G:143:ARG:CD	1:G:143:ARG:H	2.30	0.45
1:G:236:LYS:HG2	1:G:237:LYS:N	2.32	0.45
1:H:420:ILE:HG12	1:H:577:ASP:HB3	1.98	0.45
1:I:487:ILE:HG23	1:I:488:GLN:N	2.32	0.45
1:J:77:CYS:SG	1:J:78:ASP:N	2.90	0.45
1:L:143:ARG:HH21	1:L:143:ARG:HG2	1.81	0.45
1:L:273:GLU:O	1:L:277:GLN:HG3	2.17	0.45
1:A:404:SER:HB2	1:A:406:CYS:SG	2.56	0.45
1:B:191:GLU:CD	1:B:284:PRO:HB3	2.36	0.45
1:B:43:ILE:N	1:B:43:ILE:HD12	2.31	0.45
1:A:647:GLN:OE1	1:B:489:LEU:HD22	2.17	0.45
1:C:143:ARG:CD	1:C:143:ARG:H	2.30	0.45
1:C:223:HIS:O	1:C:224:HIS:HB3	2.16	0.45
1:C:26:PHE:HD2	1:C:47:ARG:HA	1.81	0.45
1:C:549:TYR:H	1:C:552:ARG:HD2	1.82	0.45
1:C:68:LEU:HD21	1:C:140:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ARG:H	1:D:143:ARG:CD	2.30	0.45
1:D:514:MET:SD	1:D:645:LYS:HD3	2.56	0.45
1:D:561:GLU:O	1:D:565:ILE:HG13	2.16	0.45
1:E:143:ARG:H	1:E:143:ARG:CD	2.30	0.45
1:E:85:ILE:HD12	1:E:89:ASP:HA	1.98	0.45
1:F:273:GLU:O	1:F:277:GLN:HG3	2.17	0.45
1:F:27:GLY:O	1:F:45:SER:HB3	2.17	0.45
1:F:408:ASN:HA	1:F:411:VAL:HG22	1.97	0.45
1:G:147:PRO:C	1:G:149:ASN:H	2.21	0.45
1:G:370:GLN:HB2	1:G:370:GLN:HE21	1.52	0.45
1:G:427:TRP:HZ2	1:G:583:SER:HA	1.81	0.45
1:H:72:ASN:ND2	1:H:127:ASP:O	2.50	0.45
1:H:370:GLN:HB2	1:H:370:GLN:HE21	1.61	0.45
1:H:473:SER:CB	1:H:527:ILE:HD11	2.47	0.45
1:J:430:ALA:O	1:J:434:VAL:HG23	2.17	0.45
1:J:497:GLN:HA	1:J:500:TYR:HD2	1.82	0.45
1:J:561:GLU:O	1:J:565:ILE:HG13	2.17	0.45
1:J:560:LEU:HB3	1:J:593:THR:HG22	1.98	0.45
1:K:192:LEU:N	1:K:192:LEU:HD12	2.31	0.45
1:K:274:ASN:HA	1:K:277:GLN:NE2	2.31	0.45
1:K:318:MET:CE	1:K:447:GLY:HA3	2.47	0.45
1:K:65:MET:SD	1:K:166:LEU:HD23	2.57	0.45
1:A:143:ARG:CD	1:A:143:ARG:H	2.30	0.45
1:B:273:GLU:O	1:B:277:GLN:HG3	2.17	0.45
1:C:452:MET:O	1:C:456:LEU:HG	2.16	0.45
1:D:126:SER:HB2	1:D:308:LEU:CD1	2.47	0.45
1:D:420:ILE:HA	1:D:423:LEU:HB2	1.98	0.45
1:E:237:LYS:CE	1:E:282:TRP:H	2.24	0.45
1:F:560:LEU:HB3	1:F:593:THR:HG22	1.98	0.45
1:F:616:GLN:O	1:F:620:ASP:HB2	2.17	0.45
1:G:9:PHE:HZ	1:G:17:MET:HG2	1.82	0.45
1:I:29:VAL:HG21	2:I:701:5TL:CAE	2.47	0.45
1:J:323:ILE:HD12	1:J:323:ILE:N	2.32	0.45
1:A:274:ASN:HA	1:A:277:GLN:NE2	2.32	0.44
1:A:373:LEU:HD21	1:A:382:TYR:HB3	1.98	0.44
1:A:420:ILE:HG21	1:A:578:HIS:H	1.82	0.44
1:B:222:LEU:HB2	1:B:230:TRP:HE1	1.81	0.44
1:D:222:LEU:HD23	1:D:230:TRP:HE1	1.81	0.44
1:F:140:ILE:HG12	1:F:171:ASP:OD2	2.16	0.44
1:F:225:LEU:O	1:F:226:GLN:C	2.54	0.44
1:F:275:TRP:CH2	1:F:279:MET:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:ASN:O	1:H:164:ILE:HG22	2.18	0.44
1:H:653:LEU:HG	1:H:656:ILE:HD11	1.98	0.44
1:I:324:ILE:N	1:I:324:ILE:HD12	2.31	0.44
1:J:541:ILE:CD1	1:J:618:ILE:HD11	2.47	0.44
1:K:222:LEU:HD13	1:K:244:ALA:O	2.17	0.44
1:K:34:HIS:CE1	1:K:37:LEU:HD23	2.52	0.44
1:K:635:ALA:HA	1:K:638:THR:OG1	2.16	0.44
1:L:143:ARG:HD2	1:L:170:LYS:HE3	1.99	0.44
1:L:274:ASN:HA	1:L:277:GLN:NE2	2.32	0.44
1:L:423:LEU:O	1:L:427:TRP:HB2	2.17	0.44
1:A:13:GLY:N	1:A:14:PRO:CD	2.76	0.44
1:A:317:ASN:ND2	1:A:319:THR:HG23	2.33	0.44
1:A:8:GLU:O	1:A:9:PHE:HB2	2.17	0.44
1:C:587:VAL:HA	1:C:590:ILE:HD12	1.98	0.44
1:C:541:ILE:HD11	1:C:618:ILE:HD11	2.00	0.44
1:D:185:LEU:HD13	1:D:186:GLN:N	2.32	0.44
1:D:502:ILE:HD13	1:D:656:ILE:HD12	1.99	0.44
1:A:249:SER:HB2	1:E:227:PRO:CG	2.47	0.44
1:E:268:ILE:O	1:E:272:MET:HB2	2.17	0.44
1:E:417:GLN:HB3	1:E:581:SER:CB	2.46	0.44
1:G:314:HIS:HB2	1:G:383:MET:HB2	1.98	0.44
1:G:334:LEU:HD22	1:G:366:LYS:O	2.17	0.44
1:G:87:ILE:HG22	1:G:88:HIS:N	2.33	0.44
1:I:452:MET:O	1:I:456:LEU:HG	2.16	0.44
1:J:311:LYS:O	1:J:372:VAL:HG11	2.17	0.44
1:J:366:LYS:CE	1:J:367:PRO:HD2	2.46	0.44
1:K:143:ARG:H	1:K:143:ARG:CD	2.30	0.44
1:K:430:ALA:O	1:K:434:VAL:HG23	2.16	0.44
1:L:218:TYR:HB2	1:L:223:HIS:ND1	2.32	0.44
1:A:268:ILE:O	1:A:272:MET:HB2	2.17	0.44
1:A:314:HIS:HB2	1:A:383:MET:HB3	1.99	0.44
1:A:410:ILE:HD12	1:A:583:SER:OG	2.17	0.44
1:B:166:LEU:N	1:B:166:LEU:HD22	2.31	0.44
1:B:616:GLN:O	1:B:620:ASP:HB2	2.18	0.44
1:C:487:ILE:HG23	1:C:488:GLN:N	2.32	0.44
1:D:395:GLU:OE2	1:D:397:PRO:HG3	2.17	0.44
1:E:190:PRO:HA	1:E:193:PHE:CD1	2.53	0.44
1:E:34:HIS:CE1	1:E:37:LEU:HD23	2.52	0.44
1:F:537:LEU:O	1:F:541:ILE:HG13	2.16	0.44
1:G:190:PRO:HA	1:G:193:PHE:CD1	2.52	0.44
1:H:598:ASP:O	1:H:602:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:462:LEU:HD22	1:H:618:ILE:HG23	1.99	0.44
1:I:34:HIS:CE1	1:I:37:LEU:HD23	2.52	0.44
1:I:452:MET:SD	1:I:611:LEU:HD22	2.57	0.44
1:I:592:HIS:CD2	4:I:706:GLC:H2	2.52	0.44
1:J:143:ARG:HH21	1:J:143:ARG:HG2	1.82	0.44
1:J:274:ASN:HA	1:J:277:GLN:NE2	2.33	0.44
1:J:411:VAL:HG12	1:J:590:ILE:HG21	1.99	0.44
1:K:35:ARG:HG3	1:K:36:GLU:HG3	2.00	0.44
1:K:427:TRP:CZ3	1:K:567:LEU:HB3	2.49	0.44
1:K:616:GLN:O	1:K:620:ASP:HB2	2.17	0.44
1:K:621:LEU:O	1:K:625:VAL:HG23	2.17	0.44
1:L:483:PHE:HZ	1:L:514:MET:HB3	1.81	0.44
1:A:635:ALA:HA	1:A:638:THR:OG1	2.16	0.44
1:A:514:MET:HE1	1:A:646:ARG:HG3	2.00	0.44
1:B:404:SER:HB2	1:B:406:CYS:SG	2.57	0.44
1:C:427:TRP:HZ2	1:C:583:SER:HA	1.82	0.44
1:D:396:GLY:N	1:D:397:PRO:CD	2.79	0.44
1:E:199:THR:HG21	1:E:285:GLN:NE2	2.32	0.44
1:E:387:PHE:CZ	1:E:451:ALA:HB2	2.52	0.44
1:F:487:ILE:HG23	1:F:488:GLN:N	2.32	0.44
1:F:498:MET:HA	1:F:503:SER:HB2	1.99	0.44
1:F:587:VAL:HA	1:F:590:ILE:HD12	1.99	0.44
1:G:180:GLU:CB	1:G:192:LEU:HD23	2.46	0.44
1:H:143:ARG:H	1:H:143:ARG:CD	2.30	0.44
1:H:334:LEU:HD11	1:H:364:PRO:HA	1.99	0.44
1:H:354:LEU:HB3	1:H:384:VAL:CG1	2.48	0.44
1:H:473:SER:HB3	1:H:527:ILE:HD11	2.00	0.44
1:I:621:LEU:O	1:I:625:VAL:HG23	2.18	0.44
1:J:383:MET:HG2	1:J:385:TYR:CE1	2.53	0.44
1:K:323:ILE:N	1:K:323:ILE:HD12	2.32	0.44
1:L:166:LEU:N	1:L:166:LEU:HD22	2.32	0.44
1:L:494:TYR:HE2	1:L:508:LEU:HD13	1.83	0.44
1:L:14:PRO:HG2	1:L:81:GLU:HG2	1.99	0.44
1:A:290:PRO:HB2	1:A:299:ARG:HB2	1.99	0.44
1:C:29:VAL:HG21	2:C:701:5TL:CAF	2.47	0.44
1:D:65:MET:SD	1:D:166:LEU:HD23	2.57	0.44
1:D:381:SER:O	1:D:383:MET:N	2.51	0.44
1:D:48:LEU:O	1:D:50:LEU:HD12	2.18	0.44
1:D:587:VAL:HA	1:D:590:ILE:HD12	1.99	0.44
1:D:616:GLN:O	1:D:620:ASP:HB2	2.17	0.44
1:E:149:ASN:O	1:E:164:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LEU:HD13	1:E:161:HIS:HA	1.99	0.44
1:E:561:GLU:O	1:E:565:ILE:HG13	2.17	0.44
1:E:541:ILE:HD11	1:E:618:ILE:HD11	2.00	0.44
1:F:231:HIS:O	1:F:235:LYS:N	2.51	0.44
1:F:323:ILE:HD12	1:F:323:ILE:N	2.32	0.44
1:F:404:SER:HB2	1:F:406:CYS:SG	2.58	0.44
1:F:445:PHE:CD1	1:F:551:ARG:HB2	2.53	0.44
1:G:116:LEU:N	1:G:116:LEU:HD12	2.30	0.44
1:G:275:TRP:HZ2	1:G:304:MET:HE2	1.82	0.44
1:G:403:LEU:HD23	1:G:403:LEU:N	2.33	0.44
1:H:275:TRP:CH2	1:H:279:MET:HG3	2.53	0.44
1:H:319:THR:HG22	1:H:394:TYR:CE1	2.52	0.44
1:H:423:LEU:HA	1:H:426:VAL:CG2	2.43	0.44
1:I:142:HIS:ND1	1:I:169:ALA:HB2	2.33	0.44
1:I:212:PHE:CD2	1:I:220:PRO:HA	2.52	0.44
1:I:51:SER:HB2	1:I:54:ASN:OD1	2.16	0.44
1:I:655:LYS:HA	1:I:658:CYS:HG	1.82	0.44
1:J:288:GLY:HA3	1:J:300:CYS:SG	2.57	0.44
1:K:497:GLN:HE22	1:L:654:LEU:HD21	1.81	0.44
1:K:561:GLU:O	1:K:565:ILE:HG13	2.17	0.44
1:K:44:LYS:HB3	1:K:93:LEU:HB3	1.99	0.44
1:L:26:PHE:HD2	1:L:47:ARG:HA	1.83	0.44
1:L:235:LYS:HA	1:L:282:TRP:CH2	2.53	0.44
1:L:393:VAL:HG13	1:L:609:SER:OG	2.18	0.44
1:A:417:GLN:HB3	1:A:581:SER:HB3	1.99	0.44
1:A:423:LEU:HA	1:A:426:VAL:CG2	2.43	0.44
1:B:149:ASN:O	1:B:164:ILE:HG22	2.18	0.44
1:B:423:LEU:O	1:B:427:TRP:HB2	2.16	0.44
1:B:48:LEU:O	1:B:50:LEU:HD12	2.17	0.44
1:C:117:LYS:HD3	1:C:117:LYS:HA	1.85	0.44
1:D:112:ASN:CB	1:D:116:LEU:HD23	2.48	0.44
1:D:209:THR:CG2	1:D:220:PRO:HG3	2.42	0.44
1:D:423:LEU:O	1:D:427:TRP:HB2	2.18	0.44
1:D:43:ILE:N	1:D:43:ILE:HD12	2.32	0.44
1:D:26:PHE:HD2	1:D:47:ARG:HA	1.83	0.44
1:D:560:LEU:HB3	1:D:593:THR:HG22	1.99	0.44
1:E:487:ILE:HG23	1:E:488:GLN:N	2.32	0.44
1:F:77:CYS:SG	1:F:94:ALA:HB3	2.58	0.44
1:G:563:ARG:HH12	4:G:706:GLC:H2	1.82	0.44
1:I:616:GLN:O	1:I:620:ASP:HB2	2.17	0.44
1:J:34:HIS:CE1	1:J:37:LEU:HD23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:404:SER:HB2	1:J:406:CYS:SG	2.57	0.44
1:J:424:ARG:HD3	1:J:572:LYS:HE2	1.99	0.44
1:J:616:GLN:O	1:J:620:ASP:HB2	2.18	0.44
1:K:396:GLY:HA2	1:K:398:PHE:CZ	2.52	0.44
1:L:541:ILE:CD1	1:L:618:ILE:HD11	2.48	0.44
1:A:219:ARG:HB2	1:A:219:ARG:HE	1.48	0.44
1:C:149:ASN:O	1:C:164:ILE:HG22	2.18	0.44
1:C:298:PRO:O	1:C:302:VAL:HG23	2.17	0.44
1:D:273:GLU:O	1:D:277:GLN:HG3	2.18	0.44
1:D:487:ILE:HG23	1:D:488:GLN:N	2.31	0.44
1:F:236:LYS:HB2	1:F:236:LYS:NZ	2.32	0.44
1:F:274:ASN:HA	1:F:277:GLN:NE2	2.33	0.44
1:H:561:GLU:O	1:H:565:ILE:HG13	2.17	0.44
1:H:84:ASN:CG	1:H:85:ILE:H	2.21	0.44
1:I:238:ASP:HB3	1:I:239:PRO:HD2	1.99	0.44
1:I:279:MET:C	1:I:280:LEU:HD12	2.38	0.44
1:I:283:ASP:OD1	1:I:285:GLN:HB2	2.18	0.44
1:I:613:GLY:O	1:I:617:LYS:HG3	2.17	0.44
1:J:43:ILE:HD12	1:J:43:ILE:N	2.32	0.44
1:J:473:SER:OG	1:J:524:VAL:HG13	2.18	0.44
1:J:621:LEU:O	1:J:625:VAL:HG23	2.18	0.44
1:K:653:LEU:HG	1:K:656:ILE:HD11	1.98	0.44
1:L:116:LEU:O	1:L:121:ILE:HD11	2.17	0.44
1:L:219:ARG:HB2	1:L:223:HIS:HB3	1.99	0.44
1:L:473:SER:HB3	1:L:632:ILE:HD13	1.98	0.44
1:L:633:LYS:HA	1:L:636:ASP:HB3	1.98	0.44
1:A:237:LYS:CD	1:A:241:CYS:HB3	2.48	0.44
1:A:283:ASP:HB3	1:A:286:GLN:HB3	2.00	0.44
1:A:507:MET:HB3	1:A:511:TRP:CD1	2.53	0.44
1:A:507:MET:CE	1:A:653:LEU:HD22	2.47	0.44
1:C:395:GLU:HG2	1:C:396:GLY:H	1.83	0.44
1:D:149:ASN:O	1:D:164:ILE:HG22	2.18	0.44
1:E:21:LEU:HD23	1:E:29:VAL:C	2.38	0.44
1:E:423:LEU:O	1:E:427:TRP:HB2	2.18	0.44
1:E:459:ASN:HD21	1:E:538:HIS:CD2	2.36	0.44
1:E:598:ASP:O	1:E:602:LYS:HG2	2.18	0.44
1:F:279:MET:C	1:F:280:LEU:HD12	2.38	0.44
1:F:320:SER:CA	1:F:398:PHE:HB3	2.47	0.44
1:F:328:LEU:HD21	1:F:337:LEU:HD22	2.00	0.44
1:F:393:VAL:HG13	1:F:609:SER:OG	2.18	0.44
1:F:26:PHE:HD2	1:F:47:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:LYS:HE2	1:G:117:LYS:N	2.33	0.44
1:G:185:LEU:HD21	1:G:188:LEU:CB	2.48	0.44
1:G:237:LYS:C	1:G:237:LYS:HD2	2.37	0.44
1:G:317:ASN:ND2	1:G:319:THR:HG23	2.33	0.44
1:G:469:LEU:HD11	1:G:628:ALA:HB3	1.99	0.44
1:G:615:LYS:O	1:G:619:ILE:HG13	2.17	0.44
1:G:633:LYS:HA	1:G:636:ASP:HB3	1.98	0.44
1:H:177:LEU:HD11	1:H:198:TYR:OH	2.18	0.44
1:H:186:GLN:HG2	1:H:219:ARG:NH1	2.33	0.44
1:H:238:ASP:HB3	1:H:239:PRO:CD	2.43	0.44
1:H:404:SER:HB2	1:H:406:CYS:SG	2.58	0.44
1:J:393:VAL:HG13	1:J:609:SER:OG	2.18	0.44
1:K:118:GLU:HA	1:K:121:ILE:HD12	2.00	0.44
1:K:74:VAL:HB	1:K:164:ILE:HG13	2.00	0.44
1:K:404:SER:HB2	1:K:406:CYS:SG	2.57	0.44
1:K:502:ILE:CG1	1:K:656:ILE:HD12	2.47	0.44
1:L:275:TRP:CH2	1:L:279:MET:HG3	2.52	0.44
1:L:485:LYS:HD3	1:L:485:LYS:O	2.18	0.44
1:L:53:LYS:HG3	1:L:54:ASN:OD1	2.18	0.44
1:L:598:ASP:O	1:L:602:LYS:HG2	2.16	0.44
1:L:613:GLY:O	1:L:617:LYS:HG3	2.18	0.44
1:A:231:HIS:O	1:A:235:LYS:N	2.51	0.44
1:A:27:GLY:O	1:A:45:SER:HB3	2.18	0.44
1:A:35:ARG:HG3	1:A:36:GLU:HG3	1.99	0.44
1:A:577:ASP:HB3	1:A:578:HIS:H	1.58	0.44
1:B:587:VAL:HA	1:B:590:ILE:HD12	2.00	0.44
1:C:116:LEU:O	1:C:121:ILE:HD11	2.18	0.44
1:C:220:PRO:O	1:C:243:PHE:HA	2.18	0.44
1:D:219:ARG:HB2	1:D:223:HIS:HA	1.99	0.44
1:D:452:MET:O	1:D:456:LEU:HG	2.18	0.44
1:D:560:LEU:O	1:D:563:ARG:HB2	2.17	0.44
1:E:404:SER:HB2	1:E:406:CYS:SG	2.58	0.44
1:F:190:PRO:HA	1:F:193:PHE:CD1	2.53	0.44
1:F:423:LEU:O	1:F:427:TRP:HB2	2.18	0.44
1:F:614:CYS:HA	1:F:617:LYS:HD3	2.00	0.44
1:G:234:ILE:HD11	1:G:282:TRP:CZ3	2.53	0.44
1:C:174:GLN:HG2	1:H:350:GLY:HA2	2.00	0.44
1:I:317:ASN:ND2	1:I:319:THR:HG23	2.32	0.44
1:J:236:LYS:HG3	1:J:236:LYS:H	1.63	0.44
1:J:88:HIS:CD2	1:J:90:VAL:HG22	2.53	0.44
1:K:27:GLY:O	1:K:45:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:PHE:HD2	1:K:47:ARG:HA	1.83	0.44
1:L:577:ASP:O	1:L:578:HIS:HB2	2.18	0.44
1:A:152:LEU:HD13	1:A:161:HIS:HA	1.99	0.43
1:A:43:ILE:N	1:A:43:ILE:HD12	2.32	0.43
1:B:251:GLU:HA	1:D:228:PHE:CD1	2.53	0.43
1:B:420:ILE:HG21	1:B:578:HIS:N	2.32	0.43
1:B:452:MET:O	1:B:456:LEU:HG	2.17	0.43
1:B:485:LYS:O	1:B:485:LYS:HD3	2.17	0.43
1:C:170:LYS:HD3	1:C:198:TYR:CZ	2.53	0.43
1:D:395:GLU:HG3	1:D:397:PRO:CD	2.38	0.43
1:D:487:ILE:HA	1:D:646:ARG:HD2	1.99	0.43
1:D:424:ARG:HD3	1:D:572:LYS:HE2	1.99	0.43
1:E:65:MET:SD	1:E:166:LEU:HD23	2.57	0.43
1:E:273:GLU:O	1:E:277:GLN:HG3	2.18	0.43
1:E:274:ASN:HA	1:E:277:GLN:NE2	2.32	0.43
1:F:84:ASN:HB3	1:F:85:ILE:H	1.68	0.43
1:G:274:ASN:HA	1:G:277:GLN:NE2	2.33	0.43
1:G:507:MET:HB3	1:G:511:TRP:CD1	2.53	0.43
1:G:95:MET:HE2	2:G:701:5TL:CAF	2.48	0.43
1:H:581:SER:O	1:H:582:ASP:HB2	2.17	0.43
1:I:166:LEU:HD22	1:I:166:LEU:N	2.33	0.43
1:I:265:CYS:SG	1:I:267:LEU:HB2	2.58	0.43
1:J:275:TRP:NE1	1:J:300:CYS:O	2.51	0.43
1:J:452:MET:O	1:J:456:LEU:HG	2.18	0.43
1:L:185:LEU:HD12	1:L:193:PHE:CZ	2.49	0.43
1:L:81:GLU:HG3	1:L:82:GLU:N	2.34	0.43
1:A:328:LEU:HD21	1:A:337:LEU:HD22	2.01	0.43
1:B:152:LEU:HD13	1:B:161:HIS:HA	1.99	0.43
1:C:265:CYS:SG	1:C:267:LEU:HB2	2.58	0.43
1:C:485:LYS:HD3	1:C:485:LYS:O	2.17	0.43
1:C:613:GLY:O	1:C:617:LYS:HG3	2.18	0.43
1:C:621:LEU:O	1:C:625:VAL:HG23	2.18	0.43
1:D:215:ILE:HG21	1:D:258:LEU:HD21	2.00	0.43
1:D:420:ILE:HD11	1:D:571:LEU:HG	1.98	0.43
1:D:6:ASP:N	1:D:7:PRO:CD	2.82	0.43
1:E:333:SER:HA	1:E:367:PRO:HB2	2.00	0.43
1:E:548:PRO:CB	1:E:552:ARG:HG3	2.49	0.43
1:E:560:LEU:O	1:E:563:ARG:HB2	2.17	0.43
1:E:655:LYS:HA	1:E:658:CYS:HG	1.83	0.43
1:F:143:ARG:CD	1:F:143:ARG:H	2.31	0.43
1:F:392:THR:HG22	1:F:616:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:VAL:CG2	1:G:163:ILE:HB	2.45	0.43
1:G:219:ARG:H	1:G:219:ARG:NE	2.16	0.43
1:G:26:PHE:HD2	1:G:47:ARG:HA	1.83	0.43
1:G:548:PRO:CB	1:G:552:ARG:HG3	2.48	0.43
1:I:592:HIS:CG	4:I:706:GLC:H4	2.53	0.43
1:J:149:ASN:O	1:J:164:ILE:HG22	2.18	0.43
1:K:187:TYR:CZ	1:K:219:ARG:HD2	2.53	0.43
1:K:334:LEU:HD22	1:K:366:LYS:O	2.18	0.43
1:L:143:ARG:CD	1:L:143:ARG:H	2.31	0.43
1:L:48:LEU:O	1:L:50:LEU:HD12	2.19	0.43
1:L:550:GLY:H	1:L:552:ARG:HG2	1.82	0.43
1:A:192:LEU:HD12	1:A:192:LEU:H	1.82	0.43
1:A:560:LEU:O	1:A:563:ARG:HB2	2.18	0.43
1:B:118:GLU:HB2	1:B:263:SER:O	2.18	0.43
1:B:323:ILE:HD12	1:B:323:ILE:N	2.33	0.43
1:B:328:LEU:HD21	1:B:337:LEU:HD22	2.00	0.43
1:B:560:LEU:O	1:B:563:ARG:HB2	2.17	0.43
1:A:227:PRO:CG	1:C:249:SER:HB2	2.48	0.43
1:C:293:LEU:HD22	1:C:293:LEU:N	2.33	0.43
1:D:621:LEU:O	1:D:625:VAL:HG23	2.18	0.43
1:E:192:LEU:N	1:E:192:LEU:HD12	2.33	0.43
1:E:324:ILE:HD12	1:E:324:ILE:N	2.33	0.43
1:E:80:PRO:HB2	1:E:81:GLU:OE2	2.18	0.43
1:F:317:ASN:ND2	1:F:319:THR:HG23	2.34	0.43
1:F:598:ASP:O	1:F:602:LYS:HG2	2.17	0.43
1:G:141:ILE:O	1:G:169:ALA:HB1	2.17	0.43
1:G:485:LYS:O	1:G:485:LYS:HD3	2.18	0.43
1:H:328:LEU:HD21	1:H:337:LEU:HD22	2.00	0.43
1:H:507:MET:HB3	1:H:511:TRP:CD1	2.53	0.43
1:H:78:ASP:HB3	1:H:79:VAL:H	1.59	0.43
1:I:190:PRO:HA	1:I:193:PHE:CD1	2.53	0.43
1:I:26:PHE:HD2	1:I:47:ARG:HA	1.83	0.43
1:I:8:GLU:HB2	1:I:86:LEU:HD12	2.00	0.43
1:J:423:LEU:O	1:J:427:TRP:HB2	2.18	0.43
1:J:487:ILE:HG23	1:J:488:GLN:N	2.32	0.43
1:L:452:MET:O	1:L:456:LEU:HG	2.18	0.43
1:A:192:LEU:N	1:A:192:LEU:HD12	2.33	0.43
1:A:258:LEU:HB2	1:A:273:GLU:HG2	2.00	0.43
1:A:424:ARG:NH1	1:A:572:LYS:HG2	2.33	0.43
1:A:455:LEU:HD13	1:A:615:LYS:CG	2.49	0.43
1:B:507:MET:HB3	1:B:511:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LEU:O	1:C:563:ARG:HB2	2.19	0.43
1:C:7:PRO:HG3	1:C:32:TYR:OH	2.17	0.43
1:B:248:MET:HB3	1:D:184:THR:HG22	2.00	0.43
1:E:396:GLY:H	1:E:397:PRO:CD	2.22	0.43
1:F:387:PHE:CZ	1:F:451:ALA:HB2	2.54	0.43
1:F:424:ARG:NH1	1:F:572:LYS:HG2	2.33	0.43
1:F:613:GLY:O	1:F:617:LYS:HG3	2.18	0.43
1:G:180:GLU:H	1:G:180:GLU:CD	2.21	0.43
1:G:473:SER:HB2	1:G:524:VAL:HG22	1.99	0.43
1:G:648:LYS:HE3	1:H:489:LEU:CD1	2.46	0.43
1:H:423:LEU:O	1:H:427:TRP:HB2	2.17	0.43
1:H:441:TYR:HE2	1:H:551:ARG:HA	1.83	0.43
1:I:273:GLU:O	1:I:277:GLN:HG3	2.18	0.43
1:K:324:ILE:N	1:K:324:ILE:HD12	2.33	0.43
1:L:149:ASN:O	1:L:164:ILE:HG22	2.19	0.43
1:B:411:VAL:HG23	1:B:412:GLN:N	2.34	0.43
1:C:223:HIS:C	1:C:225:LEU:H	2.22	0.43
1:C:239:PRO:O	1:C:240:LYS:HB2	2.17	0.43
1:C:324:ILE:N	1:C:324:ILE:HD12	2.32	0.43
1:C:74:VAL:HG22	1:C:95:MET:HB2	2.01	0.43
1:D:275:TRP:CH2	1:D:279:MET:HG3	2.53	0.43
1:D:317:ASN:ND2	1:D:319:THR:HG23	2.34	0.43
1:D:410:ILE:HD12	1:D:583:SER:OG	2.19	0.43
1:E:338:GLN:HA	1:E:341:ILE:HD12	2.01	0.43
1:E:35:ARG:HG3	1:E:36:GLU:HG3	2.01	0.43
1:E:502:ILE:HB	1:F:654:LEU:HD21	2.00	0.43
1:E:502:ILE:HD12	1:F:654:LEU:CD1	2.49	0.43
1:E:639:VAL:O	1:E:642:MET:HB2	2.19	0.43
1:E:109:LYS:HZ3	4:E:703:GLC:H4	1.84	0.43
1:F:283:ASP:OD2	1:F:286:GLN:HB2	2.19	0.43
1:F:401:ARG:NH2	1:F:440:ASP:HB2	2.33	0.43
1:E:489:LEU:HD11	1:F:648:LYS:HE3	2.01	0.43
1:F:74:VAL:HG11	1:F:164:ILE:HD12	1.99	0.43
1:G:27:GLY:O	1:G:45:SER:HB3	2.19	0.43
1:G:35:ARG:HG3	1:G:36:GLU:HG3	2.00	0.43
1:G:37:LEU:HB3	1:G:38:ASP:H	1.65	0.43
1:G:430:ALA:O	1:G:434:VAL:HG23	2.17	0.43
1:G:95:MET:CE	1:G:164:ILE:HD11	2.48	0.43
1:H:7:PRO:HD2	1:H:17:MET:SD	2.58	0.43
1:I:515:GLU:O	1:I:519:ILE:HG13	2.19	0.43
1:J:275:TRP:CH2	1:J:279:MET:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:541:ILE:HD11	1:J:618:ILE:HD11	2.00	0.43
1:J:613:GLY:O	1:J:617:LYS:HG3	2.19	0.43
1:K:141:ILE:HG23	1:K:170:LYS:HB2	2.00	0.43
1:L:487:ILE:HG23	1:L:488:GLN:N	2.33	0.43
1:L:515:GLU:O	1:L:519:ILE:HG13	2.18	0.43
1:A:324:ILE:N	1:A:324:ILE:HD12	2.30	0.43
1:A:411:VAL:HG23	1:A:412:GLN:N	2.33	0.43
1:A:423:LEU:O	1:A:427:TRP:HB2	2.19	0.43
1:B:462:LEU:HD22	1:B:618:ILE:HG23	2.00	0.43
1:D:152:LEU:HD13	1:D:161:HIS:HA	2.00	0.43
1:D:281:ASN:H	1:D:287:ARG:HH12	1.65	0.43
1:D:485:LYS:HD3	1:D:485:LYS:O	2.18	0.43
1:F:222:LEU:HD12	1:F:244:ALA:O	2.18	0.43
1:H:324:ILE:N	1:H:324:ILE:HD12	2.32	0.43
1:H:48:LEU:O	1:H:50:LEU:HD12	2.17	0.43
1:H:621:LEU:O	1:H:625:VAL:HG23	2.19	0.43
1:H:49:GLU:HA	1:H:88:HIS:HB2	2.01	0.43
1:I:191:GLU:CD	1:I:284:PRO:HB3	2.38	0.43
1:I:281:ASN:ND2	1:I:286:GLN:HB2	2.33	0.43
1:I:75:LYS:HD2	1:I:76:ALA:H	1.83	0.43
1:J:587:VAL:HA	1:J:590:ILE:HD12	2.00	0.43
1:J:83:LEU:HD12	1:J:92:LEU:HD13	2.00	0.43
1:K:560:LEU:O	1:K:563:ARG:HB2	2.18	0.43
1:K:598:ASP:O	1:K:602:LYS:HG2	2.19	0.43
1:L:227:PRO:HA	1:L:230:TRP:CB	2.41	0.43
1:L:190:PRO:HB3	1:L:231:HIS:CD2	2.53	0.43
1:B:147:PRO:C	1:B:149:ASN:H	2.22	0.43
1:B:333:SER:HA	1:B:368:ALA:H	1.84	0.43
1:B:26:PHE:HD2	1:B:47:ARG:HA	1.83	0.43
1:C:328:LEU:HD21	1:C:337:LEU:HD22	2.01	0.43
1:C:359:GLY:HA3	1:C:453:LEU:HB2	2.01	0.43
1:C:543:GLU:O	1:C:546:LYS:HD3	2.19	0.43
1:C:640:MET:HE1	1:D:485:LYS:HG2	2.00	0.43
1:D:117:LYS:O	1:D:121:ILE:HG13	2.19	0.43
1:D:142:HIS:HA	1:D:169:ALA:HB1	1.99	0.43
1:D:190:PRO:HA	1:D:193:PHE:CD1	2.54	0.43
1:C:648:LYS:HE3	1:D:489:LEU:HD11	2.01	0.43
1:E:473:SER:OG	1:E:524:VAL:HG13	2.19	0.43
1:F:515:GLU:O	1:F:519:ILE:HG13	2.19	0.43
1:F:71:ALA:C	1:F:73:VAL:N	2.72	0.43
1:G:324:ILE:N	1:G:324:ILE:HD12	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:GLU:HA	1:I:121:ILE:HD12	2.01	0.43
1:I:223:HIS:O	1:I:224:HIS:HB3	2.18	0.43
1:I:323:ILE:HD12	1:I:323:ILE:N	2.33	0.43
1:I:395:GLU:CG	1:I:396:GLY:H	2.30	0.43
1:J:116:LEU:CD1	1:J:116:LEU:H	2.31	0.43
1:J:27:GLY:O	1:J:45:SER:HB3	2.19	0.43
1:I:227:PRO:CG	1:K:249:SER:HB2	2.48	0.43
1:K:487:ILE:HG23	1:K:488:GLN:N	2.33	0.43
1:L:190:PRO:HA	1:L:193:PHE:CD1	2.54	0.43
1:H:227:PRO:CG	1:L:249:SER:HB2	2.48	0.43
1:L:408:ASN:HA	1:L:411:VAL:HG22	1.99	0.43
1:L:614:CYS:HA	1:L:617:LYS:HD3	2.01	0.43
1:A:147:PRO:C	1:A:149:ASN:H	2.22	0.43
1:A:234:ILE:HA	1:A:236:LYS:NZ	2.33	0.43
1:A:237:LYS:HD2	1:A:241:CYS:HB3	2.00	0.43
1:A:403:LEU:HD12	1:A:407:VAL:HG12	2.01	0.43
1:A:427:TRP:CZ3	1:A:567:LEU:HB3	2.53	0.43
1:A:57:ARG:O	1:A:60:HIS:HB3	2.18	0.43
1:A:560:LEU:HB3	1:A:593:THR:HG22	2.01	0.43
1:B:586:MET:O	1:B:590:ILE:HG13	2.18	0.43
1:C:236:LYS:O	1:C:237:LYS:O	2.35	0.43
1:D:244:ALA:HA	1:D:253:ARG:O	2.19	0.43
1:D:34:HIS:CE1	1:D:37:LEU:HD23	2.54	0.43
1:E:219:ARG:HE	1:E:219:ARG:HB2	1.66	0.43
1:E:445:PHE:HA	1:E:604:LEU:HD21	2.01	0.43
1:E:26:PHE:HD2	1:E:47:ARG:HA	1.84	0.43
1:G:114:CYS:HB2	1:G:432:HIS:CD2	2.54	0.43
1:I:231:HIS:N	1:I:231:HIS:ND1	2.66	0.43
1:I:489:LEU:HD22	1:J:647:GLN:OE1	2.19	0.43
1:I:427:TRP:HZ2	1:I:583:SER:HA	1.84	0.43
1:J:10:GLY:C	1:J:12:GLY:H	2.22	0.43
1:J:152:LEU:HD13	1:J:161:HIS:HA	2.00	0.43
1:K:410:ILE:O	1:K:587:VAL:HG22	2.18	0.43
1:B:274:ASN:HA	1:B:277:GLN:NE2	2.34	0.43
1:B:334:LEU:HD11	1:B:364:PRO:HA	2.01	0.43
1:A:655:LYS:HE2	1:B:501:GLY:HA3	2.01	0.43
1:B:473:SER:CB	1:B:527:ILE:HD11	2.49	0.43
1:C:152:LEU:HD13	1:C:161:HIS:HA	2.00	0.43
1:C:507:MET:HB3	1:C:511:TRP:CD1	2.53	0.43
1:D:186:GLN:NE2	1:D:219:ARG:HG2	2.34	0.43
1:D:35:ARG:HG3	1:D:36:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:THR:HG22	1:D:616:GLN:HE22	1.82	0.43
1:D:8:GLU:OE2	1:D:87:ILE:HG23	2.19	0.43
1:F:621:LEU:O	1:F:625:VAL:HG23	2.18	0.43
1:G:613:GLY:O	1:G:617:LYS:HG3	2.19	0.43
1:H:147:PRO:C	1:H:149:ASN:H	2.22	0.43
1:H:392:THR:HG22	1:H:616:GLN:HE22	1.84	0.43
1:I:228:PHE:HA	1:K:251:GLU:OE2	2.19	0.43
1:I:415:LYS:HA	1:I:584:THR:HB	2.01	0.43
1:J:204:TYR:HA	1:J:279:MET:HE1	2.01	0.43
1:K:224:HIS:C	1:K:225:LEU:HD22	2.39	0.43
1:K:57:ARG:O	1:K:60:HIS:HB3	2.19	0.43
1:L:275:TRP:CZ2	1:L:304:MET:HE2	2.53	0.43
1:L:34:HIS:CE1	1:L:37:LEU:HD23	2.54	0.43
1:L:507:MET:HB3	1:L:511:TRP:CD1	2.53	0.43
1:A:270:GLU:N	1:A:271:PRO:HD2	2.34	0.43
1:A:613:GLY:O	1:A:617:LYS:HG3	2.19	0.43
1:B:515:GLU:O	1:B:519:ILE:HG13	2.19	0.43
1:C:273:GLU:O	1:C:277:GLN:HG3	2.18	0.43
1:C:35:ARG:HG3	1:C:36:GLU:HG3	2.00	0.43
1:C:515:GLU:O	1:C:519:ILE:HG13	2.19	0.43
1:C:581:SER:O	1:C:582:ASP:HB2	2.19	0.43
1:C:614:CYS:HA	1:C:617:LYS:HD3	2.00	0.43
1:D:27:GLY:O	1:D:45:SER:HB3	2.19	0.43
1:D:473:SER:CB	1:D:527:ILE:HD11	2.49	0.43
1:E:201:THR:O	1:E:287:ARG:NH1	2.52	0.43
1:E:27:GLY:O	1:E:45:SER:HB3	2.18	0.43
1:E:289:GLY:O	1:E:291:VAL:N	2.52	0.43
1:E:90:VAL:HG13	1:E:91:PRO:HD2	2.00	0.43
1:F:315:ILE:CD1	1:F:384:VAL:HB	2.49	0.43
1:F:589:ILE:O	1:F:593:THR:HG23	2.18	0.43
1:E:497:GLN:OE1	1:F:655:LYS:HE3	2.18	0.43
1:G:480:LEU:CD2	1:G:518:ALA:HB1	2.49	0.43
1:H:240:LYS:O	1:H:277:GLN:HG2	2.19	0.43
1:H:412:GLN:OE1	1:J:20:ARG:HB3	2.19	0.43
1:H:613:GLY:O	1:H:617:LYS:HG3	2.19	0.43
1:I:143:ARG:HD3	1:I:143:ARG:H	1.84	0.43
1:I:328:LEU:HD21	1:I:337:LEU:HD22	2.01	0.43
1:I:86:LEU:N	1:I:86:LEU:HD22	2.34	0.43
1:J:244:ALA:HA	1:J:253:ARG:O	2.18	0.43
1:J:589:ILE:O	1:J:593:THR:HG23	2.18	0.43
1:K:95:MET:CE	1:K:164:ILE:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:ALA:HA	1:L:253:ARG:O	2.19	0.43
1:L:317:ASN:ND2	1:L:319:THR:HG23	2.34	0.43
1:L:420:ILE:HG21	1:L:578:HIS:N	2.34	0.43
1:A:95:MET:CE	1:A:164:ILE:HD11	2.49	0.42
1:A:574:ARG:O	1:A:576:SER:N	2.52	0.42
1:B:118:GLU:HA	1:B:121:ILE:HD12	2.00	0.42
1:B:180:GLU:HB3	1:B:181:PHE:H	1.68	0.42
1:C:655:LYS:HA	1:C:658:CYS:HG	1.83	0.42
1:E:236:LYS:NZ	1:E:236:LYS:HB2	2.33	0.42
1:F:86:LEU:C	1:F:87:ILE:HD12	2.38	0.42
1:G:515:GLU:O	1:G:519:ILE:HG13	2.19	0.42
1:G:57:ARG:O	1:G:60:HIS:HB3	2.19	0.42
1:G:79:VAL:HG11	1:G:83:LEU:HD23	2.00	0.42
1:H:106:LEU:HD11	1:H:152:LEU:HG	2.01	0.42
1:H:395:GLU:H	1:H:395:GLU:CD	2.22	0.42
1:H:515:GLU:O	1:H:519:ILE:HG13	2.19	0.42
1:H:548:PRO:HB2	1:H:552:ARG:HG3	2.01	0.42
1:J:143:ARG:H	1:J:143:ARG:CD	2.32	0.42
1:K:507:MET:HB3	1:K:511:TRP:CD1	2.54	0.42
1:K:515:GLU:O	1:K:519:ILE:HG13	2.19	0.42
1:L:328:LEU:HD21	1:L:337:LEU:HD22	2.01	0.42
1:A:46:CYS:SG	1:A:90:VAL:HB	2.59	0.42
1:B:190:PRO:HA	1:B:193:PHE:CD1	2.54	0.42
1:C:533:GLN:HE21	1:C:621:LEU:HD21	1.84	0.42
1:D:212:PHE:CE2	1:D:220:PRO:HA	2.54	0.42
1:E:48:LEU:HB2	1:E:49:GLU:H	1.64	0.42
1:E:507:MET:HB3	1:E:511:TRP:CD1	2.53	0.42
1:F:502:ILE:HD13	1:F:656:ILE:HD12	2.01	0.42
1:F:83:LEU:HB3	1:F:84:ASN:H	1.70	0.42
1:G:258:LEU:HB2	1:G:273:GLU:HG2	2.01	0.42
1:G:240:LYS:O	1:G:277:GLN:HG2	2.19	0.42
1:G:473:SER:HA	1:G:632:ILE:CG2	2.49	0.42
1:G:507:MET:HA	1:G:510:ALA:HB3	2.01	0.42
1:G:658:CYS:SG	1:H:502:ILE:HG13	2.59	0.42
1:H:199:THR:OG1	1:H:284:PRO:HB2	2.18	0.42
1:H:215:ILE:HG21	1:H:258:LEU:HD21	2.00	0.42
1:H:229:THR:C	1:H:231:HIS:H	2.22	0.42
1:H:622:LEU:N	1:H:623:PRO:CD	2.82	0.42
1:I:220:PRO:HG2	1:I:221:PHE:CD2	2.54	0.42
1:G:184:THR:H	1:I:248:MET:HB2	1.83	0.42
1:I:27:GLY:O	1:I:45:SER:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:GLU:HA	1:J:121:ILE:HD12	2.01	0.42
1:J:236:LYS:HD3	1:J:237:LYS:H	1.84	0.42
1:J:410:ILE:HG23	1:J:583:SER:HG	1.83	0.42
1:K:463:THR:HA	1:K:534:ILE:HD11	1.99	0.42
1:K:560:LEU:HB3	1:K:593:THR:HG22	2.01	0.42
1:A:338:GLN:HA	1:A:341:ILE:HD12	2.02	0.42
1:A:485:LYS:HD3	1:A:485:LYS:O	2.19	0.42
1:A:53:LYS:HG3	1:A:54:ASN:OD1	2.19	0.42
1:B:265:CYS:SG	1:B:267:LEU:HB2	2.60	0.42
1:B:473:SER:OG	1:B:524:VAL:HG13	2.18	0.42
1:B:561:GLU:O	1:B:565:ILE:HG13	2.19	0.42
1:B:621:LEU:O	1:B:625:VAL:HG23	2.19	0.42
1:C:190:PRO:HA	1:C:193:PHE:CD1	2.53	0.42
1:C:401:ARG:H	1:C:401:ARG:HG2	1.72	0.42
1:C:561:GLU:O	1:C:565:ILE:HG13	2.19	0.42
1:C:576:SER:OG	1:E:580:TYR:HB2	2.19	0.42
1:C:596:SER:O	1:C:600:VAL:HG22	2.19	0.42
1:C:449:ARG:HH22	10:C:709:Z4K:C6	2.32	0.42
1:D:287:ARG:HG3	1:D:287:ARG:HH11	1.84	0.42
1:D:473:SER:OG	1:D:524:VAL:HG13	2.18	0.42
1:D:79:VAL:HG21	1:D:83:LEU:CD1	2.49	0.42
1:E:275:TRP:CH2	1:E:279:MET:HG3	2.54	0.42
1:F:170:LYS:HA	1:F:177:LEU:HA	2.00	0.42
1:G:147:PRO:HB2	1:G:148:GLU:OE2	2.20	0.42
1:G:270:GLU:N	1:G:271:PRO:HD2	2.35	0.42
1:G:396:GLY:HA2	1:G:398:PHE:CE2	2.54	0.42
1:G:511:TRP:CZ3	1:G:646:ARG:HA	2.54	0.42
1:H:152:LEU:HD13	1:H:161:HIS:HA	2.00	0.42
1:H:244:ALA:HA	1:H:253:ARG:O	2.20	0.42
1:H:485:LYS:HD3	1:H:485:LYS:O	2.18	0.42
1:I:507:MET:HB3	1:I:511:TRP:CD1	2.53	0.42
1:I:549:TYR:H	1:I:552:ARG:HD2	1.85	0.42
1:J:26:PHE:HD2	1:J:47:ARG:HA	1.85	0.42
1:J:410:ILE:O	1:J:587:VAL:HG22	2.19	0.42
1:K:53:LYS:HG3	1:K:54:ASN:OD1	2.19	0.42
1:K:29:VAL:HG21	2:K:701:5TL:CAE	2.50	0.42
1:L:118:GLU:HB2	1:L:263:SER:O	2.19	0.42
1:J:403:LEU:HD23	1:L:26:PHE:HE1	1.84	0.42
1:L:550:GLY:HA3	1:L:604:LEU:HD13	2.01	0.42
1:L:561:GLU:O	1:L:565:ILE:HG13	2.19	0.42
1:L:77:CYS:HB3	1:L:94:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HB3	1:A:38:ASP:H	1.65	0.42
1:A:420:ILE:HG21	1:A:578:HIS:N	2.34	0.42
1:B:237:LYS:HE3	1:B:281:ASN:HA	2.02	0.42
1:B:35:ARG:HG3	1:B:36:GLU:HG3	2.00	0.42
1:B:387:PHE:HD1	1:B:394:TYR:OH	2.01	0.42
1:B:396:GLY:N	1:B:397:PRO:CD	2.80	0.42
1:E:614:CYS:O	1:E:618:ILE:HG13	2.19	0.42
1:F:35:ARG:HG3	1:F:36:GLU:HG3	2.00	0.42
1:F:53:LYS:HG3	1:F:54:ASN:OD1	2.20	0.42
1:E:489:LEU:HD13	1:F:643:GLN:CG	2.50	0.42
1:G:411:VAL:HG23	1:G:412:GLN:N	2.34	0.42
1:G:504:SER:OG	1:G:653:LEU:HD21	2.18	0.42
1:C:174:GLN:CG	1:H:350:GLY:HA2	2.49	0.42
1:J:235:LYS:HA	1:J:282:TRP:CH2	2.54	0.42
1:J:28:ASN:HB2	1:J:29:VAL:H	1.67	0.42
1:J:313:VAL:HG11	1:J:371:CYS:SG	2.59	0.42
1:J:6:ASP:HB3	1:J:7:PRO:HD2	2.00	0.42
1:K:274:ASN:O	1:K:277:GLN:HB2	2.19	0.42
1:B:70:HIS:HB2	1:B:134:TYR:CD2	2.54	0.42
1:B:21:LEU:HD23	1:B:29:VAL:C	2.39	0.42
1:B:244:ALA:HA	1:B:253:ARG:O	2.20	0.42
1:B:473:SER:HB3	1:B:527:ILE:HD11	2.01	0.42
1:B:53:LYS:HG3	1:B:54:ASN:OD1	2.20	0.42
1:B:412:GLN:HB3	1:D:21:LEU:O	2.20	0.42
1:D:393:VAL:HG22	1:D:609:SER:HB3	2.02	0.42
1:D:613:GLY:O	1:D:617:LYS:HG3	2.20	0.42
1:E:118:GLU:HB2	1:E:263:SER:O	2.20	0.42
1:E:411:VAL:HG23	1:E:412:GLN:N	2.35	0.42
1:F:485:LYS:HD3	1:F:485:LYS:O	2.19	0.42
1:G:118:GLU:HB2	1:G:263:SER:O	2.20	0.42
1:G:222:LEU:HD22	1:G:230:TRP:HA	2.01	0.42
1:G:219:ARG:HH12	1:G:224:HIS:CA	2.33	0.42
1:H:265:CYS:SG	1:H:267:LEU:HB2	2.60	0.42
1:I:149:ASN:O	1:I:164:ILE:HG22	2.20	0.42
1:I:98:CYS:HB3	1:I:152:LEU:O	2.20	0.42
1:I:376:VAL:O	1:I:377:ARG:HG2	2.19	0.42
1:I:589:ILE:O	1:I:593:THR:HG23	2.20	0.42
1:J:507:MET:HB3	1:J:511:TRP:CD1	2.54	0.42
1:K:270:GLU:N	1:K:271:PRO:HD2	2.35	0.42
1:K:613:GLY:O	1:K:617:LYS:HG3	2.20	0.42
1:K:68:LEU:HD21	1:K:140:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:HA	1:C:251:GLU:OE2	2.19	0.42
1:A:26:PHE:HD2	1:A:47:ARG:HA	1.83	0.42
1:B:410:ILE:HD12	1:B:583:SER:OG	2.19	0.42
1:B:415:LYS:HD3	1:B:584:THR:CG2	2.50	0.42
1:C:318:MET:CE	1:C:447:GLY:HA3	2.50	0.42
1:D:363:ASP:N	1:D:364:PRO:HD3	2.34	0.42
1:D:319:THR:HG22	1:D:394:TYR:CE1	2.55	0.42
1:D:411:VAL:CG1	1:D:590:ILE:HG21	2.49	0.42
1:D:57:ARG:O	1:D:60:HIS:HB3	2.20	0.42
1:E:270:GLU:N	1:E:271:PRO:HD2	2.35	0.42
1:E:268:ILE:C	1:E:271:PRO:HD2	2.39	0.42
1:F:34:HIS:CE1	1:F:37:LEU:HD23	2.55	0.42
1:F:355:LEU:HD12	1:F:355:LEU:N	2.35	0.42
1:F:48:LEU:O	1:F:50:LEU:HD12	2.20	0.42
1:F:507:MET:HB3	1:F:511:TRP:CD1	2.54	0.42
1:F:560:LEU:O	1:F:563:ARG:HB2	2.18	0.42
1:G:152:LEU:HD13	1:G:161:HIS:HA	2.00	0.42
1:G:275:TRP:CH2	1:G:279:MET:HG3	2.55	0.42
1:I:281:ASN:HD22	1:I:286:GLN:HB2	1.84	0.42
1:I:514:MET:HA	1:I:642:MET:HE1	2.00	0.42
1:I:639:VAL:O	1:I:642:MET:HB2	2.19	0.42
1:I:50:LEU:HD22	1:I:90:VAL:HG11	2.01	0.42
1:J:514:MET:HA	1:J:642:MET:HE1	2.01	0.42
1:J:14:PRO:HG2	1:J:82:GLU:OE1	2.19	0.42
1:I:578:HIS:HB2	1:K:579:SER:HB2	2.01	0.42
1:K:655:LYS:HA	1:K:658:CYS:HG	1.84	0.42
1:L:560:LEU:O	1:L:563:ARG:HB2	2.18	0.42
1:L:621:LEU:O	1:L:625:VAL:HG23	2.19	0.42
1:L:68:LEU:HD21	1:L:140:ILE:HD12	2.01	0.42
1:A:655:LYS:N	1:A:655:LYS:HD2	2.35	0.42
1:B:549:TYR:H	1:B:552:ARG:HD2	1.85	0.42
1:B:614:CYS:O	1:B:618:ILE:HG13	2.19	0.42
1:C:497:GLN:C	1:C:499:THR:H	2.22	0.42
1:E:328:LEU:HD21	1:E:337:LEU:HD22	2.01	0.42
1:E:395:GLU:HG3	1:E:396:GLY:H	1.85	0.42
1:E:515:GLU:O	1:E:519:ILE:HG13	2.20	0.42
1:F:424:ARG:HH11	1:F:572:LYS:HG2	1.85	0.42
1:G:265:CYS:SG	1:G:267:LEU:HB2	2.60	0.42
1:G:588:LYS:HB3	1:G:589:ILE:HD12	2.01	0.42
1:H:238:ASP:CB	1:H:239:PRO:HD2	2.40	0.42
1:H:28:ASN:HB2	1:H:29:VAL:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:ARG:HG3	1:I:36:GLU:HG3	2.00	0.42
1:I:485:LYS:HD3	1:I:485:LYS:O	2.19	0.42
1:I:614:CYS:HA	1:I:617:LYS:HD3	2.01	0.42
1:J:485:LYS:O	1:J:485:LYS:HD3	2.19	0.42
1:J:57:ARG:O	1:J:60:HIS:HB3	2.20	0.42
1:K:152:LEU:HD13	1:K:161:HIS:HA	2.01	0.42
1:L:547:SER:HB2	1:L:548:PRO:HD2	2.01	0.42
1:L:392:THR:HG22	1:L:616:GLN:HE22	1.84	0.42
1:L:83:LEU:O	1:L:92:LEU:HD13	2.20	0.42
1:A:412:GLN:NE2	1:E:27:GLY:HA2	2.35	0.42
1:A:549:TYR:HB2	1:A:552:ARG:NE	2.35	0.42
1:A:630:SER:O	1:A:634:GLU:HB2	2.20	0.42
1:B:230:TRP:O	1:B:234:ILE:HD13	2.19	0.42
1:B:535:MET:HA	1:B:538:HIS:HB3	2.02	0.42
1:C:191:GLU:OE2	1:C:284:PRO:HB3	2.20	0.42
1:C:27:GLY:O	1:C:45:SER:HB3	2.19	0.42
1:C:403:LEU:HD12	1:C:407:VAL:HG12	2.02	0.42
1:C:449:ARG:HH22	10:C:709:Z4K:C5	2.32	0.42
1:F:324:ILE:N	1:F:324:ILE:HD12	2.32	0.42
1:F:561:GLU:O	1:F:565:ILE:HG13	2.19	0.42
1:G:107:LEU:HD23	1:G:116:LEU:HD11	2.02	0.42
1:G:338:GLN:HA	1:G:341:ILE:HD12	2.02	0.42
1:G:614:CYS:HA	1:G:617:LYS:HD3	2.01	0.42
1:H:396:GLY:N	1:H:397:PRO:CD	2.82	0.42
1:I:223:HIS:C	1:I:225:LEU:H	2.22	0.42
1:I:411:VAL:HG23	1:I:412:GLN:N	2.35	0.42
1:J:237:LYS:HE3	1:J:282:TRP:HB2	2.02	0.42
1:J:317:ASN:ND2	1:J:319:THR:HG23	2.35	0.42
1:J:35:ARG:HG3	1:J:36:GLU:HG3	2.01	0.42
1:J:53:LYS:HG3	1:J:54:ASN:OD1	2.19	0.42
1:K:279:MET:O	1:K:287:ARG:HD2	2.20	0.42
1:L:596:SER:O	1:L:600:VAL:HG22	2.20	0.42
1:A:125:LEU:HD23	1:A:207:PHE:CZ	2.54	0.42
1:A:86:LEU:HB3	1:A:87:ILE:H	1.60	0.42
1:B:240:LYS:H	1:B:240:LYS:NZ	2.18	0.42
1:B:28:ASN:HB2	1:B:29:VAL:H	1.68	0.42
1:B:420:ILE:HG21	1:B:578:HIS:H	1.85	0.42
1:B:639:VAL:O	1:B:642:MET:HB2	2.20	0.42
1:C:653:LEU:CD1	1:C:656:ILE:HD11	2.50	0.42
1:D:142:HIS:HA	1:D:169:ALA:CB	2.50	0.42
1:D:319:THR:HG22	1:D:394:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:HG3	1:D:90:VAL:HG13	2.02	0.42
1:E:403:LEU:HD12	1:E:407:VAL:HG12	2.02	0.42
1:F:342:GLU:HB2	1:F:352:GLN:HE22	1.85	0.42
1:F:363:ASP:HB3	1:F:370:GLN:NE2	2.34	0.42
1:F:411:VAL:HG23	1:F:412:GLN:N	2.35	0.42
1:F:567:LEU:CD2	1:F:589:ILE:HD13	2.50	0.42
1:G:219:ARG:NH1	1:G:224:HIS:N	2.66	0.42
1:H:186:GLN:HG2	1:H:219:ARG:HH11	1.85	0.42
1:H:452:MET:O	1:H:456:LEU:HG	2.19	0.42
1:K:167:GLY:O	1:K:178:CYS:HB3	2.20	0.42
1:K:221:PHE:O	1:K:223:HIS:N	2.53	0.42
1:K:244:ALA:HA	1:K:253:ARG:O	2.20	0.42
1:K:275:TRP:CH2	1:K:279:MET:HG3	2.55	0.42
1:L:313:VAL:HG11	1:L:371:CYS:SG	2.60	0.42
1:L:411:VAL:HG23	1:L:412:GLN:N	2.34	0.42
1:L:639:VAL:O	1:L:642:MET:HB2	2.19	0.42
1:B:223:HIS:O	1:B:225:LEU:HD23	2.19	0.42
1:B:415:LYS:CA	1:B:584:THR:HB	2.44	0.42
1:C:477:LYS:HE3	1:C:524:VAL:CG1	2.46	0.42
1:C:507:MET:HA	1:C:510:ALA:HB3	2.02	0.42
1:C:643:GLN:HG3	1:D:489:LEU:HD13	2.01	0.42
1:D:507:MET:HB3	1:D:511:TRP:CD1	2.54	0.42
1:D:541:ILE:HD11	1:D:618:ILE:HD11	2.00	0.42
1:E:13:GLY:H	1:E:14:PRO:CD	2.24	0.42
1:E:13:GLY:N	1:E:14:PRO:HD3	2.21	0.42
1:E:34:HIS:ND1	1:E:37:LEU:HB2	2.35	0.42
1:E:401:ARG:HH22	1:E:440:ASP:CB	2.32	0.42
1:E:485:LYS:O	1:E:485:LYS:HD3	2.20	0.42
1:E:536:SER:O	1:E:540:GLU:HB2	2.20	0.42
1:F:401:ARG:HB2	1:F:433:TYR:HE1	1.83	0.42
1:G:268:ILE:O	1:G:272:MET:HB2	2.20	0.42
1:H:411:VAL:HG23	1:H:412:GLN:N	2.35	0.42
1:G:651:TRP:HZ2	1:H:490:ASP:HB3	1.83	0.42
1:H:589:ILE:O	1:H:593:THR:HG23	2.20	0.42
1:I:186:GLN:OE1	1:I:227:PRO:HD3	2.19	0.42
1:I:473:SER:HB3	1:I:632:ILE:HD13	2.01	0.42
1:K:13:GLY:N	1:K:14:PRO:CD	2.80	0.42
1:K:48:LEU:HB2	1:K:49:GLU:H	1.64	0.42
1:K:630:SER:O	1:K:634:GLU:HB2	2.20	0.42
1:L:404:SER:HB2	1:L:406:CYS:SG	2.60	0.42
1:A:151:VAL:C	1:A:152:LEU:HD22	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HD12	1:B:407:VAL:HG12	2.02	0.41
1:B:458:TYR:HB3	1:B:618:ILE:HG21	2.02	0.41
1:C:560:LEU:HB3	1:C:593:THR:HG22	2.01	0.41
1:D:417:GLN:HB3	1:D:581:SER:CB	2.48	0.41
1:D:95:MET:CE	1:D:164:ILE:HD11	2.50	0.41
1:E:139:LYS:HD2	1:E:172:VAL:CG1	2.50	0.41
1:E:316:LEU:HB2	1:E:383:MET:HE1	2.01	0.41
1:E:73:VAL:HG22	1:E:74:VAL:N	2.35	0.41
1:F:37:LEU:HB3	1:F:38:ASP:H	1.67	0.41
1:G:215:ILE:HD13	1:G:264:LEU:HD11	2.01	0.41
1:G:219:ARG:H	1:G:219:ARG:HE	1.68	0.41
1:G:401:ARG:HH22	1:G:437:LEU:N	2.18	0.41
1:H:118:GLU:HA	1:H:121:ILE:HD12	2.01	0.41
1:C:63:GLN:NE2	1:H:349:THR:OG1	2.52	0.41
1:H:560:LEU:HB3	1:H:593:THR:HG22	2.02	0.41
1:I:482:PHE:HD2	1:J:482:PHE:HD2	1.67	0.41
1:I:561:GLU:O	1:I:565:ILE:HG13	2.19	0.41
1:I:57:ARG:O	1:I:60:HIS:HB3	2.20	0.41
1:J:630:SER:O	1:J:634:GLU:HB2	2.20	0.41
1:K:411:VAL:HG23	1:K:412:GLN:N	2.35	0.41
1:L:9:PHE:CZ	1:L:82:GLU:HB2	2.55	0.41
1:A:185:LEU:HD21	1:A:188:LEU:CD2	2.51	0.41
1:A:25:GLY:HA3	1:A:47:ARG:NH1	2.35	0.41
1:A:34:HIS:CE1	1:A:37:LEU:HD23	2.55	0.41
1:A:411:VAL:HG12	1:A:590:ILE:HG21	2.03	0.41
1:B:171:ASP:HB3	1:B:173:ASP:OD1	2.20	0.41
1:B:270:GLU:N	1:B:271:PRO:HD2	2.36	0.41
1:B:396:GLY:C	1:B:398:PHE:H	2.22	0.41
1:B:480:LEU:HD22	1:B:518:ALA:HB1	2.02	0.41
1:C:411:VAL:HG23	1:C:412:GLN:N	2.35	0.41
1:C:7:PRO:HB2	1:C:86:LEU:CD1	2.50	0.41
1:D:118:GLU:HA	1:D:121:ILE:HD12	2.02	0.41
1:D:403:LEU:N	1:D:403:LEU:HD23	2.34	0.41
1:D:403:LEU:HD12	1:D:407:VAL:HG12	2.02	0.41
1:D:473:SER:HB3	1:D:527:ILE:HD11	2.01	0.41
1:E:410:ILE:O	1:E:587:VAL:HG22	2.20	0.41
1:E:53:LYS:HG3	1:E:54:ASN:OD1	2.20	0.41
1:E:452:MET:SD	1:E:611:LEU:HD22	2.61	0.41
1:F:149:ASN:O	1:F:164:ILE:HG22	2.20	0.41
1:F:295:LEU:HD12	1:F:295:LEU:N	2.34	0.41
1:E:478:ALA:HB2	1:F:475:GLN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:LEU:HD11	1:G:408:ASN:HA	2.03	0.41
1:G:53:LYS:HG3	1:G:54:ASN:OD1	2.20	0.41
1:G:622:LEU:N	1:G:623:PRO:CD	2.83	0.41
1:H:170:LYS:HD3	1:H:198:TYR:CZ	2.55	0.41
1:H:614:CYS:HA	1:H:617:LYS:HD3	2.02	0.41
1:I:507:MET:HA	1:I:510:ALA:HB3	2.03	0.41
1:I:563:ARG:HH12	4:I:706:GLC:C2	2.33	0.41
1:I:630:SER:O	1:I:634:GLU:HB2	2.20	0.41
1:J:283:ASP:HB2	1:J:286:GLN:HB2	2.02	0.41
1:J:485:LYS:HE2	1:J:485:LYS:HB2	1.91	0.41
3:J:704:5LS:C6	4:J:705:GLC:C5	2.98	0.41
1:K:237:LYS:NZ	1:K:240:LYS:H	2.18	0.41
1:K:328:LEU:HD21	1:K:337:LEU:HD22	2.01	0.41
1:K:455:LEU:HD22	1:K:611:LEU:O	2.20	0.41
1:K:614:CYS:O	1:K:618:ILE:HG13	2.20	0.41
1:A:227:PRO:HG2	1:C:249:SER:HB2	2.02	0.41
1:A:515:GLU:O	1:A:519:ILE:HG13	2.20	0.41
1:C:117:LYS:O	1:C:121:ILE:HG13	2.20	0.41
1:C:244:ALA:HA	1:C:253:ARG:O	2.20	0.41
1:C:34:HIS:CE1	1:C:37:LEU:HD23	2.55	0.41
1:E:274:ASN:O	1:E:277:GLN:HB2	2.21	0.41
1:E:489:LEU:HD13	1:F:643:GLN:HG3	2.01	0.41
1:E:70:HIS:HB3	1:E:73:VAL:HG12	2.02	0.41
1:F:211:VAL:HG21	1:F:275:TRP:CH2	2.56	0.41
1:F:240:LYS:CD	1:F:277:GLN:HB3	2.50	0.41
1:F:639:VAL:O	1:F:642:MET:HB2	2.19	0.41
1:G:142:HIS:ND1	1:G:169:ALA:HB2	2.35	0.41
1:G:517:LYS:HD2	1:G:642:MET:HE1	2.02	0.41
1:H:26:PHE:HD2	1:H:47:ARG:HA	1.85	0.41
1:H:536:SER:O	1:H:540:GLU:HB2	2.21	0.41
1:I:152:LEU:HD13	1:I:161:HIS:HA	2.01	0.41
1:I:215:ILE:HD13	1:I:264:LEU:HD11	2.02	0.41
1:I:489:LEU:HD21	1:J:648:LYS:HG3	2.01	0.41
1:K:423:LEU:O	1:K:427:TRP:HB2	2.21	0.41
1:K:596:SER:O	1:K:600:VAL:HG22	2.20	0.41
1:K:653:LEU:CD1	1:K:656:ILE:HD11	2.50	0.41
1:K:45:SER:HA	1:K:86:LEU:HD21	2.02	0.41
1:L:311:LYS:CD	1:L:372:VAL:HG21	2.44	0.41
1:L:396:GLY:H	1:L:397:PRO:HD3	1.84	0.41
1:L:394:TYR:CE2	1:L:612:LEU:HD22	2.56	0.41
1:A:233:LYS:O	1:A:236:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:MET:CE	1:B:447:GLY:HA3	2.50	0.41
1:C:143:ARG:H	1:C:143:ARG:HD3	1.86	0.41
1:C:237:LYS:HG3	1:C:237:LYS:O	2.20	0.41
1:D:342:GLU:HB2	1:D:352:GLN:HE22	1.85	0.41
1:D:366:LYS:HB3	1:D:367:PRO:HD2	2.01	0.41
1:D:158:LYS:NZ	1:D:377:ARG:HH21	2.18	0.41
1:D:53:LYS:HG3	1:D:54:ASN:OD1	2.19	0.41
1:D:596:SER:O	1:D:600:VAL:HG22	2.21	0.41
1:D:393:VAL:HG13	1:D:609:SER:OG	2.19	0.41
1:E:523:GLU:HA	1:E:526:VAL:HG23	2.03	0.41
1:E:567:LEU:CD2	1:E:589:ILE:HD13	2.51	0.41
1:E:596:SER:O	1:E:600:VAL:HG22	2.20	0.41
1:F:118:GLU:HA	1:F:121:ILE:HD12	2.01	0.41
1:G:143:ARG:HD3	1:G:143:ARG:H	1.86	0.41
1:G:234:ILE:O	1:G:237:LYS:N	2.54	0.41
1:G:69:ASN:ND2	1:G:75:LYS:HE2	2.35	0.41
1:H:445:PHE:CG	1:H:551:ARG:HB2	2.55	0.41
1:H:8:GLU:HB3	1:H:86:LEU:HG	2.02	0.41
1:I:219:ARG:CZ	1:I:224:HIS:H	2.33	0.41
1:I:53:LYS:HG3	1:I:54:ASN:OD1	2.20	0.41
1:J:614:CYS:HA	1:J:617:LYS:HD3	2.01	0.41
1:G:249:SER:O	1:K:227:PRO:HG2	2.20	0.41
1:K:510:ALA:O	1:K:645:LYS:HE2	2.21	0.41
1:K:639:VAL:O	1:K:642:MET:HB2	2.21	0.41
1:L:240:LYS:HD2	1:L:277:GLN:HB3	2.01	0.41
1:A:295:LEU:C	1:A:297:GLN:H	2.24	0.41
1:A:392:THR:O	1:A:612:LEU:HD23	2.20	0.41
1:B:141:ILE:CG2	1:B:170:LYS:HB2	2.49	0.41
1:B:313:VAL:HG21	1:B:371:CYS:HB2	2.03	0.41
1:A:658:CYS:HB3	1:B:501:GLY:HA2	2.03	0.41
1:B:507:MET:HA	1:B:510:ALA:HB3	2.02	0.41
1:B:577:ASP:HB2	1:B:578:HIS:H	1.58	0.41
1:C:158:LYS:HE3	1:C:377:ARG:HH21	1.85	0.41
1:C:536:SER:O	1:C:540:GLU:HB2	2.21	0.41
1:C:639:VAL:O	1:C:642:MET:HB2	2.20	0.41
7:C:710:5TK:C6	8:C:711:5TH:O2	2.68	0.41
1:D:328:LEU:HD21	1:D:337:LEU:HD22	2.01	0.41
1:D:515:GLU:O	1:D:519:ILE:HG13	2.19	0.41
1:C:501:GLY:HA2	1:D:658:CYS:HB3	2.02	0.41
1:E:147:PRO:C	1:E:149:ASN:H	2.24	0.41
1:E:589:ILE:O	1:E:593:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:LEU:HD13	1:F:161:HIS:HA	2.02	0.41
1:F:168:TYR:CD1	1:F:182:VAL:HG22	2.56	0.41
1:F:168:TYR:CE1	1:F:182:VAL:HG22	2.56	0.41
1:F:452:MET:O	1:F:456:LEU:HG	2.19	0.41
1:G:143:ARG:C	1:G:145:LEU:H	2.24	0.41
1:G:328:LEU:HD21	1:G:337:LEU:HD22	2.03	0.41
1:G:452:MET:O	1:G:456:LEU:HG	2.20	0.41
1:G:560:LEU:HB3	1:G:593:THR:HG22	2.03	0.41
1:H:283:ASP:HB3	1:H:286:GLN:HB2	2.01	0.41
1:I:180:GLU:HB3	1:I:181:PHE:H	1.62	0.41
1:I:258:LEU:HB2	1:I:273:GLU:HG2	2.00	0.41
1:I:423:LEU:O	1:I:427:TRP:HB2	2.20	0.41
1:I:536:SER:O	1:I:540:GLU:HB2	2.21	0.41
1:I:596:SER:O	1:I:600:VAL:HG22	2.21	0.41
1:J:560:LEU:O	1:J:563:ARG:HB2	2.20	0.41
1:K:151:VAL:C	1:K:152:LEU:HD22	2.41	0.41
1:K:268:ILE:C	1:K:271:PRO:HD2	2.40	0.41
1:K:485:LYS:O	1:K:485:LYS:HD3	2.21	0.41
1:L:35:ARG:HG3	1:L:36:GLU:HG3	2.01	0.41
1:K:478:ALA:HB1	1:L:475:GLN:HA	2.03	0.41
1:A:463:THR:HG21	1:A:538:HIS:HD2	1.86	0.41
1:B:414:SER:HA	1:B:587:VAL:HG21	2.02	0.41
1:C:142:HIS:HA	1:C:169:ALA:HB1	2.02	0.41
1:C:21:LEU:HD12	2:C:701:5TL:CAJ	2.50	0.41
1:D:589:ILE:O	1:D:593:THR:HG23	2.20	0.41
1:D:87:ILE:O	1:D:89:ASP:N	2.54	0.41
1:E:118:GLU:HA	1:E:121:ILE:HD12	2.03	0.41
1:E:231:HIS:O	1:E:235:LYS:N	2.54	0.41
1:E:613:GLY:O	1:E:617:LYS:HG3	2.21	0.41
1:E:95:MET:CE	1:E:164:ILE:HD11	2.51	0.41
1:E:74:VAL:HG21	1:E:95:MET:HE1	2.02	0.41
1:F:244:ALA:HA	1:F:253:ARG:O	2.20	0.41
1:F:596:SER:O	1:F:600:VAL:HG22	2.21	0.41
1:G:126:SER:HB2	1:G:308:LEU:CD1	2.51	0.41
1:H:201:THR:C	1:H:287:ARG:HH21	2.23	0.41
1:H:53:LYS:HG3	1:H:54:ASN:OD1	2.21	0.41
1:H:630:SER:O	1:H:634:GLU:HB2	2.20	0.41
1:I:142:HIS:HA	1:I:169:ALA:CB	2.50	0.41
1:I:77:CYS:O	1:I:94:ALA:HB3	2.20	0.41
1:I:97:TYR:HA	2:I:701:5TL:OAO	2.21	0.41
1:J:190:PRO:HA	1:J:193:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:639:VAL:O	1:J:642:MET:HB2	2.20	0.41
1:K:589:ILE:O	1:K:593:THR:HG23	2.21	0.41
1:K:97:TYR:HA	2:K:701:5TL:OAO	2.20	0.41
1:L:237:LYS:HD2	1:L:238:ASP:N	2.25	0.41
1:A:372:VAL:O	1:A:373:LEU:HD13	2.20	0.41
1:A:475:GLN:HA	1:B:478:ALA:HB2	2.02	0.41
1:A:507:MET:HA	1:A:510:ALA:HB3	2.02	0.41
1:A:473:SER:CB	1:A:524:VAL:HA	2.44	0.41
1:A:614:CYS:HA	1:A:617:LYS:HD3	2.01	0.41
1:B:258:LEU:HB2	1:B:273:GLU:HG2	2.03	0.41
1:B:34:HIS:ND1	1:B:37:LEU:HB2	2.35	0.41
1:B:595:GLN:CG	4:B:705:GLC:H62	2.49	0.41
1:C:275:TRP:CH2	1:C:279:MET:HG3	2.56	0.41
1:C:342:GLU:HB2	1:C:352:GLN:HE22	1.86	0.41
1:C:574:ARG:NH1	1:C:575:PRO:HD2	2.36	0.41
1:C:589:ILE:O	1:C:593:THR:HG23	2.21	0.41
1:D:221:PHE:HB2	1:D:230:TRP:CZ2	2.54	0.41
1:D:41:ILE:O	1:D:41:ILE:HG13	2.21	0.41
1:D:485:LYS:HE2	1:D:485:LYS:HB2	1.92	0.41
1:F:147:PRO:C	1:F:149:ASN:H	2.23	0.41
1:F:215:ILE:HD13	1:F:264:LEU:HD11	2.02	0.41
1:H:165:ASP:O	1:H:166:LEU:HD13	2.20	0.41
1:I:21:LEU:HD23	1:I:29:VAL:C	2.41	0.41
1:J:109:LYS:HB3	1:J:111:GLU:HG2	2.03	0.41
1:J:143:ARG:HD2	1:J:170:LYS:HG3	2.03	0.41
1:J:170:LYS:HZ1	1:J:192:LEU:HD11	1.85	0.41
1:J:371:CYS:HB2	1:J:372:VAL:H	1.62	0.41
1:J:655:LYS:N	1:J:655:LYS:HD2	2.36	0.41
1:K:567:LEU:CD2	1:K:589:ILE:HD13	2.51	0.41
1:L:324:ILE:HD12	1:L:324:ILE:N	2.33	0.41
1:L:122:LEU:HD12	1:L:379:CYS:SG	2.60	0.41
1:L:86:LEU:HD13	1:L:87:ILE:HG13	2.03	0.41
1:A:143:ARG:H	1:A:143:ARG:HD3	1.86	0.41
1:A:536:SER:O	1:A:540:GLU:HB2	2.21	0.41
1:A:658:CYS:HB3	1:B:500:TYR:O	2.20	0.41
1:B:125:LEU:HD23	1:B:207:PHE:CZ	2.56	0.41
1:B:234:ILE:HD12	1:B:234:ILE:H	1.85	0.41
1:B:560:LEU:HB3	1:B:593:THR:HG22	2.02	0.41
1:B:579:SER:HB2	1:D:578:HIS:CE1	2.55	0.41
1:C:176:GLU:O	1:C:177:LEU:HB2	2.21	0.41
1:C:158:LYS:HE3	1:C:377:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLU:HG2	1:C:396:GLY:N	2.36	0.41
1:C:465:MET:O	1:C:469:LEU:HB2	2.21	0.41
1:C:541:ILE:CD1	1:C:618:ILE:HD11	2.51	0.41
1:C:630:SER:O	1:C:634:GLU:HB2	2.20	0.41
1:D:536:SER:O	1:D:540:GLU:HB2	2.20	0.41
1:D:614:CYS:HA	1:D:617:LYS:HD3	2.02	0.41
1:D:69:ASN:HD22	1:D:69:ASN:HA	1.61	0.41
1:E:143:ARG:HD3	1:E:143:ARG:H	1.85	0.41
1:E:507:MET:HA	1:E:510:ALA:HB3	2.03	0.41
1:E:535:MET:HA	1:E:538:HIS:HB3	2.03	0.41
1:E:83:LEU:O	1:E:92:LEU:HD13	2.20	0.41
1:F:199:THR:OG1	1:F:284:PRO:HB2	2.20	0.41
1:G:237:LYS:HD2	1:G:241:CYS:HB3	2.03	0.41
1:G:237:LYS:NZ	1:G:240:LYS:H	2.19	0.41
1:G:34:HIS:CE1	1:G:37:LEU:HD23	2.56	0.41
1:H:141:ILE:HG13	1:H:203:ASP:CG	2.40	0.41
1:H:35:ARG:HG3	1:H:36:GLU:HG3	2.01	0.41
1:H:57:ARG:O	1:H:60:HIS:HB3	2.21	0.41
1:I:278:LEU:O	1:I:287:ARG:HG3	2.21	0.41
1:I:348:ASN:O	1:I:352:GLN:HG3	2.21	0.41
1:J:395:GLU:HG3	1:J:397:PRO:CD	2.45	0.41
1:J:549:TYR:H	1:J:552:ARG:HD2	1.85	0.41
1:K:143:ARG:H	1:K:143:ARG:HD3	1.85	0.41
1:K:193:PHE:CE2	1:K:231:HIS:NE2	2.86	0.41
1:K:535:MET:HA	1:K:538:HIS:HB3	2.03	0.41
1:K:536:SER:O	1:K:540:GLU:HB2	2.21	0.41
1:K:70:HIS:HB2	1:K:134:TYR:CD2	2.55	0.41
1:K:79:VAL:CG1	1:K:83:LEU:HD13	2.46	0.41
1:A:141:ILE:HG13	1:A:203:ASP:CG	2.42	0.41
1:A:521:TYR:CD1	1:A:635:ALA:HB1	2.56	0.41
1:B:275:TRP:CH2	1:B:279:MET:HG3	2.56	0.41
1:B:296:LYS:HB3	1:B:296:LYS:NZ	2.35	0.41
1:B:653:LEU:CD1	1:B:656:ILE:HD11	2.50	0.41
1:C:274:ASN:O	1:C:277:GLN:HB2	2.21	0.41
1:C:455:LEU:HD22	1:C:611:LEU:O	2.21	0.41
1:D:125:LEU:HD23	1:D:207:PHE:CZ	2.56	0.41
1:D:342:GLU:HB2	1:D:352:GLN:NE2	2.36	0.41
1:D:630:SER:O	1:D:634:GLU:HB2	2.21	0.41
1:E:289:GLY:N	1:E:290:PRO:CD	2.84	0.41
1:F:225:LEU:HD13	1:F:225:LEU:HA	1.91	0.41
1:G:403:LEU:HD12	1:G:407:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:PRO:HA	1:H:193:PHE:CD1	2.56	0.41
1:H:21:LEU:HD23	1:H:29:VAL:C	2.40	0.41
1:I:342:GLU:HB2	1:I:352:GLN:HE22	1.86	0.41
1:I:37:LEU:HB3	1:I:38:ASP:H	1.68	0.41
1:I:393:VAL:HG13	1:I:609:SER:OG	2.20	0.41
1:I:64:ILE:O	1:I:67:LYS:HB3	2.20	0.41
1:J:328:LEU:HD21	1:J:337:LEU:HD22	2.01	0.41
1:J:403:LEU:HD12	1:J:407:VAL:HG12	2.02	0.41
1:J:515:GLU:O	1:J:519:ILE:HG13	2.19	0.41
1:J:71:ALA:C	1:J:73:VAL:H	2.24	0.41
1:K:147:PRO:C	1:K:149:ASN:H	2.24	0.41
1:K:342:GLU:HB2	1:K:352:GLN:HE22	1.85	0.41
1:K:469:LEU:HD12	1:K:625:VAL:HG13	2.03	0.41
1:L:112:ASN:OD1	1:L:116:LEU:HA	2.21	0.41
1:L:118:GLU:HA	1:L:121:ILE:HD12	2.01	0.41
1:L:125:LEU:HD23	1:L:207:PHE:CZ	2.56	0.41
1:L:147:PRO:C	1:L:149:ASN:H	2.23	0.41
1:L:574:ARG:NH1	1:L:575:PRO:HD2	2.36	0.41
1:A:589:ILE:O	1:A:593:THR:HG23	2.21	0.41
1:B:41:ILE:O	1:B:41:ILE:HG13	2.21	0.41
1:B:613:GLY:O	1:B:617:LYS:HG3	2.20	0.41
1:C:319:THR:HG22	1:C:394:TYR:CE1	2.56	0.41
1:C:396:GLY:N	1:C:397:PRO:CD	2.80	0.41
1:C:423:LEU:O	1:C:427:TRP:HB2	2.20	0.41
1:C:540:GLU:O	1:C:544:LEU:HG	2.21	0.41
1:C:548:PRO:CB	1:C:552:ARG:HG3	2.49	0.41
1:D:372:VAL:O	1:D:372:VAL:HG13	2.20	0.41
1:E:221:PHE:HB2	1:E:230:TRP:CE2	2.56	0.41
1:E:258:LEU:HB2	1:E:273:GLU:HG2	2.02	0.41
1:E:342:GLU:HB2	1:E:352:GLN:HE22	1.85	0.41
1:E:37:LEU:HB3	1:E:38:ASP:H	1.67	0.41
1:E:424:ARG:HH11	1:E:572:LYS:HG2	1.86	0.41
1:E:560:LEU:HB3	1:E:593:THR:HG22	2.03	0.41
1:E:630:SER:O	1:E:634:GLU:HB2	2.21	0.41
1:F:186:GLN:HG2	1:F:219:ARG:HD3	2.02	0.41
1:G:273:GLU:O	1:G:277:GLN:HG3	2.20	0.41
1:H:342:GLU:HB2	1:H:352:GLN:HE22	1.86	0.41
1:H:34:HIS:ND1	1:H:37:LEU:HB2	2.35	0.41
1:I:117:LYS:HD3	1:I:117:LYS:HA	1.94	0.41
1:I:653:LEU:CD1	1:I:656:ILE:HD11	2.51	0.41
1:J:279:MET:SD	1:J:300:CYS:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:342:GLU:HB2	1:J:352:GLN:HE22	1.85	0.41
1:K:622:LEU:N	1:K:623:PRO:CD	2.84	0.41
1:K:86:LEU:HB3	1:K:87:ILE:H	1.59	0.41
1:L:106:LEU:HD11	1:L:152:LEU:HG	2.03	0.41
1:L:567:LEU:CD2	1:L:589:ILE:HD13	2.51	0.41
1:A:186:GLN:OE1	1:A:219:ARG:HD2	2.21	0.41
1:B:143:ARG:HD3	1:B:143:ARG:H	1.85	0.41
1:C:173:ASP:O	1:C:175:GLY:N	2.53	0.41
1:C:209:THR:HG22	1:C:280:LEU:HD11	2.03	0.41
1:C:338:GLN:HA	1:C:341:ILE:HD12	2.02	0.41
1:D:34:HIS:ND1	1:D:37:LEU:HB2	2.35	0.41
1:D:70:HIS:C	1:D:72:ASN:H	2.24	0.41
1:F:95:MET:CE	1:F:164:ILE:HD11	2.50	0.41
1:D:408:ASN:ND2	1:F:26:PHE:HA	2.36	0.41
1:F:420:ILE:HG21	1:F:578:HIS:H	1.86	0.41
1:G:423:LEU:O	1:G:427:TRP:HB2	2.21	0.41
1:G:627:VAL:HG12	1:G:631:ASN:ND2	2.35	0.41
1:H:103:LEU:HB2	1:H:150:ILE:HB	2.03	0.41
1:H:219:ARG:HD2	1:H:223:HIS:HA	2.03	0.41
1:H:473:SER:OG	1:H:524:VAL:HG13	2.20	0.41
1:H:627:VAL:HG12	1:H:631:ASN:ND2	2.36	0.41
1:H:653:LEU:CD1	1:H:656:ILE:HD11	2.50	0.41
1:H:507:MET:CE	1:H:653:LEU:HD13	2.51	0.41
1:I:550:GLY:C	1:I:552:ARG:H	2.25	0.41
1:J:41:ILE:O	1:J:41:ILE:HG13	2.21	0.41
1:K:338:GLN:HA	1:K:341:ILE:HD12	2.03	0.41
1:K:47:ARG:O	1:K:87:ILE:HB	2.20	0.41
1:K:85:ILE:HB	1:K:90:VAL:H	1.86	0.41
1:L:418:LEU:O	1:L:581:SER:HA	2.21	0.41
1:L:653:LEU:CD1	1:L:656:ILE:HD11	2.51	0.41
1:A:21:LEU:HD23	1:A:29:VAL:C	2.41	0.40
1:B:455:LEU:HD12	1:B:618:ILE:HD12	2.03	0.40
1:B:465:MET:SD	1:B:625:VAL:HG11	2.61	0.40
1:C:125:LEU:HD23	1:C:207:PHE:CZ	2.56	0.40
1:C:231:HIS:C	1:C:233:LYS:N	2.74	0.40
1:C:53:LYS:HG3	1:C:54:ASN:OD1	2.20	0.40
1:D:507:MET:HA	1:D:510:ALA:HB3	2.03	0.40
1:E:244:ALA:HA	1:E:253:ARG:O	2.22	0.40
1:E:563:ARG:HB3	1:E:589:ILE:CG1	2.52	0.40
1:E:57:ARG:O	1:E:60:HIS:HB3	2.21	0.40
1:F:32:TYR:HD2	1:F:43:ILE:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:ASN:O	1:F:352:GLN:HG3	2.21	0.40
1:F:57:ARG:O	1:F:60:HIS:HB3	2.20	0.40
1:G:141:ILE:HG13	1:G:203:ASP:CG	2.42	0.40
1:G:383:MET:SD	1:G:385:TYR:CE1	3.14	0.40
1:G:639:VAL:O	1:G:642:MET:HB2	2.21	0.40
1:H:507:MET:HA	1:H:510:ALA:HB3	2.02	0.40
1:H:535:MET:HA	1:H:538:HIS:HB3	2.03	0.40
1:I:268:ILE:C	1:I:271:PRO:HD2	2.42	0.40
1:I:270:GLU:N	1:I:271:PRO:HD2	2.35	0.40
1:I:50:LEU:HD13	1:I:90:VAL:HG21	2.02	0.40
1:J:34:HIS:ND1	1:J:37:LEU:HB2	2.35	0.40
1:L:270:GLU:N	1:L:271:PRO:HD2	2.36	0.40
1:L:355:LEU:HD12	1:L:355:LEU:N	2.36	0.40
1:K:478:ALA:HB2	1:L:475:GLN:HA	2.02	0.40
1:A:588:LYS:HB3	1:A:589:ILE:HD12	2.03	0.40
1:A:89:ASP:O	1:A:90:VAL:HG13	2.21	0.40
1:B:237:LYS:HD3	1:B:238:ASP:O	2.20	0.40
1:B:317:ASN:HD21	1:B:319:THR:HG23	1.86	0.40
1:B:342:GLU:HB2	1:B:352:GLN:HE22	1.87	0.40
1:B:574:ARG:NH1	1:B:575:PRO:HD2	2.36	0.40
1:B:57:ARG:O	1:B:60:HIS:HB3	2.21	0.40
1:C:147:PRO:HB2	1:C:148:GLU:OE2	2.21	0.40
1:C:270:GLU:N	1:C:271:PRO:HD2	2.35	0.40
1:C:284:PRO:HG2	1:C:285:GLN:H	1.86	0.40
1:C:473:SER:HA	1:C:632:ILE:HG21	2.04	0.40
1:C:567:LEU:CD2	1:C:589:ILE:HD13	2.52	0.40
1:C:65:MET:HB3	1:C:76:ALA:HB2	2.03	0.40
1:D:147:PRO:C	1:D:149:ASN:H	2.23	0.40
1:D:639:VAL:O	1:D:642:MET:HB2	2.20	0.40
1:D:72:ASN:HD21	1:D:127:ASP:HA	1.87	0.40
1:F:141:ILE:HG13	1:F:203:ASP:CG	2.41	0.40
1:F:342:GLU:HB2	1:F:352:GLN:NE2	2.36	0.40
1:F:76:ALA:HA	1:F:94:ALA:O	2.20	0.40
1:G:268:ILE:C	1:G:271:PRO:HD2	2.41	0.40
1:G:482:PHE:HD2	1:H:482:PHE:HD2	1.69	0.40
1:G:448:GLN:OE1	1:G:549:TYR:HB3	2.22	0.40
1:G:630:SER:O	1:G:634:GLU:HB2	2.22	0.40
1:H:574:ARG:HH11	1:H:575:PRO:HD2	1.85	0.40
1:I:34:HIS:ND1	1:I:37:LEU:HB2	2.35	0.40
1:I:455:LEU:HD22	1:I:611:LEU:O	2.21	0.40
1:I:588:LYS:HB3	1:I:589:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ILE:C	1:I:86:LEU:HD22	2.41	0.40
1:J:617:LYS:O	1:J:621:LEU:HG	2.22	0.40
1:K:223:HIS:O	1:K:225:LEU:HD23	2.20	0.40
1:K:37:LEU:HB3	1:K:38:ASP:H	1.65	0.40
1:K:507:MET:HA	1:K:510:ALA:HB3	2.03	0.40
1:L:141:ILE:HG13	1:L:203:ASP:CG	2.41	0.40
1:L:215:ILE:HG21	1:L:258:LEU:HD21	2.04	0.40
1:L:265:CYS:SG	1:L:267:LEU:HB2	2.61	0.40
1:L:373:LEU:O	1:L:378:GLY:HA3	2.22	0.40
1:L:37:LEU:HB3	1:L:38:ASP:H	1.67	0.40
1:L:627:VAL:HG12	1:L:631:ASN:ND2	2.36	0.40
1:L:85:ILE:O	1:L:90:VAL:HG23	2.21	0.40
1:A:244:ALA:HA	1:A:253:ARG:O	2.21	0.40
1:A:268:ILE:C	1:A:271:PRO:HD2	2.41	0.40
1:A:577:ASP:H	1:C:579:SER:CB	2.31	0.40
1:A:644:GLY:O	1:A:648:LYS:HB2	2.22	0.40
1:B:238:ASP:CB	1:B:239:PRO:HD2	2.51	0.40
1:B:237:LYS:NZ	1:B:281:ASN:HA	2.35	0.40
1:B:445:PHE:HA	1:B:604:LEU:HD21	2.03	0.40
1:B:536:SER:O	1:B:540:GLU:HB2	2.21	0.40
1:B:563:ARG:HB3	1:B:589:ILE:CG1	2.51	0.40
1:B:589:ILE:O	1:B:593:THR:HG23	2.22	0.40
1:B:596:SER:O	1:B:600:VAL:HG22	2.21	0.40
1:B:655:LYS:N	1:B:655:LYS:HD2	2.36	0.40
1:C:147:PRO:C	1:C:149:ASN:H	2.23	0.40
1:C:317:ASN:HD21	1:C:319:THR:HG23	1.86	0.40
1:D:109:LYS:HB3	1:D:111:GLU:HG2	2.04	0.40
1:D:324:ILE:HD12	1:D:324:ILE:N	2.32	0.40
1:D:655:LYS:N	1:D:655:LYS:HD2	2.36	0.40
1:E:171:ASP:OD1	1:E:172:VAL:N	2.52	0.40
1:E:32:TYR:HD2	1:E:43:ILE:H	1.70	0.40
1:F:523:GLU:HA	1:F:526:VAL:HG23	2.04	0.40
1:F:550:GLY:HA3	1:F:604:LEU:HD13	2.02	0.40
1:G:314:HIS:O	1:G:315:ILE:HD13	2.21	0.40
1:H:484:HIS:O	1:H:488:GLN:HG2	2.22	0.40
1:I:125:LEU:HD23	1:I:207:PHE:CZ	2.56	0.40
1:I:392:THR:HG22	1:I:616:GLN:NE2	2.35	0.40
1:I:560:LEU:HB3	1:I:593:THR:HG22	2.02	0.40
1:J:222:LEU:HD12	1:J:225:LEU:HD23	2.03	0.40
1:J:653:LEU:CD1	1:J:656:ILE:HD11	2.51	0.40
1:K:128:ILE:O	1:K:132:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:ASP:O	1:K:166:LEU:HD13	2.21	0.40
1:K:21:LEU:HD23	1:K:29:VAL:C	2.41	0.40
1:L:21:LEU:HD23	1:L:29:VAL:C	2.42	0.40
1:L:258:LEU:HB2	1:L:273:GLU:HG2	2.02	0.40
1:L:342:GLU:HB2	1:L:352:GLN:HE22	1.87	0.40
1:L:473:SER:HA	1:L:632:ILE:HG21	2.03	0.40
1:A:73:VAL:HA	1:A:162:LYS:HB3	2.03	0.40
1:A:222:LEU:N	1:A:222:LEU:HD22	2.36	0.40
1:A:354:LEU:HB3	1:A:384:VAL:CG1	2.51	0.40
1:A:396:GLY:HA2	1:A:398:PHE:CE2	2.57	0.40
1:A:639:VAL:O	1:A:642:MET:HB2	2.22	0.40
1:B:182:VAL:HG12	1:B:183:GLY:H	1.86	0.40
1:B:630:SER:O	1:B:634:GLU:HB2	2.21	0.40
3:C:702:5LS:C1	5:C:704:PDX:H5	2.52	0.40
1:D:557:MET:HE1	1:D:597:GLN:HA	2.02	0.40
1:E:151:VAL:C	1:E:152:LEU:HD22	2.42	0.40
1:E:29:VAL:HG12	1:E:30:CYS:N	2.37	0.40
1:E:355:LEU:N	1:E:355:LEU:HD12	2.36	0.40
1:A:579:SER:OG	1:E:577:ASP:HB2	2.22	0.40
1:E:653:LEU:CD1	1:E:656:ILE:HD11	2.51	0.40
1:E:97:TYR:HA	2:E:701:5TL:OAO	2.22	0.40
1:F:258:LEU:HB2	1:F:273:GLU:HG2	2.02	0.40
1:F:41:ILE:O	1:F:41:ILE:HG13	2.22	0.40
1:F:653:LEU:CD1	1:F:656:ILE:HD11	2.51	0.40
1:G:536:SER:O	1:G:540:GLU:HB2	2.21	0.40
1:H:403:LEU:HD12	1:H:407:VAL:HG12	2.04	0.40
1:I:147:PRO:C	1:I:149:ASN:H	2.23	0.40
1:I:226:GLN:O	1:I:230:TRP:HB2	2.21	0.40
1:I:271:PRO:HB2	1:I:307:ILE:HD11	2.02	0.40
1:I:627:VAL:HG12	1:I:631:ASN:ND2	2.36	0.40
1:J:342:GLU:HB2	1:J:352:GLN:NE2	2.37	0.40
1:J:396:GLY:N	1:J:397:PRO:CD	2.80	0.40
1:J:473:SER:O	1:J:524:VAL:HG22	2.22	0.40
1:J:98:CYS:HA	1:J:153:GLN:NE2	2.36	0.40
1:K:317:ASN:ND2	1:K:319:THR:HG23	2.35	0.40
1:K:34:HIS:ND1	1:K:37:LEU:HB2	2.36	0.40
1:K:46:CYS:H	1:K:86:LEU:CD2	2.25	0.40
1:K:25:GLY:HA3	1:K:47:ARG:NH1	2.36	0.40
1:L:41:ILE:HG13	1:L:41:ILE:O	2.22	0.40
1:L:465:MET:O	1:L:469:LEU:HB2	2.21	0.40
1:L:536:SER:O	1:L:540:GLU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:549:TYR:H	1:L:552:ARG:HD2	1.87	0.40
1:A:234:ILE:HA	1:A:236:LYS:HZ2	1.85	0.40
1:A:487:ILE:HD11	1:A:511:TRP:O	2.21	0.40
1:B:27:GLY:HA2	1:F:412:GLN:CD	2.42	0.40
1:C:237:LYS:HD3	1:C:282:TRP:H	1.86	0.40
1:C:237:LYS:HZ3	1:C:281:ASN:HA	1.85	0.40
1:C:363:ASP:HB3	1:C:370:GLN:NE2	2.34	0.40
1:D:588:LYS:HB3	1:D:589:ILE:HD12	2.04	0.40
1:E:128:ILE:O	1:E:132:ILE:HG22	2.21	0.40
1:F:427:TRP:CZ3	1:F:567:LEU:HB3	2.55	0.40
1:F:630:SER:O	1:F:634:GLU:HB2	2.21	0.40
1:H:465:MET:O	1:H:469:LEU:HB2	2.20	0.40
1:H:596:SER:O	1:H:600:VAL:HG22	2.21	0.40
1:I:244:ALA:HA	1:I:253:ARG:O	2.21	0.40
1:J:141:ILE:HG13	1:J:203:ASP:CG	2.42	0.40
1:J:222:LEU:HD13	1:J:222:LEU:HA	1.89	0.40
1:K:239:PRO:O	1:K:240:LYS:HB2	2.20	0.40
1:K:126:SER:HB2	1:K:308:LEU:CD1	2.51	0.40
1:K:334:LEU:HD21	1:K:364:PRO:HA	2.03	0.40
1:K:523:GLU:HA	1:K:526:VAL:HG23	2.04	0.40
1:K:420:ILE:HD11	1:K:571:LEU:HG	2.03	0.40
1:L:313:VAL:HG21	1:L:371:CYS:SG	2.61	0.40
1:L:79:VAL:HG23	1:L:79:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	653/655 (100%)	504 (77%)	113 (17%)	36 (6%)	2 29
1	B	653/655 (100%)	514 (79%)	106 (16%)	33 (5%)	2 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	653/655 (100%)	511 (78%)	105 (16%)	37 (6%)	2 28
1	D	653/655 (100%)	515 (79%)	104 (16%)	34 (5%)	2 30
1	E	653/655 (100%)	511 (78%)	104 (16%)	38 (6%)	2 28
1	F	653/655 (100%)	505 (77%)	111 (17%)	37 (6%)	2 28
1	G	653/655 (100%)	508 (78%)	114 (18%)	31 (5%)	3 32
1	H	653/655 (100%)	507 (78%)	99 (15%)	47 (7%)	1 22
1	I	653/655 (100%)	502 (77%)	110 (17%)	41 (6%)	2 26
1	J	653/655 (100%)	515 (79%)	98 (15%)	40 (6%)	2 27
1	K	653/655 (100%)	506 (78%)	105 (16%)	42 (6%)	2 26
1	L	653/655 (100%)	500 (77%)	113 (17%)	40 (6%)	2 27
All	All	7836/7860 (100%)	6098 (78%)	1282 (16%)	456 (6%)	2 28

All (456) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	521	TYR
1	A	549	TYR
1	B	48	LEU
1	B	173	ASP
1	B	180	GLU
1	B	521	TYR
1	C	7	PRO
1	C	48	LEU
1	C	180	GLU
1	C	186	GLN
1	C	237	LYS
1	C	521	TYR
1	C	549	TYR
1	D	8	GLU
1	D	48	LEU
1	D	282	TRP
1	D	521	TYR
1	E	48	LEU
1	E	89	ASP
1	E	173	ASP
1	E	180	GLU
1	E	186	GLN

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Mol	Chain	Res	Type
1	E	521	TYR
1	F	48	LEU
1	F	70	HIS
1	F	521	TYR
1	F	579	SER
1	G	48	LEU
1	G	395	GLU
1	G	521	TYR
1	H	8	GLU
1	H	14	PRO
1	H	48	LEU
1	H	80	PRO
1	H	87	ILE
1	H	172	VAL
1	H	173	ASP
1	H	180	GLU
1	H	365	ARG
1	H	521	TYR
1	I	48	LEU
1	I	184	THR
1	I	370	GLN
1	I	521	TYR
1	I	549	TYR
1	J	48	LEU
1	J	395	GLU
1	J	521	TYR
1	J	549	TYR
1	K	14	PRO
1	K	48	LEU
1	K	186	GLN
1	K	365	ARG
1	K	521	TYR
1	L	14	PRO
1	L	48	LEU
1	L	80	PRO
1	L	521	TYR
1	A	28	ASN
1	A	47	ARG
1	A	86	LEU
1	A	237	LYS
1	A	583	SER
1	B	28	ASN

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Mol	Chain	Res	Type
1	B	47	ARG
1	B	175	GLY
1	B	549	TYR
1	B	575	PRO
1	B	583	SER
1	C	28	ASN
1	C	47	ARG
1	C	174	GLN
1	C	367	PRO
1	C	377	ARG
1	C	395	GLU
1	C	501	GLY
1	C	583	SER
1	D	28	ASN
1	D	47	ARG
1	D	89	ASP
1	D	186	GLN
1	D	237	LYS
1	D	579	SER
1	D	583	SER
1	E	14	PRO
1	E	28	ASN
1	E	222	LEU
1	E	579	SER
1	E	583	SER
1	F	28	ASN
1	F	47	ARG
1	F	365	ARG
1	F	583	SER
1	G	14	PRO
1	G	28	ASN
1	G	73	VAL
1	G	91	PRO
1	G	367	PRO
1	G	579	SER
1	G	583	SER
1	H	28	ASN
1	H	47	ARG
1	H	78	ASP
1	H	186	GLN
1	H	233	LYS
1	H	575	PRO

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Mol	Chain	Res	Type
1	H	579	SER
1	H	583	SER
1	I	11	ALA
1	I	28	ASN
1	I	47	ARG
1	I	83	LEU
1	I	237	LYS
1	I	365	ARG
1	I	395	GLU
1	I	579	SER
1	I	583	SER
1	J	28	ASN
1	J	87	ILE
1	J	173	ASP
1	J	175	GLY
1	J	186	GLN
1	J	579	SER
1	J	583	SER
1	K	28	ASN
1	K	172	VAL
1	K	222	LEU
1	K	237	LYS
1	K	395	GLU
1	K	549	TYR
1	K	579	SER
1	K	583	SER
1	L	28	ASN
1	L	47	ARG
1	L	73	VAL
1	L	77	CYS
1	L	81	GLU
1	L	174	GLN
1	L	365	ARG
1	L	367	PRO
1	L	400	SER
1	L	579	SER
1	L	583	SER
1	A	13	GLY
1	A	14	PRO
1	A	71	ALA
1	A	165	ASP
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	361	SER
1	A	362	LEU
1	A	550	GLY
1	A	575	PRO
1	A	579	SER
1	A	588	LYS
1	B	165	ASP
1	B	169	ALA
1	B	186	GLN
1	B	361	SER
1	B	362	LEU
1	B	365	ARG
1	B	588	LYS
1	C	14	PRO
1	C	80	PRO
1	C	165	ASP
1	C	361	SER
1	C	362	LEU
1	C	505	GLU
1	C	550	GLY
1	C	588	LYS
1	D	86	LEU
1	D	88	HIS
1	D	165	ASP
1	D	177	LEU
1	D	361	SER
1	D	362	LEU
1	D	382	TYR
1	D	395	GLU
1	D	575	PRO
1	D	588	LYS
1	E	13	GLY
1	E	47	ARG
1	E	165	ASP
1	E	169	ALA
1	E	182	VAL
1	E	237	LYS
1	E	290	PRO
1	E	361	SER
1	E	362	LEU
1	E	365	ARG
1	E	396	GLY

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Mol	Chain	Res	Type
1	E	575	PRO
1	E	588	LYS
1	F	9	PHE
1	F	69	ASN
1	F	88	HIS
1	F	165	ASP
1	F	180	GLU
1	F	237	LYS
1	F	290	PRO
1	F	292	ASP
1	F	361	SER
1	F	362	LEU
1	F	367	PRO
1	F	575	PRO
1	F	588	LYS
1	G	9	PHE
1	G	47	ARG
1	G	80	PRO
1	G	165	ASP
1	G	237	LYS
1	G	361	SER
1	G	362	LEU
1	G	575	PRO
1	G	588	LYS
1	H	11	ALA
1	H	165	ASP
1	H	237	LYS
1	H	290	PRO
1	H	361	SER
1	H	362	LEU
1	H	367	PRO
1	H	549	TYR
1	H	588	LYS
1	I	9	PHE
1	I	80	PRO
1	I	165	ASP
1	I	361	SER
1	I	362	LEU
1	I	505	GLU
1	I	588	LYS
1	J	47	ARG
1	J	88	HIS

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Mol	Chain	Res	Type
1	J	165	ASP
1	J	180	GLU
1	J	224	HIS
1	J	237	LYS
1	J	361	SER
1	J	362	LEU
1	J	400	SER
1	J	550	GLY
1	J	575	PRO
1	J	588	LYS
1	K	47	ARG
1	K	165	ASP
1	K	179	THR
1	K	290	PRO
1	K	361	SER
1	K	362	LEU
1	K	575	PRO
1	K	588	LYS
1	L	8	GLU
1	L	165	ASP
1	L	180	GLU
1	L	361	SER
1	L	362	LEU
1	L	395	GLU
1	L	575	PRO
1	L	588	LYS
1	A	8	GLU
1	A	91	PRO
1	A	157	GLY
1	A	186	GLN
1	A	284	PRO
1	A	414	SER
1	B	237	LYS
1	B	414	SER
1	C	85	ILE
1	C	157	GLY
1	C	365	ARG
1	C	414	SER
1	C	575	PRO
1	D	14	PRO
1	D	157	GLY
1	D	290	PRO

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Mol	Chain	Res	Type
1	D	414	SER
1	E	157	GLY
1	E	414	SER
1	F	113	CYS
1	F	173	ASP
1	F	381	SER
1	F	396	GLY
1	F	414	SER
1	G	157	GLY
1	G	414	SER
1	H	9	PHE
1	H	414	SER
1	H	576	SER
1	I	10	GLY
1	I	70	HIS
1	I	157	GLY
1	I	381	SER
1	I	414	SER
1	J	157	GLY
1	J	284	PRO
1	J	414	SER
1	K	77	CYS
1	K	80	PRO
1	K	89	ASP
1	K	157	GLY
1	K	180	GLU
1	K	367	PRO
1	K	383	MET
1	K	414	SER
1	K	576	SER
1	L	222	LEU
1	L	237	LYS
1	L	290	PRO
1	L	414	SER
1	L	576	SER
1	A	290	PRO
1	A	367	PRO
1	A	396	GLY
1	A	522	ALA
1	B	83	LEU
1	B	157	GLY
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	312	ILE
1	B	379	CYS
1	B	522	ALA
1	C	182	VAL
1	C	312	ILE
1	C	522	ALA
1	D	37	LEU
1	D	312	ILE
1	D	522	ALA
1	E	88	HIS
1	E	367	PRO
1	E	395	GLU
1	E	522	ALA
1	F	117	LYS
1	F	157	GLY
1	F	312	ILE
1	F	522	ALA
1	G	84	ASN
1	G	178	CYS
1	G	522	ALA
1	H	10	GLY
1	H	77	CYS
1	H	157	GLY
1	H	182	VAL
1	H	312	ILE
1	H	522	ALA
1	I	85	ILE
1	I	290	PRO
1	I	312	ILE
1	I	504	SER
1	I	522	ALA
1	I	575	PRO
1	I	576	SER
1	J	14	PRO
1	J	37	LEU
1	J	290	PRO
1	J	312	ILE
1	J	379	CYS
1	J	522	ALA
1	K	312	ILE
1	K	400	SER

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Mol	Chain	Res	Type
1	K	522	ALA
1	K	550	GLY
1	L	84	ASN
1	L	85	ILE
1	L	157	GLY
1	L	522	ALA
1	A	312	ILE
1	B	37	LEU
1	C	37	LEU
1	E	37	LEU
1	E	312	ILE
1	F	14	PRO
1	F	284	PRO
1	G	312	ILE
1	H	37	LEU
1	H	89	ASP
1	I	37	LEU
1	I	175	GLY
1	I	377	ARG
1	I	550	GLY
1	J	13	GLY
1	K	37	LEU
1	K	182	VAL
1	K	399	ALA
1	L	37	LEU
1	L	312	ILE
1	A	182	VAL
1	A	197	PRO
1	B	197	PRO
1	B	550	GLY
1	C	197	PRO
1	D	197	PRO
1	E	197	PRO
1	F	197	PRO
1	G	197	PRO
1	H	13	GLY
1	H	197	PRO
1	I	197	PRO
1	J	80	PRO
1	J	197	PRO
1	J	376	VAL
1	K	197	PRO

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Mol	Chain	Res	Type
1	L	10	GLY
1	L	197	PRO
1	B	290	PRO
1	E	85	ILE
1	E	115	GLY
1	H	550	GLY
1	A	155	VAL
1	B	155	VAL
1	C	91	PRO
1	C	155	VAL
1	C	239	PRO
1	D	80	PRO
1	D	155	VAL
1	E	155	VAL
1	G	155	VAL
1	G	376	VAL
1	H	155	VAL
1	I	155	VAL
1	J	10	GLY
1	J	375	GLY
1	K	73	VAL
1	K	155	VAL
1	L	155	VAL
1	A	121	ILE
1	A	175	GLY
1	B	22	GLY
1	B	121	ILE
1	C	22	GLY
1	E	121	ILE
1	F	22	GLY
1	F	121	ILE
1	F	155	VAL
1	F	550	GLY
1	G	259	PRO
1	G	550	GLY
1	H	22	GLY
1	H	121	ILE
1	H	259	PRO
1	H	376	VAL
1	J	22	GLY
1	J	155	VAL
1	K	121	ILE

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Mol	Chain	Res	Type
1	L	22	GLY
1	L	182	VAL
1	A	259	PRO
1	D	22	GLY
1	D	121	ILE
1	D	259	PRO
1	E	22	GLY
1	G	121	ILE
1	H	397	PRO
1	I	22	GLY
1	I	259	PRO
1	K	22	GLY
1	L	121	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/589 (100%)	557 (95%)	32 (5%)	27	66
1	B	589/589 (100%)	557 (95%)	32 (5%)	27	66
1	C	589/589 (100%)	563 (96%)	26 (4%)	35	71
1	D	589/589 (100%)	567 (96%)	22 (4%)	41	75
1	E	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	F	589/589 (100%)	561 (95%)	28 (5%)	31	69
1	G	589/589 (100%)	555 (94%)	34 (6%)	25	64
1	H	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	I	589/589 (100%)	561 (95%)	28 (5%)	31	69
1	J	589/589 (100%)	560 (95%)	29 (5%)	31	68
1	K	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	L	589/589 (100%)	557 (95%)	32 (5%)	27	66
All	All	7068/7068 (100%)	6715 (95%)	353 (5%)	30	68

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	47	ARG
1	A	48	LEU
1	A	56	GLU
1	A	81	GLU
1	A	83	LEU
1	A	90	VAL
1	A	113	CYS
1	A	127	ASP
1	A	143	ARG
1	A	170	LYS
1	A	180	GLU
1	A	185	LEU
1	A	191	GLU
1	A	219	ARG
1	A	223	HIS
1	A	231	HIS
1	A	236	LYS
1	A	237	LYS
1	A	295	LEU
1	A	317	ASN
1	A	373	LEU
1	A	377	ARG
1	A	382	TYR
1	A	485	LYS
1	A	506	LYS
1	A	543	GLU
1	A	552	ARG
1	A	574	ARG
1	A	601	LEU
1	A	646	ARG
1	A	655	LYS
1	B	9	PHE
1	B	20	ARG
1	B	47	ARG
1	B	48	LEU
1	B	56	GLU
1	B	81	GLU
1	B	88	HIS
1	B	90	VAL
1	B	127	ASP
1	B	143	ARG

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Mol	Chain	Res	Type
1	B	176	GLU
1	B	185	LEU
1	B	191	GLU
1	B	219	ARG
1	B	230	TRP
1	B	238	ASP
1	B	281	ASN
1	B	297	GLN
1	B	317	ASN
1	B	366	LYS
1	B	382	TYR
1	B	395	GLU
1	B	401	ARG
1	B	485	LYS
1	B	506	LYS
1	B	543	GLU
1	B	552	ARG
1	B	574	ARG
1	B	577	ASP
1	B	601	LEU
1	B	646	ARG
1	B	655	LYS
1	C	20	ARG
1	C	47	ARG
1	C	48	LEU
1	C	56	GLU
1	C	82	GLU
1	C	83	LEU
1	C	90	VAL
1	C	127	ASP
1	C	143	ARG
1	C	178	CYS
1	C	185	LEU
1	C	191	GLU
1	C	219	ARG
1	C	297	GLN
1	C	317	ASN
1	C	366	LYS
1	C	377	ARG
1	C	485	LYS
1	C	506	LYS
1	C	543	GLU

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Mol	Chain	Res	Type
1	C	552	ARG
1	C	574	ARG
1	C	579	SER
1	C	601	LEU
1	C	646	ARG
1	C	655	LYS
1	D	20	ARG
1	D	47	ARG
1	D	48	LEU
1	D	56	GLU
1	D	127	ASP
1	D	143	ARG
1	D	174	GLN
1	D	185	LEU
1	D	191	GLU
1	D	317	ASN
1	D	370	GLN
1	D	382	TYR
1	D	401	ARG
1	D	485	LYS
1	D	506	LYS
1	D	543	GLU
1	D	544	LEU
1	D	552	ARG
1	D	574	ARG
1	D	601	LEU
1	D	646	ARG
1	D	655	LYS
1	E	20	ARG
1	E	47	ARG
1	E	48	LEU
1	E	56	GLU
1	E	81	GLU
1	E	82	GLU
1	E	83	LEU
1	E	86	LEU
1	E	127	ASP
1	E	143	ARG
1	E	177	LEU
1	E	185	LEU
1	E	191	GLU
1	E	219	ARG

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Mol	Chain	Res	Type
1	E	236	LYS
1	E	237	LYS
1	E	238	ASP
1	E	287	ARG
1	E	317	ASN
1	E	371	CYS
1	E	377	ARG
1	E	395	GLU
1	E	485	LYS
1	E	506	LYS
1	E	543	GLU
1	E	552	ARG
1	E	574	ARG
1	E	601	LEU
1	E	646	ARG
1	E	655	LYS
1	F	20	ARG
1	F	47	ARG
1	F	48	LEU
1	F	56	GLU
1	F	75	LYS
1	F	81	GLU
1	F	116	LEU
1	F	127	ASP
1	F	143	ARG
1	F	176	GLU
1	F	184	THR
1	F	185	LEU
1	F	191	GLU
1	F	222	LEU
1	F	225	LEU
1	F	231	HIS
1	F	232	GLU
1	F	281	ASN
1	F	317	ASN
1	F	371	CYS
1	F	485	LYS
1	F	506	LYS
1	F	543	GLU
1	F	552	ARG
1	F	574	ARG
1	F	601	LEU

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Mol	Chain	Res	Type
1	F	646	ARG
1	F	655	LYS
1	G	20	ARG
1	G	47	ARG
1	G	48	LEU
1	G	56	GLU
1	G	84	ASN
1	G	86	LEU
1	G	90	VAL
1	G	127	ASP
1	G	143	ARG
1	G	170	LYS
1	G	173	ASP
1	G	174	GLN
1	G	191	GLU
1	G	219	ARG
1	G	222	LEU
1	G	225	LEU
1	G	231	HIS
1	G	237	LYS
1	G	281	ASN
1	G	317	ASN
1	G	370	GLN
1	G	373	LEU
1	G	383	MET
1	G	395	GLU
1	G	401	ARG
1	G	485	LYS
1	G	503	SER
1	G	506	LYS
1	G	543	GLU
1	G	552	ARG
1	G	574	ARG
1	G	601	LEU
1	G	646	ARG
1	G	655	LYS
1	H	9	PHE
1	H	20	ARG
1	H	47	ARG
1	H	48	LEU
1	H	56	GLU
1	H	86	LEU

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Mol	Chain	Res	Type
1	H	90	VAL
1	H	114	CYS
1	H	127	ASP
1	H	143	ARG
1	H	171	ASP
1	H	173	ASP
1	H	191	GLU
1	H	219	ARG
1	H	224	HIS
1	H	235	LYS
1	H	237	LYS
1	H	317	ASN
1	H	370	GLN
1	H	373	LEU
1	H	382	TYR
1	H	401	ARG
1	H	485	LYS
1	H	506	LYS
1	H	543	GLU
1	H	552	ARG
1	H	574	ARG
1	H	601	LEU
1	H	646	ARG
1	H	655	LYS
1	I	20	ARG
1	I	47	ARG
1	I	48	LEU
1	I	56	GLU
1	I	69	ASN
1	I	83	LEU
1	I	86	LEU
1	I	90	VAL
1	I	127	ASP
1	I	143	ARG
1	I	191	GLU
1	I	231	HIS
1	I	236	LYS
1	I	237	LYS
1	I	287	ARG
1	I	317	ASN
1	I	366	LYS
1	I	370	GLN

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Mol	Chain	Res	Type
1	I	377	ARG
1	I	401	ARG
1	I	485	LYS
1	I	506	LYS
1	I	543	GLU
1	I	552	ARG
1	I	574	ARG
1	I	601	LEU
1	I	646	ARG
1	I	655	LYS
1	J	20	ARG
1	J	47	ARG
1	J	48	LEU
1	J	56	GLU
1	J	73	VAL
1	J	114	CYS
1	J	127	ASP
1	J	143	ARG
1	J	178	CYS
1	J	191	GLU
1	J	219	ARG
1	J	223	HIS
1	J	225	LEU
1	J	230	TRP
1	J	236	LYS
1	J	237	LYS
1	J	283	ASP
1	J	317	ASN
1	J	370	GLN
1	J	379	CYS
1	J	485	LYS
1	J	499	THR
1	J	506	LYS
1	J	543	GLU
1	J	552	ARG
1	J	574	ARG
1	J	601	LEU
1	J	646	ARG
1	J	655	LYS
1	K	20	ARG
1	K	47	ARG
1	K	48	LEU

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Mol	Chain	Res	Type
1	K	56	GLU
1	K	78	ASP
1	K	114	CYS
1	K	127	ASP
1	K	143	ARG
1	K	168	TYR
1	K	174	GLN
1	K	185	LEU
1	K	191	GLU
1	K	219	ARG
1	K	235	LYS
1	K	236	LYS
1	K	237	LYS
1	K	238	ASP
1	K	317	ASN
1	K	373	LEU
1	K	374	ASP
1	K	382	TYR
1	K	395	GLU
1	K	485	LYS
1	K	506	LYS
1	K	543	GLU
1	K	552	ARG
1	K	574	ARG
1	K	601	LEU
1	K	646	ARG
1	K	655	LYS
1	L	20	ARG
1	L	47	ARG
1	L	48	LEU
1	L	56	GLU
1	L	70	HIS
1	L	72	ASN
1	L	84	ASN
1	L	86	LEU
1	L	88	HIS
1	L	127	ASP
1	L	143	ARG
1	L	173	ASP
1	L	184	THR
1	L	191	GLU
1	L	223	HIS

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Mol	Chain	Res	Type
1	L	237	LYS
1	L	238	ASP
1	L	286	GLN
1	L	317	ASN
1	L	370	GLN
1	L	373	LEU
1	L	377	ARG
1	L	395	GLU
1	L	401	ARG
1	L	485	LYS
1	L	506	LYS
1	L	543	GLU
1	L	552	ARG
1	L	574	ARG
1	L	601	LEU
1	L	646	ARG
1	L	655	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (276) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN
1	A	112	ASN
1	A	195	ASN
1	A	260	GLN
1	A	262	ASN
1	A	309	ASN
1	A	317	ASN
1	A	370	GLN
1	A	408	ASN
1	A	422	GLN
1	A	459	ASN
1	A	475	GLN
1	A	488	GLN
1	A	538	HIS
1	A	573	HIS
1	A	597	GLN
1	A	616	GLN
1	A	631	ASN
1	A	643	GLN
1	B	28	ASN

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	72	ASN
1	B	84	ASN
1	B	112	ASN
1	B	195	ASN
1	B	226	GLN
1	B	260	GLN
1	B	262	ASN
1	B	281	ASN
1	B	286	GLN
1	B	309	ASN
1	B	317	ASN
1	B	370	GLN
1	B	408	ASN
1	B	422	GLN
1	B	475	GLN
1	B	488	GLN
1	B	538	HIS
1	B	545	GLN
1	B	573	HIS
1	B	595	GLN
1	B	597	GLN
1	B	616	GLN
1	B	631	ASN
1	B	643	GLN
1	C	28	ASN
1	C	33	GLN
1	C	63	GLN
1	C	72	ASN
1	C	195	ASN
1	C	260	GLN
1	C	262	ASN
1	C	281	ASN
1	C	297	GLN
1	C	309	ASN
1	C	317	ASN
1	C	370	GLN
1	C	412	GLN
1	C	422	GLN
1	C	475	GLN
1	C	488	GLN
1	C	533	GLN

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Mol	Chain	Res	Type
1	C	538	HIS
1	C	573	HIS
1	C	597	GLN
1	C	616	GLN
1	C	631	ASN
1	C	643	GLN
1	D	28	ASN
1	D	33	GLN
1	D	69	ASN
1	D	84	ASN
1	D	88	HIS
1	D	174	GLN
1	D	186	GLN
1	D	195	ASN
1	D	260	GLN
1	D	262	ASN
1	D	309	ASN
1	D	317	ASN
1	D	408	ASN
1	D	412	GLN
1	D	422	GLN
1	D	459	ASN
1	D	475	GLN
1	D	488	GLN
1	D	538	HIS
1	D	573	HIS
1	D	597	GLN
1	D	616	GLN
1	D	631	ASN
1	D	643	GLN
1	E	28	ASN
1	E	33	GLN
1	E	70	HIS
1	E	84	ASN
1	E	195	ASN
1	E	260	GLN
1	E	262	ASN
1	E	285	GLN
1	E	297	GLN
1	E	309	ASN
1	E	408	ASN
1	E	422	GLN

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Mol	Chain	Res	Type
1	E	475	GLN
1	E	488	GLN
1	E	533	GLN
1	E	538	HIS
1	E	573	HIS
1	E	597	GLN
1	E	616	GLN
1	E	631	ASN
1	E	643	GLN
1	F	28	ASN
1	F	33	GLN
1	F	84	ASN
1	F	186	GLN
1	F	195	ASN
1	F	226	GLN
1	F	260	GLN
1	F	262	ASN
1	F	281	ASN
1	F	309	ASN
1	F	317	ASN
1	F	370	GLN
1	F	408	ASN
1	F	422	GLN
1	F	459	ASN
1	F	475	GLN
1	F	488	GLN
1	F	545	GLN
1	F	573	HIS
1	F	597	GLN
1	F	616	GLN
1	F	631	ASN
1	F	643	GLN
1	G	33	GLN
1	G	69	ASN
1	G	84	ASN
1	G	112	ASN
1	G	186	GLN
1	G	195	ASN
1	G	260	GLN
1	G	262	ASN
1	G	281	ASN
1	G	285	GLN

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Mol	Chain	Res	Type
1	G	286	GLN
1	G	309	ASN
1	G	317	ASN
1	G	370	GLN
1	G	408	ASN
1	G	422	GLN
1	G	459	ASN
1	G	475	GLN
1	G	488	GLN
1	G	538	HIS
1	G	573	HIS
1	G	597	GLN
1	G	616	GLN
1	G	631	ASN
1	G	643	GLN
1	H	28	ASN
1	H	33	GLN
1	H	69	ASN
1	H	72	ASN
1	H	84	ASN
1	H	186	GLN
1	H	195	ASN
1	H	260	GLN
1	H	262	ASN
1	H	297	GLN
1	H	309	ASN
1	H	317	ASN
1	H	370	GLN
1	H	422	GLN
1	H	475	GLN
1	H	488	GLN
1	H	533	GLN
1	H	538	HIS
1	H	545	GLN
1	H	573	HIS
1	H	597	GLN
1	H	616	GLN
1	H	631	ASN
1	H	643	GLN
1	I	28	ASN
1	I	33	GLN
1	I	60	HIS

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Mol	Chain	Res	Type
1	I	69	ASN
1	I	195	ASN
1	I	260	GLN
1	I	262	ASN
1	I	281	ASN
1	I	309	ASN
1	I	317	ASN
1	I	370	GLN
1	I	412	GLN
1	I	422	GLN
1	I	475	GLN
1	I	488	GLN
1	I	533	GLN
1	I	545	GLN
1	I	573	HIS
1	I	597	GLN
1	I	616	GLN
1	I	631	ASN
1	I	643	GLN
1	J	28	ASN
1	J	33	GLN
1	J	63	GLN
1	J	88	HIS
1	J	112	ASN
1	J	186	GLN
1	J	195	ASN
1	J	260	GLN
1	J	262	ASN
1	J	297	GLN
1	J	309	ASN
1	J	370	GLN
1	J	408	ASN
1	J	422	GLN
1	J	459	ASN
1	J	475	GLN
1	J	488	GLN
1	J	533	GLN
1	J	538	HIS
1	J	573	HIS
1	J	597	GLN
1	J	616	GLN
1	J	631	ASN

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Mol	Chain	Res	Type
1	J	643	GLN
1	K	28	ASN
1	K	33	GLN
1	K	72	ASN
1	K	195	ASN
1	K	260	GLN
1	K	262	ASN
1	K	309	ASN
1	K	317	ASN
1	K	408	ASN
1	K	422	GLN
1	K	475	GLN
1	K	488	GLN
1	K	497	GLN
1	K	533	GLN
1	K	538	HIS
1	K	573	HIS
1	K	595	GLN
1	K	597	GLN
1	K	616	GLN
1	K	631	ASN
1	K	643	GLN
1	L	28	ASN
1	L	33	GLN
1	L	72	ASN
1	L	186	GLN
1	L	195	ASN
1	L	231	HIS
1	L	260	GLN
1	L	262	ASN
1	L	297	GLN
1	L	309	ASN
1	L	317	ASN
1	L	408	ASN
1	L	422	GLN
1	L	459	ASN
1	L	475	GLN
1	L	484	HIS
1	L	488	GLN
1	L	538	HIS
1	L	573	HIS
1	L	597	GLN

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Mol	Chain	Res	Type
1	L	616	GLN
1	L	631	ASN
1	L	643	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

112 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5TL	A	701	-	28,28,28	2.68	11 (39%)	36,41,41	5.12	20 (55%)
3	5LS	A	702	4	19,20,20	1.09	0	26,31,31	1.04	2 (7%)
4	GLC	A	703	3,5	11,11,12	0.56	0	15,15,17	0.43	0
5	PDX	A	704	4	19,19,20	1.39	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	A	705	4	19,20,20	1.11	0	26,31,31	1.03	2 (7%)
4	GLC	A	706	3,5	11,11,12	0.85	0	15,15,17	1.15	1 (6%)
5	PDX	A	707	4	19,19,20	1.35	2 (10%)	24,29,31	0.83	1 (4%)
6	5TJ	A	708	9,3	14,17,18	1.01	0	19,24,26	0.92	1 (5%)
6	5TJ	A	709	9,10	14,17,18	1.02	0	19,24,26	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	5TK	A	710	10,8	10,13,14	0.56	0	13,17,19	0.40	0
8	5TH	A	711	7	14,17,18	1.41	2 (14%)	17,24,26	0.50	0
2	5TL	B	701	-	28,28,28	2.72	11 (39%)	36,41,41	5.06	21 (58%)
4	GLC	B	702	3,5	11,11,12	0.65	0	15,15,17	0.45	0
5	PDX	B	703	4	19,19,20	1.30	2 (10%)	24,29,31	0.62	0
3	5LS	B	704	4	19,20,20	1.14	0	26,31,31	1.06	2 (7%)
4	GLC	B	705	3,5	11,11,12	0.55	0	15,15,17	0.42	0
5	PDX	B	706	4	19,19,20	1.41	2 (10%)	24,29,31	0.91	2 (8%)
3	5LS	B	707	6	19,20,20	1.08	0	26,31,31	1.06	2 (7%)
9	5TM	B	708	6	14,17,18	1.22	1 (7%)	17,24,26	0.53	0
10	Z4K	B	709	7,6	15,15,16	1.21	1 (6%)	19,22,24	0.55	0
2	5TL	C	701	-	28,28,28	2.67	11 (39%)	36,41,41	5.15	20 (55%)
3	5LS	C	702	4	19,20,20	1.06	0	26,31,31	1.02	2 (7%)
4	GLC	C	703	3,5	11,11,12	0.52	0	15,15,17	0.37	0
5	PDX	C	704	4	19,19,20	1.41	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	C	705	4	19,20,20	1.03	0	26,31,31	0.96	1 (3%)
4	GLC	C	706	3,5	11,11,12	0.45	0	15,15,17	0.38	0
5	PDX	C	707	4	19,19,20	1.41	2 (10%)	24,29,31	0.82	1 (4%)
9	5TM	C	708	6	14,17,18	1.18	1 (7%)	17,24,26	0.63	0
10	Z4K	C	709	7,6	15,15,16	1.15	1 (6%)	19,22,24	0.54	0
7	5TK	C	710	10,8	10,13,14	0.62	0	13,17,19	0.56	0
8	5TH	C	711	7	14,17,18	1.43	2 (14%)	17,24,26	0.63	0
2	5TL	D	701	-	28,28,28	2.71	10 (35%)	36,41,41	5.18	20 (55%)
3	5LS	D	702	4	19,20,20	1.08	0	26,31,31	1.03	2 (7%)
4	GLC	D	703	3,5	11,11,12	0.54	0	15,15,17	0.39	0
5	PDX	D	704	4	19,19,20	1.38	2 (10%)	24,29,31	0.79	1 (4%)
3	5LS	D	705	4	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
4	GLC	D	706	3,5	11,11,12	0.58	0	15,15,17	0.52	0
5	PDX	D	707	4	19,19,20	1.37	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	D	708	4	19,20,20	1.11	0	26,31,31	1.06	2 (7%)
3	5LS	D	709	6	19,20,20	1.10	0	26,31,31	1.04	2 (7%)
6	5TJ	D	710	9,3	14,17,18	0.99	0	19,24,26	0.86	1 (5%)
6	5TJ	D	711	9,10	14,17,18	0.98	0	19,24,26	0.88	1 (5%)
2	5TL	E	701	-	28,28,28	2.66	10 (35%)	36,41,41	5.11	18 (50%)
3	5LS	E	702	4	19,20,20	1.11	0	26,31,31	1.04	3 (11%)
4	GLC	E	703	3,5	11,11,12	0.64	0	15,15,17	0.71	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PDX	E	704	4	19,19,20	1.41	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	E	705	4	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
4	GLC	E	706	3,5	11,11,12	0.58	0	15,15,17	0.59	0
5	PDX	E	707	4	19,19,20	1.38	2 (10%)	24,29,31	0.78	1 (4%)
2	5TL	F	701	-	28,28,28	2.71	10 (35%)	36,41,41	5.09	21 (58%)
3	5LS	F	702	4	19,20,20	1.11	0	26,31,31	1.06	2 (7%)
4	GLC	F	703	3,5	11,11,12	0.59	0	15,15,17	0.56	0
5	PDX	F	704	4	19,19,20	1.47	2 (10%)	24,29,31	1.00	2 (8%)
3	5LS	F	705	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	F	706	3,5	11,11,12	0.67	0	15,15,17	0.52	0
5	PDX	F	707	4	19,19,20	1.38	2 (10%)	24,29,31	0.83	1 (4%)
2	5TL	G	701	-	28,28,28	2.67	11 (39%)	36,41,41	5.17	21 (58%)
3	5LS	G	702	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	G	703	3,5	11,11,12	0.56	0	15,15,17	0.34	0
5	PDX	G	704	4	19,19,20	1.39	2 (10%)	24,29,31	0.85	1 (4%)
3	5LS	G	705	4	19,20,20	1.09	0	26,31,31	1.06	2 (7%)
4	GLC	G	706	3,5	11,11,12	0.54	0	15,15,17	0.50	0
5	PDX	G	707	4	19,19,20	1.36	2 (10%)	24,29,31	0.83	1 (4%)
9	5TM	G	708	6	14,17,18	1.28	2 (14%)	17,24,26	0.54	0
7	5TK	G	709	10,8	10,13,14	0.62	0	13,17,19	0.39	0
8	5TH	G	710	7	14,17,18	1.30	2 (14%)	17,24,26	0.55	0
2	5TL	H	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.08	21 (58%)
3	5LS	H	702	4	19,20,20	1.09	0	26,31,31	1.05	2 (7%)
4	GLC	H	703	3,5	11,11,12	0.79	0	15,15,17	0.51	0
5	PDX	H	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.84	1 (4%)
3	5LS	H	705	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	H	706	3,5	11,11,12	0.66	0	15,15,17	0.44	0
3	5LS	H	707	6	19,20,20	1.07	0	26,31,31	1.02	2 (7%)
6	5TJ	H	708	9,3	14,17,18	1.00	0	19,24,26	0.83	1 (5%)
6	5TJ	H	709	9,10	14,17,18	1.03	0	19,24,26	0.89	1 (5%)
10	Z4K	H	710	7,6	15,15,16	1.19	1 (6%)	19,22,24	0.66	0
2	5TL	I	701	-	28,28,28	2.69	10 (35%)	36,41,41	5.09	20 (55%)
3	5LS	I	702	4	19,20,20	1.12	0	26,31,31	1.10	2 (7%)
4	GLC	I	703	3,5	11,11,12	0.65	0	15,15,17	0.60	0
5	PDX	I	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.90	2 (8%)
3	5LS	I	705	4	19,20,20	1.09	0	26,31,31	1.05	2 (7%)
4	GLC	I	706	3,5	11,11,12	0.57	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PDX	I	707	4	19,19,20	1.37	2 (10%)	24,29,31	0.83	1 (4%)
6	5TJ	I	708	9,3	14,17,18	1.01	0	19,24,26	0.92	1 (5%)
6	5TJ	I	709	9,10	14,17,18	1.00	0	19,24,26	0.93	1 (5%)
7	5TK	I	710	10,8	10,13,14	0.52	0	13,17,19	0.36	0
8	5TH	I	711	7	14,17,18	1.37	2 (14%)	17,24,26	0.57	0
2	5TL	J	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.21	20 (55%)
4	GLC	J	702	3,5	11,11,12	0.81	0	15,15,17	1.24	1 (6%)
5	PDX	J	703	4	19,19,20	1.39	2 (10%)	24,29,31	0.79	1 (4%)
3	5LS	J	704	4	19,20,20	1.10	0	26,31,31	1.10	2 (7%)
4	GLC	J	705	3,5	11,11,12	0.89	0	15,15,17	1.15	2 (13%)
5	PDX	J	706	4	19,19,20	1.43	2 (10%)	24,29,31	1.05	2 (8%)
3	5LS	J	707	6	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
9	5TM	J	708	6	14,17,18	1.24	1 (7%)	17,24,26	0.60	0
10	Z4K	J	709	7,6	15,15,16	1.24	1 (6%)	19,22,24	0.55	0
2	5TL	K	701	-	28,28,28	2.63	10 (35%)	36,41,41	5.24	20 (55%)
3	5LS	K	702	4	19,20,20	1.09	0	26,31,31	1.02	2 (7%)
4	GLC	K	703	3,5	11,11,12	0.58	0	15,15,17	0.32	0
5	PDX	K	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.84	1 (4%)
3	5LS	K	705	4	19,20,20	1.04	0	26,31,31	0.94	1 (3%)
4	GLC	K	706	3,5	11,11,12	0.52	0	15,15,17	0.51	0
5	PDX	K	707	4	19,19,20	1.39	2 (10%)	24,29,31	0.82	1 (4%)
2	5TL	L	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.12	19 (52%)
3	5LS	L	702	4	19,20,20	1.08	0	26,31,31	1.06	2 (7%)
5	PDX	L	703	4	19,19,20	1.52	2 (10%)	24,29,31	1.02	2 (8%)
3	5LS	L	704	4	19,20,20	1.08	0	26,31,31	1.03	2 (7%)
4	GLC	L	705	3,5	11,11,12	0.60	0	15,15,17	0.51	0
5	PDX	L	706	4	19,19,20	1.46	2 (10%)	24,29,31	1.03	2 (8%)
3	5LS	L	707	4	19,20,20	1.01	0	26,31,31	1.45	2 (7%)
4	GLC	L	708	3,5	11,11,12	0.56	0	15,15,17	0.47	0
5	PDX	L	709	4	19,19,20	1.40	2 (10%)	24,29,31	0.82	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5TL	A	701	-	-	0/18/18/18	0/3/3/3
3	5LS	A	702	4	-	0/12/32/32	0/1/1/1
4	GLC	A	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	A	704	4	-	0/12/29/32	0/1/1/1
3	5LS	A	705	4	-	0/12/32/32	0/1/1/1
4	GLC	A	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	A	707	4	-	0/12/29/32	0/1/1/1
6	5TJ	A	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	A	709	9,10	-	0/9/27/30	0/1/1/1
7	5TK	A	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	A	711	7	-	0/9/27/30	0/1/1/1
2	5TL	B	701	-	-	0/18/18/18	0/3/3/3
4	GLC	B	702	3,5	-	0/2/19/22	0/1/1/1
5	PDX	B	703	4	-	0/12/29/32	0/1/1/1
3	5LS	B	704	4	-	0/12/32/32	0/1/1/1
4	GLC	B	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	B	706	4	-	0/12/29/32	0/1/1/1
3	5LS	B	707	6	-	0/12/32/32	0/1/1/1
9	5TM	B	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	B	709	7,6	-	0/7/24/27	0/1/1/1
2	5TL	C	701	-	-	0/18/18/18	0/3/3/3
3	5LS	C	702	4	-	0/12/32/32	0/1/1/1
4	GLC	C	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	C	704	4	-	0/12/29/32	0/1/1/1
3	5LS	C	705	4	-	0/12/32/32	0/1/1/1
4	GLC	C	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	C	707	4	-	0/12/29/32	0/1/1/1
9	5TM	C	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	C	709	7,6	-	0/7/24/27	0/1/1/1
7	5TK	C	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	C	711	7	-	0/9/27/30	0/1/1/1
2	5TL	D	701	-	-	0/18/18/18	0/3/3/3
3	5LS	D	702	4	-	0/12/32/32	0/1/1/1
4	GLC	D	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	D	704	4	-	0/12/29/32	0/1/1/1
3	5LS	D	705	4	-	0/12/32/32	0/1/1/1
4	GLC	D	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	D	707	4	-	0/12/29/32	0/1/1/1
3	5LS	D	708	4	-	0/12/32/32	0/1/1/1
3	5LS	D	709	6	-	0/12/32/32	0/1/1/1
6	5TJ	D	710	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	D	711	9,10	-	0/9/27/30	0/1/1/1
2	5TL	E	701	-	-	0/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5LS	E	702	4	-	0/12/32/32	0/1/1/1
4	GLC	E	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	E	704	4	-	0/12/29/32	0/1/1/1
3	5LS	E	705	4	-	0/12/32/32	0/1/1/1
4	GLC	E	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	E	707	4	-	0/12/29/32	0/1/1/1
2	5TL	F	701	-	-	0/18/18/18	0/3/3/3
3	5LS	F	702	4	-	0/12/32/32	0/1/1/1
4	GLC	F	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	F	704	4	-	0/12/29/32	0/1/1/1
3	5LS	F	705	4	-	0/12/32/32	0/1/1/1
4	GLC	F	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	F	707	4	-	0/12/29/32	0/1/1/1
2	5TL	G	701	-	-	0/18/18/18	0/3/3/3
3	5LS	G	702	4	-	0/12/32/32	0/1/1/1
4	GLC	G	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	G	704	4	-	0/12/29/32	0/1/1/1
3	5LS	G	705	4	-	0/12/32/32	0/1/1/1
4	GLC	G	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	G	707	4	-	0/12/29/32	0/1/1/1
9	5TM	G	708	6	-	0/9/27/30	0/1/1/1
7	5TK	G	709	10,8	-	0/4/22/25	0/1/1/1
8	5TH	G	710	7	-	0/9/27/30	0/1/1/1
2	5TL	H	701	-	-	0/18/18/18	0/3/3/3
3	5LS	H	702	4	-	0/12/32/32	0/1/1/1
4	GLC	H	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	H	704	4	-	0/12/29/32	0/1/1/1
3	5LS	H	705	4	-	0/12/32/32	0/1/1/1
4	GLC	H	706	3,5	-	0/2/19/22	0/1/1/1
3	5LS	H	707	6	-	0/12/32/32	0/1/1/1
6	5TJ	H	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	H	709	9,10	-	0/9/27/30	0/1/1/1
10	Z4K	H	710	7,6	-	0/7/24/27	0/1/1/1
2	5TL	I	701	-	-	0/18/18/18	0/3/3/3
3	5LS	I	702	4	-	0/12/32/32	0/1/1/1
4	GLC	I	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	I	704	4	-	0/12/29/32	0/1/1/1
3	5LS	I	705	4	-	0/12/32/32	0/1/1/1
4	GLC	I	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	I	707	4	-	0/12/29/32	0/1/1/1
6	5TJ	I	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	I	709	9,10	-	0/9/27/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	5TK	I	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	I	711	7	-	0/9/27/30	0/1/1/1
2	5TL	J	701	-	-	0/18/18/18	0/3/3/3
4	GLC	J	702	3,5	-	0/2/19/22	0/1/1/1
5	PDX	J	703	4	-	0/12/29/32	0/1/1/1
3	5LS	J	704	4	-	0/12/32/32	0/1/1/1
4	GLC	J	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	J	706	4	-	0/12/29/32	0/1/1/1
3	5LS	J	707	6	-	0/12/32/32	0/1/1/1
9	5TM	J	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	J	709	7,6	-	0/7/24/27	0/1/1/1
2	5TL	K	701	-	-	0/18/18/18	0/3/3/3
3	5LS	K	702	4	-	0/12/32/32	0/1/1/1
4	GLC	K	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	K	704	4	-	0/12/29/32	0/1/1/1
3	5LS	K	705	4	-	0/12/32/32	0/1/1/1
4	GLC	K	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	K	707	4	-	0/12/29/32	0/1/1/1
2	5TL	L	701	-	-	0/18/18/18	0/3/3/3
3	5LS	L	702	4	-	0/12/32/32	0/1/1/1
5	PDX	L	703	4	-	0/12/29/32	0/1/1/1
3	5LS	L	704	4	-	0/12/32/32	0/1/1/1
4	GLC	L	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	L	706	4	-	0/12/29/32	0/1/1/1
3	5LS	L	707	4	-	0/12/32/32	0/1/1/1
4	GLC	L	708	3,5	-	0/2/19/22	0/1/1/1
5	PDX	L	709	4	-	0/12/29/32	0/1/1/1

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	5TL	S-N1	-7.07	1.48	1.60
2	H	701	5TL	S-N1	-7.02	1.48	1.60
2	F	701	5TL	S-N1	-6.99	1.48	1.60
2	B	701	5TL	S-N1	-6.92	1.48	1.60
2	L	701	5TL	S-N1	-6.82	1.48	1.60
2	I	701	5TL	S-N1	-6.81	1.48	1.60
2	J	701	5TL	S-N1	-6.76	1.48	1.60
2	C	701	5TL	S-N1	-6.73	1.48	1.60
2	A	701	5TL	S-N1	-6.54	1.49	1.60
2	D	701	5TL	S-N1	-6.51	1.49	1.60
2	K	701	5TL	S-N1	-6.46	1.49	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	5TL	S-N1	-6.45	1.49	1.60
2	G	701	5TL	CAQ-CAR	-4.50	1.33	1.42
2	I	701	5TL	CAQ-CAR	-4.45	1.33	1.42
2	A	701	5TL	CAQ-CAR	-4.39	1.34	1.42
2	C	701	5TL	CAQ-CAR	-4.38	1.34	1.42
2	J	701	5TL	CAQ-CAR	-4.34	1.34	1.42
2	H	701	5TL	CAQ-CAR	-4.33	1.34	1.42
2	F	701	5TL	CAQ-CAR	-4.32	1.34	1.42
2	B	701	5TL	CAQ-CAR	-4.23	1.34	1.42
2	D	701	5TL	CAQ-CAR	-4.20	1.34	1.42
2	K	701	5TL	CAQ-CAR	-4.17	1.34	1.42
2	E	701	5TL	CAQ-CAR	-4.16	1.34	1.42
2	L	701	5TL	CAQ-CAR	-4.11	1.34	1.42
5	G	707	PDX	O2-C2	-3.39	1.42	1.47
2	A	701	5TL	CAG-CAH	-3.34	1.40	1.49
5	I	707	PDX	O2-C2	-3.33	1.42	1.47
5	A	707	PDX	O2-C2	-3.30	1.42	1.47
5	K	707	PDX	O2-C2	-3.29	1.42	1.47
5	C	704	PDX	O2-C2	-3.29	1.42	1.47
5	G	704	PDX	O2-C2	-3.27	1.42	1.47
2	E	701	5TL	CAG-CAH	-3.26	1.40	1.49
8	I	711	5TH	O2-C2	-3.25	1.42	1.47
5	B	706	PDX	O2-C2	-3.24	1.42	1.47
2	L	701	5TL	CAG-CAH	-3.23	1.40	1.49
5	A	704	PDX	O2-C2	-3.23	1.42	1.47
5	F	707	PDX	O2-C2	-3.22	1.42	1.47
2	B	701	5TL	CAG-CAH	-3.21	1.40	1.49
2	H	701	5TL	CAG-CAH	-3.20	1.40	1.49
2	I	701	5TL	CAG-CAH	-3.18	1.40	1.49
5	L	709	PDX	O2-C2	-3.18	1.42	1.47
9	J	708	5TM	O2-C2	-3.18	1.42	1.47
10	J	709	Z4K	O2-C2	-3.16	1.42	1.47
2	L	701	5TL	CAS-CAL	-3.14	1.32	1.39
2	K	701	5TL	CAG-CAH	-3.13	1.40	1.49
8	A	711	5TH	O2-C2	-3.13	1.42	1.47
10	B	709	Z4K	O2-C2	-3.13	1.42	1.47
5	J	703	PDX	O2-C2	-3.12	1.42	1.47
5	L	703	PDX	O2-C2	-3.11	1.42	1.47
2	H	701	5TL	CAS-CAL	-3.11	1.32	1.39
5	D	707	PDX	O2-C2	-3.11	1.42	1.47
5	E	707	PDX	O2-C2	-3.10	1.42	1.47
5	D	704	PDX	O2-C2	-3.10	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	704	PDX	O2-C2	-3.09	1.42	1.47
2	C	701	5TL	CAG-CAH	-3.09	1.41	1.49
5	C	707	PDX	O2-C2	-3.09	1.42	1.47
5	K	704	PDX	O2-C2	-3.09	1.42	1.47
5	E	704	PDX	O2-C2	-3.08	1.42	1.47
9	G	708	5TM	O2-C2	-3.08	1.42	1.47
2	D	701	5TL	CAG-CAH	-3.07	1.41	1.49
2	J	701	5TL	CAG-CAH	-3.06	1.41	1.49
2	G	701	5TL	CAG-CAH	-3.06	1.41	1.49
5	L	706	PDX	O2-C2	-3.05	1.42	1.47
10	C	709	Z4K	O2-C2	-3.04	1.42	1.47
9	C	708	5TM	O2-C2	-3.04	1.42	1.47
5	H	704	PDX	O2-C2	-3.03	1.42	1.47
2	A	701	5TL	CAS-CAL	-3.01	1.33	1.39
5	B	703	PDX	O2-C2	-3.00	1.42	1.47
2	G	701	5TL	CAS-CAL	-2.99	1.33	1.39
2	C	701	5TL	CAS-CAL	-2.98	1.33	1.39
5	J	706	PDX	O2-C2	-2.98	1.42	1.47
10	H	710	Z4K	O2-C2	-2.97	1.42	1.47
2	F	701	5TL	CAG-CAH	-2.96	1.41	1.49
5	I	704	PDX	O2-C2	-2.92	1.43	1.47
2	B	701	5TL	CAS-CAL	-2.92	1.33	1.39
9	B	708	5TM	O2-C2	-2.92	1.43	1.47
8	C	711	5TH	O2-C2	-2.92	1.43	1.47
2	D	701	5TL	CAS-CAL	-2.89	1.33	1.39
2	E	701	5TL	CAS-CAL	-2.86	1.33	1.39
2	J	701	5TL	CAS-CAL	-2.85	1.33	1.39
2	I	701	5TL	CAS-CAL	-2.84	1.33	1.39
2	F	701	5TL	CAS-CAL	-2.79	1.33	1.39
2	G	701	5TL	CAQ-CAV	-2.74	1.46	1.50
8	G	710	5TH	O2-C2	-2.72	1.43	1.47
2	K	701	5TL	CAS-CAL	-2.71	1.33	1.39
2	J	701	5TL	CAQ-CAV	-2.51	1.46	1.50
2	A	701	5TL	CAI-CAJ	-2.41	1.36	1.39
2	D	701	5TL	CAQ-CAV	-2.40	1.46	1.50
2	H	701	5TL	CAQ-CAV	-2.34	1.46	1.50
2	L	701	5TL	CAQ-CAV	-2.29	1.47	1.50
2	I	701	5TL	CAI-CAJ	-2.28	1.36	1.39
2	E	701	5TL	CAI-CAJ	-2.28	1.36	1.39
2	C	701	5TL	CAI-CAJ	-2.28	1.36	1.39
2	F	701	5TL	CAI-CAJ	-2.26	1.36	1.39
2	B	701	5TL	CAQ-CAV	-2.18	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	701	5TL	CAI-CAJ	-2.18	1.36	1.39
2	G	701	5TL	CAI-CAJ	-2.17	1.36	1.39
2	C	701	5TL	CAQ-CAV	-2.15	1.47	1.50
2	B	701	5TL	CAI-CAJ	-2.12	1.36	1.39
2	A	701	5TL	CAQ-CAV	-2.09	1.47	1.50
2	L	701	5TL	CAI-CAJ	-2.05	1.36	1.39
2	H	701	5TL	CAI-CAJ	-2.05	1.36	1.39
2	J	701	5TL	CAI-CAJ	-2.04	1.36	1.39
5	A	707	PDX	C1-C2	2.06	1.55	1.51
5	G	707	PDX	C1-C2	2.21	1.55	1.51
9	G	708	5TM	C1-C2	2.33	1.55	1.51
5	B	703	PDX	C1-C2	2.43	1.55	1.51
8	G	710	5TH	C1-C2	2.49	1.55	1.51
5	I	707	PDX	C1-C2	2.49	1.55	1.51
5	K	707	PDX	C1-C2	2.53	1.55	1.51
5	G	704	PDX	C1-C2	2.59	1.56	1.51
5	F	707	PDX	C1-C2	2.60	1.56	1.51
5	J	703	PDX	C1-C2	2.73	1.56	1.51
8	I	711	5TH	C1-C2	2.73	1.56	1.51
5	D	704	PDX	C1-C2	2.76	1.56	1.51
5	A	704	PDX	C1-C2	2.80	1.56	1.51
5	C	704	PDX	C1-C2	2.80	1.56	1.51
5	E	707	PDX	C1-C2	2.81	1.56	1.51
5	B	706	PDX	C1-C2	2.82	1.56	1.51
5	D	707	PDX	C1-C2	2.83	1.56	1.51
5	L	709	PDX	C1-C2	2.84	1.56	1.51
5	C	707	PDX	C1-C2	2.97	1.56	1.51
5	E	704	PDX	C1-C2	2.99	1.56	1.51
5	K	704	PDX	C1-C2	3.05	1.56	1.51
8	A	711	5TH	C1-C2	3.09	1.56	1.51
8	C	711	5TH	C1-C2	3.24	1.57	1.51
5	H	704	PDX	C1-C2	3.27	1.57	1.51
5	I	704	PDX	C1-C2	3.31	1.57	1.51
5	J	706	PDX	C1-C2	3.37	1.57	1.51
5	L	706	PDX	C1-C2	3.47	1.57	1.51
5	F	704	PDX	C1-C2	3.55	1.57	1.51
2	G	701	5TL	CAU-S	3.74	1.82	1.77
2	C	701	5TL	CAR-NAY	3.82	1.48	1.37
2	I	701	5TL	CAR-NAY	3.84	1.48	1.37
2	B	701	5TL	CAR-NAY	3.84	1.48	1.37
2	E	701	5TL	CAR-NAY	3.88	1.48	1.37
5	L	703	PDX	C1-C2	3.90	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	5TL	CAR-NAY	3.91	1.48	1.37
2	A	701	5TL	CAR-NAY	3.91	1.48	1.37
2	K	701	5TL	CAR-NAY	3.94	1.48	1.37
2	H	701	5TL	CAR-NAY	3.94	1.49	1.37
2	K	701	5TL	CAU-S	3.95	1.82	1.77
2	J	701	5TL	CAV-NAW	3.95	1.41	1.33
2	F	701	5TL	CAV-NAW	3.95	1.41	1.33
2	J	701	5TL	CAR-NAY	3.96	1.49	1.37
2	L	701	5TL	CAV-NAW	3.96	1.41	1.33
2	H	701	5TL	CAV-NAW	3.97	1.41	1.33
2	L	701	5TL	CAR-NAY	3.98	1.49	1.37
2	F	701	5TL	CAR-NAY	3.99	1.49	1.37
2	G	701	5TL	CAV-NAW	4.01	1.41	1.33
2	D	701	5TL	CAV-NAW	4.01	1.41	1.33
2	D	701	5TL	CAR-NAY	4.04	1.49	1.37
2	G	701	5TL	CAN-CAU	4.05	1.45	1.38
2	C	701	5TL	CAN-CAU	4.09	1.45	1.38
2	G	701	5TL	CAT-CAU	4.10	1.45	1.38
2	B	701	5TL	CAV-NAW	4.11	1.41	1.33
2	A	701	5TL	CAV-NAW	4.11	1.41	1.33
2	E	701	5TL	CAN-CAU	4.12	1.45	1.38
2	I	701	5TL	CAV-NAW	4.12	1.41	1.33
2	C	701	5TL	CAV-NAW	4.12	1.41	1.33
2	F	701	5TL	CAU-S	4.13	1.83	1.77
2	A	701	5TL	CAU-S	4.15	1.83	1.77
2	F	701	5TL	CAN-CAU	4.16	1.45	1.38
2	A	701	5TL	CAN-CAU	4.16	1.45	1.38
2	H	701	5TL	CAU-S	4.17	1.83	1.77
2	I	701	5TL	CAN-CAU	4.21	1.45	1.38
2	C	701	5TL	CAU-S	4.25	1.83	1.77
2	K	701	5TL	CAN-CAU	4.25	1.45	1.38
2	K	701	5TL	CAV-NAW	4.28	1.41	1.33
2	I	701	5TL	CAU-S	4.32	1.83	1.77
2	J	701	5TL	CAU-S	4.33	1.83	1.77
2	E	701	5TL	CAU-S	4.35	1.83	1.77
2	H	701	5TL	CAN-CAU	4.35	1.45	1.38
2	E	701	5TL	CAV-NAW	4.37	1.41	1.33
2	F	701	5TL	CAT-CAU	4.38	1.45	1.38
2	H	701	5TL	CAT-CAU	4.41	1.45	1.38
2	L	701	5TL	CAN-CAU	4.43	1.45	1.38
2	B	701	5TL	CAN-CAU	4.44	1.45	1.38
2	J	701	5TL	CAN-CAU	4.44	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	5TL	CAU-S	4.45	1.83	1.77
2	K	701	5TL	CAT-CAU	4.46	1.46	1.38
2	E	701	5TL	CAT-CAU	4.48	1.46	1.38
2	A	701	5TL	CAT-CAU	4.48	1.46	1.38
2	D	701	5TL	CAU-S	4.51	1.83	1.77
2	B	701	5TL	CAT-CAU	4.54	1.46	1.38
2	C	701	5TL	CAT-CAU	4.56	1.46	1.38
2	I	701	5TL	CAT-CAU	4.56	1.46	1.38
2	J	701	5TL	CAT-CAU	4.59	1.46	1.38
2	L	701	5TL	CAT-CAU	4.62	1.46	1.38
2	L	701	5TL	CAU-S	4.62	1.83	1.77
2	D	701	5TL	CAN-CAU	4.63	1.46	1.38
2	D	701	5TL	CAT-CAU	4.65	1.46	1.38

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	5TL	CAT-CAS-CAL	-13.49	102.19	121.15
2	J	701	5TL	CAT-CAS-CAL	-13.45	102.24	121.15
2	L	701	5TL	CAT-CAS-CAL	-13.42	102.29	121.15
2	A	701	5TL	CAT-CAS-CAL	-13.38	102.34	121.15
2	C	701	5TL	CAT-CAS-CAL	-13.34	102.40	121.15
2	K	701	5TL	CAT-CAS-CAL	-13.32	102.43	121.15
2	G	701	5TL	CAT-CAS-CAL	-13.27	102.50	121.15
2	E	701	5TL	CAT-CAS-CAL	-13.26	102.52	121.15
2	H	701	5TL	CAT-CAS-CAL	-13.25	102.53	121.15
2	I	701	5TL	CAT-CAS-CAL	-13.22	102.56	121.15
2	B	701	5TL	CAT-CAS-CAL	-13.04	102.82	121.15
2	F	701	5TL	CAT-CAS-CAL	-12.49	103.60	121.15
2	K	701	5TL	CAM-CAN-CAU	-10.78	108.00	119.49
2	C	701	5TL	CAM-CAN-CAU	-10.70	108.08	119.49
2	G	701	5TL	CAM-CAN-CAU	-10.62	108.17	119.49
2	E	701	5TL	CAM-CAN-CAU	-10.58	108.21	119.49
2	A	701	5TL	CAM-CAN-CAU	-10.54	108.25	119.49
2	I	701	5TL	CAM-CAN-CAU	-10.45	108.35	119.49
2	J	701	5TL	CAM-CAN-CAU	-10.43	108.37	119.49
2	D	701	5TL	CAM-CAN-CAU	-10.41	108.39	119.49
2	H	701	5TL	CAM-CAN-CAU	-10.34	108.47	119.49
2	B	701	5TL	CAM-CAN-CAU	-10.31	108.49	119.49
2	L	701	5TL	CAM-CAN-CAU	-10.31	108.50	119.49
2	F	701	5TL	CAN-CAU-S	-9.51	105.75	119.75
2	F	701	5TL	CAM-CAN-CAU	-9.40	109.47	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	701	5TL	CAS-CAL-CAJ	-9.26	106.63	120.92
2	B	701	5TL	CAS-CAL-CAJ	-9.22	106.68	120.92
2	K	701	5TL	O4-S-O2	-9.21	106.49	118.87
2	L	701	5TL	CAS-CAL-CAJ	-9.20	106.73	120.92
2	H	701	5TL	CAS-CAL-CAJ	-9.14	106.81	120.92
2	K	701	5TL	CAS-CAL-CAJ	-9.10	106.87	120.92
2	D	701	5TL	CAS-CAL-CAJ	-9.10	106.88	120.92
2	E	701	5TL	CAS-CAL-CAJ	-9.08	106.91	120.92
2	G	701	5TL	CAS-CAL-CAJ	-9.04	106.97	120.92
2	J	701	5TL	O4-S-O2	-8.99	106.78	118.87
2	A	701	5TL	CAS-CAL-CAJ	-8.97	107.07	120.92
2	C	701	5TL	CAS-CAL-CAJ	-8.87	107.24	120.92
2	I	701	5TL	CAS-CAL-CAJ	-8.81	107.33	120.92
2	F	701	5TL	CAM-CAL-CAJ	-8.74	107.43	120.92
2	G	701	5TL	O4-S-O2	-8.58	107.34	118.87
2	E	701	5TL	CAN-CAU-S	-8.55	107.16	119.75
2	F	701	5TL	O4-S-O2	-8.53	107.41	118.87
2	C	701	5TL	CAN-CAU-S	-8.49	107.25	119.75
2	K	701	5TL	CAN-CAU-S	-8.40	107.39	119.75
2	A	701	5TL	CAN-CAU-S	-8.34	107.47	119.75
2	F	701	5TL	CAS-CAL-CAJ	-8.34	108.05	120.92
2	I	701	5TL	CAN-CAU-S	-8.33	107.48	119.75
2	G	701	5TL	CAN-CAU-S	-8.30	107.53	119.75
2	D	701	5TL	O4-S-O2	-8.29	107.73	118.87
2	D	701	5TL	CAN-CAU-S	-8.23	107.64	119.75
2	L	701	5TL	CAN-CAU-S	-8.21	107.67	119.75
2	C	701	5TL	O4-S-O2	-8.20	107.84	118.87
2	D	701	5TL	CAM-CAL-CAJ	-8.18	108.29	120.92
2	B	701	5TL	CAN-CAU-S	-8.17	107.73	119.75
2	A	701	5TL	O4-S-O2	-8.13	107.94	118.87
2	I	701	5TL	O4-S-O2	-8.12	107.95	118.87
2	J	701	5TL	CAN-CAU-S	-8.07	107.87	119.75
2	H	701	5TL	CAN-CAU-S	-8.05	107.91	119.75
2	J	701	5TL	CAM-CAL-CAJ	-8.03	108.53	120.92
2	L	701	5TL	CAM-CAL-CAJ	-8.02	108.55	120.92
2	E	701	5TL	CAM-CAL-CAJ	-7.93	108.68	120.92
2	I	701	5TL	CAM-CAL-CAJ	-7.89	108.74	120.92
2	K	701	5TL	CAM-CAL-CAJ	-7.86	108.78	120.92
2	L	701	5TL	O4-S-O2	-7.86	108.30	118.87
2	H	701	5TL	CAM-CAL-CAJ	-7.86	108.80	120.92
2	B	701	5TL	CAM-CAL-CAJ	-7.83	108.83	120.92
2	C	701	5TL	CAM-CAL-CAJ	-7.76	108.95	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	5TL	O4-S-O2	-7.75	108.46	118.87
2	G	701	5TL	CAM-CAL-CAJ	-7.69	109.06	120.92
2	A	701	5TL	CAM-CAL-CAJ	-7.67	109.08	120.92
2	H	701	5TL	O4-S-O2	-7.63	108.61	118.87
2	E	701	5TL	O4-S-O2	-7.37	108.97	118.87
2	F	701	5TL	CAN-CAM-CAL	-4.76	114.45	121.15
2	E	701	5TL	OAO-CAV-NAW	-4.71	115.86	122.58
2	K	701	5TL	OAO-CAV-NAW	-4.55	116.09	122.58
2	D	701	5TL	CAN-CAM-CAL	-4.38	114.99	121.15
2	J	701	5TL	CAN-CAM-CAL	-4.34	115.05	121.15
2	I	701	5TL	OAO-CAV-NAW	-4.25	116.52	122.58
2	C	701	5TL	OAO-CAV-NAW	-4.19	116.61	122.58
2	L	701	5TL	CAN-CAM-CAL	-4.18	115.28	121.15
2	H	701	5TL	CAN-CAM-CAL	-4.14	115.33	121.15
2	K	701	5TL	CAN-CAM-CAL	-4.12	115.36	121.15
2	E	701	5TL	CAN-CAM-CAL	-4.11	115.38	121.15
2	F	701	5TL	OAO-CAV-NAW	-4.07	116.78	122.58
2	I	701	5TL	CAN-CAM-CAL	-4.03	115.48	121.15
2	B	701	5TL	CAN-CAM-CAL	-3.99	115.54	121.15
2	G	701	5TL	CAN-CAM-CAL	-3.98	115.55	121.15
2	A	701	5TL	CAN-CAM-CAL	-3.92	115.64	121.15
2	C	701	5TL	CAN-CAM-CAL	-3.90	115.67	121.15
2	A	701	5TL	OAO-CAV-NAW	-3.84	117.11	122.58
2	L	701	5TL	OAO-CAV-NAW	-3.80	117.16	122.58
2	H	701	5TL	OAO-CAV-NAW	-3.77	117.21	122.58
2	G	701	5TL	OAO-CAV-NAW	-3.69	117.32	122.58
2	B	701	5TL	OAO-CAV-NAW	-3.65	117.38	122.58
2	G	701	5TL	CAJ-CAR-NAY	-3.63	116.05	120.12
2	J	701	5TL	OAO-CAV-NAW	-3.59	117.46	122.58
2	D	701	5TL	OAO-CAV-NAW	-3.58	117.48	122.58
2	C	701	5TL	CAJ-CAR-NAY	-3.50	116.21	120.12
2	A	701	5TL	CAJ-CAR-NAY	-3.49	116.22	120.12
3	B	704	5LS	C2-O2-S1	-3.42	112.26	118.77
3	I	702	5LS	C2-O2-S1	-3.37	112.35	118.77
5	G	704	PDX	C3-O3-S'	-3.36	112.37	118.77
3	E	705	5LS	C4-O4-S2	-3.36	112.38	118.77
2	K	701	5TL	CAJ-CAR-NAY	-3.35	116.37	120.12
2	L	701	5TL	CAJ-CAR-NAY	-3.35	116.37	120.12
3	J	707	5LS	C2-O2-S1	-3.34	112.40	118.77
3	K	705	5LS	C2-O2-S1	-3.33	112.42	118.77
3	F	702	5LS	C2-O2-S1	-3.33	112.42	118.77
2	E	701	5TL	CAJ-CAR-NAY	-3.32	116.40	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	707	PDX	C3-O3-S'	-3.31	112.47	118.77
3	F	705	5LS	C2-O2-S1	-3.31	112.47	118.77
3	G	702	5LS	C4-O4-S2	-3.30	112.48	118.77
5	K	707	PDX	C3-O3-S'	-3.30	112.49	118.77
3	L	702	5LS	C4-O4-S2	-3.28	112.52	118.77
5	C	707	PDX	C3-O3-S'	-3.28	112.52	118.77
5	G	707	PDX	C3-O3-S'	-3.27	112.53	118.77
6	I	708	5TJ	C3-O3-S3	-3.27	112.54	118.77
5	L	706	PDX	C3-O3-S'	-3.27	112.54	118.77
3	I	705	5LS	C2-O2-S1	-3.27	112.55	118.77
3	D	708	5LS	C4-O4-S2	-3.27	112.55	118.77
3	J	707	5LS	C4-O4-S2	-3.26	112.57	118.77
3	A	705	5LS	C2-O2-S1	-3.25	112.58	118.77
2	H	701	5TL	CAJ-CAR-NAY	-3.25	116.48	120.12
2	A	701	5TL	O2-S-CAU	-3.25	103.75	107.41
6	I	709	5TJ	C3-O3-S3	-3.25	112.59	118.77
3	K	702	5LS	C2-O2-S1	-3.23	112.61	118.77
3	G	705	5LS	C4-O4-S2	-3.23	112.62	118.77
3	B	704	5LS	C4-O4-S2	-3.23	112.62	118.77
3	G	702	5LS	C2-O2-S1	-3.23	112.62	118.77
3	J	704	5LS	C2-O2-S1	-3.22	112.63	118.77
3	L	707	5LS	C4-O4-S2	-3.22	112.64	118.77
3	L	702	5LS	C2-O2-S1	-3.21	112.65	118.77
3	D	705	5LS	C4-O4-S2	-3.21	112.66	118.77
3	D	705	5LS	C2-O2-S1	-3.20	112.67	118.77
3	L	704	5LS	C4-O4-S2	-3.20	112.68	118.77
3	B	707	5LS	C2-O2-S1	-3.20	112.68	118.77
3	H	702	5LS	C4-O4-S2	-3.20	112.68	118.77
3	H	702	5LS	C2-O2-S1	-3.19	112.70	118.77
3	C	702	5LS	C4-O4-S2	-3.19	112.70	118.77
3	D	709	5LS	C4-O4-S2	-3.19	112.70	118.77
3	D	708	5LS	C2-O2-S1	-3.17	112.72	118.77
5	L	709	PDX	C3-O3-S'	-3.16	112.74	118.77
3	D	702	5LS	C4-O4-S2	-3.16	112.74	118.77
3	F	702	5LS	C4-O4-S2	-3.16	112.75	118.77
5	J	706	PDX	C3-O3-S'	-3.16	112.76	118.77
6	D	710	5TJ	C3-O3-S3	-3.15	112.77	118.77
6	H	708	5TJ	C3-O3-S3	-3.15	112.77	118.77
3	G	705	5LS	C2-O2-S1	-3.15	112.78	118.77
3	E	705	5LS	C2-O2-S1	-3.15	112.78	118.77
5	I	707	PDX	C3-O3-S'	-3.14	112.79	118.77
3	I	705	5LS	C4-O4-S2	-3.14	112.79	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	705	5LS	C4-O4-S2	-3.13	112.81	118.77
3	J	704	5LS	C4-O4-S2	-3.13	112.81	118.77
2	B	701	5TL	CAJ-CAR-NAY	-3.13	116.62	120.12
3	A	705	5LS	C4-O4-S2	-3.12	112.82	118.77
3	C	702	5LS	C2-O2-S1	-3.12	112.83	118.77
2	I	701	5TL	CAJ-CAR-NAY	-3.12	116.63	120.12
3	D	709	5LS	C2-O2-S1	-3.12	112.83	118.77
6	D	711	5TJ	C3-O3-S3	-3.10	112.87	118.77
6	H	709	5TJ	C3-O3-S3	-3.09	112.88	118.77
5	F	707	PDX	C3-O3-S'	-3.09	112.89	118.77
3	D	702	5LS	C2-O2-S1	-3.08	112.90	118.77
5	E	704	PDX	C3-O3-S'	-3.08	112.91	118.77
3	L	704	5LS	C2-O2-S1	-3.07	112.92	118.77
3	H	705	5LS	C4-O4-S2	-3.07	112.93	118.77
5	D	704	PDX	C3-O3-S'	-3.06	112.94	118.77
5	J	703	PDX	C3-O3-S'	-3.05	112.95	118.77
3	E	702	5LS	C4-O4-S2	-3.05	112.96	118.77
5	C	704	PDX	C3-O3-S'	-3.04	112.97	118.77
3	A	702	5LS	C4-O4-S2	-3.04	112.98	118.77
5	B	706	PDX	C3-O3-S'	-3.04	112.98	118.77
3	C	705	5LS	C2-O2-S1	-3.02	113.02	118.77
3	B	707	5LS	C4-O4-S2	-3.01	113.04	118.77
2	J	701	5TL	CAJ-CAR-NAY	-2.99	116.77	120.12
5	K	704	PDX	C3-O3-S'	-2.99	113.08	118.77
6	A	709	5TJ	C3-O3-S3	-2.99	113.08	118.77
3	H	705	5LS	C2-O2-S1	-2.99	113.08	118.77
5	I	704	PDX	C3-O3-S'	-2.98	113.09	118.77
3	K	702	5LS	C4-O4-S2	-2.97	113.11	118.77
5	H	704	PDX	C3-O3-S'	-2.96	113.12	118.77
3	H	707	5LS	C2-O2-S1	-2.96	113.12	118.77
3	I	702	5LS	C4-O4-S2	-2.96	113.12	118.77
5	A	704	PDX	C3-O3-S'	-2.94	113.16	118.77
2	D	701	5TL	CAJ-CAR-NAY	-2.94	116.83	120.12
3	A	702	5LS	C2-O2-S1	-2.94	113.17	118.77
5	E	707	PDX	C3-O3-S'	-2.92	113.21	118.77
6	A	708	5TJ	C3-O3-S3	-2.91	113.23	118.77
3	E	702	5LS	C2-O2-S1	-2.82	113.41	118.77
5	D	707	PDX	C3-O3-S'	-2.77	113.49	118.77
5	F	704	PDX	C3-O3-S'	-2.75	113.53	118.77
2	F	701	5TL	CAJ-CAR-NAY	-2.74	117.05	120.12
2	G	701	5TL	CAQ-CAP-CAH	-2.73	116.52	121.34
2	D	701	5TL	O2-S-CAU	-2.71	104.35	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	707	5LS	C4-O4-S2	-2.69	113.65	118.77
2	C	701	5TL	O2-S-CAU	-2.67	104.40	107.41
2	J	701	5TL	O2-S-CAU	-2.64	104.43	107.41
2	F	701	5TL	O2-S-CAU	-2.62	104.45	107.41
2	I	701	5TL	O2-S-CAU	-2.60	104.48	107.41
2	B	701	5TL	O2-S-CAU	-2.58	104.50	107.41
2	A	701	5TL	CAQ-CAP-CAH	-2.54	116.87	121.34
5	L	703	PDX	C3-O3-S'	-2.46	114.08	118.77
2	B	701	5TL	CAQ-CAP-CAH	-2.45	117.01	121.34
2	L	701	5TL	CAQ-CAP-CAH	-2.38	117.14	121.34
2	H	701	5TL	CAQ-CAP-CAH	-2.34	117.21	121.34
2	D	701	5TL	CAQ-CAP-CAH	-2.34	117.22	121.34
2	E	701	5TL	CAQ-CAP-CAH	-2.32	117.25	121.34
2	H	701	5TL	O2-S-CAU	-2.29	104.83	107.41
2	F	701	5TL	CAQ-CAP-CAH	-2.25	117.38	121.34
2	J	701	5TL	CAQ-CAP-CAH	-2.24	117.39	121.34
2	K	701	5TL	CAQ-CAP-CAH	-2.21	117.44	121.34
2	C	701	5TL	CAQ-CAP-CAH	-2.21	117.45	121.34
2	L	701	5TL	O2-S-CAU	-2.20	104.92	107.41
2	G	701	5TL	O2-S-CAU	-2.15	104.99	107.41
2	G	701	5TL	CAF-CAG-CAH	-2.14	117.83	121.40
2	I	701	5TL	CAQ-CAP-CAH	-2.13	117.59	121.34
2	K	701	5TL	O2-S-CAU	-2.01	105.14	107.41
2	H	701	5TL	CAD-CAG-CAF	2.00	121.48	117.56
2	F	701	5TL	CAD-CAG-CAF	2.04	121.55	117.56
2	H	701	5TL	O4-S-N1	2.06	109.81	107.25
5	J	706	PDX	C1-C2-C3	2.07	112.58	109.48
2	B	701	5TL	CAD-CAG-CAF	2.08	121.62	117.56
5	L	706	PDX	C1-C2-C3	2.10	112.63	109.48
5	B	706	PDX	C1-C2-C3	2.13	112.67	109.48
3	E	702	5LS	C4-C3-C2	2.15	113.46	109.05
5	I	704	PDX	C1-C2-C3	2.17	112.73	109.48
2	D	701	5TL	O4-S-N1	2.27	110.07	107.25
4	E	703	GLC	C1-C2-C3	2.32	112.36	109.55
4	J	705	GLC	C1-O5-C5	2.32	115.56	112.14
2	B	701	5TL	O4-S-N1	2.46	110.31	107.25
2	F	701	5TL	CAR-CAQ-CAV	2.47	123.60	121.61
2	K	701	5TL	CAT-CAU-S	2.50	123.43	119.75
2	C	701	5TL	O4-S-N1	2.52	110.38	107.25
2	G	701	5TL	O4-S-N1	2.55	110.42	107.25
2	J	701	5TL	CAT-CAU-S	2.64	123.63	119.75
2	I	701	5TL	O4-S-N1	2.66	110.55	107.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	701	5TL	CAT-CAU-S	2.78	123.84	119.75
2	H	701	5TL	CAT-CAU-S	2.80	123.86	119.75
2	A	701	5TL	O4-S-N1	2.91	110.86	107.25
2	D	701	5TL	CAT-CAU-S	2.92	124.04	119.75
2	A	701	5TL	CAT-CAU-S	2.92	124.05	119.75
2	K	701	5TL	CAU-S-N1	2.94	112.01	108.33
2	B	701	5TL	CAT-CAU-S	2.96	124.11	119.75
2	I	701	5TL	CAT-CAU-S	2.96	124.11	119.75
5	F	704	PDX	C1-C2-C3	2.98	113.94	109.48
2	E	701	5TL	CAT-CAU-S	3.00	124.16	119.75
2	E	701	5TL	CAU-S-N1	3.00	112.09	108.33
2	C	701	5TL	CAT-CAU-S	3.02	124.19	119.75
2	J	701	5TL	O4-S-N1	3.04	111.03	107.25
2	I	701	5TL	CAU-S-N1	3.05	112.15	108.33
2	C	701	5TL	CAU-S-N1	3.05	112.16	108.33
2	G	701	5TL	CAU-S-N1	3.08	112.19	108.33
2	F	701	5TL	O4-S-N1	3.10	111.10	107.25
2	A	701	5TL	CAQ-CAV-NAW	3.13	122.69	118.08
2	L	701	5TL	CAT-CAU-S	3.18	124.43	119.75
4	J	705	GLC	C1-C2-C3	3.24	113.48	109.55
2	K	701	5TL	O4-S-N1	3.31	111.35	107.25
2	A	701	5TL	CAU-S-N1	3.31	112.47	108.33
2	F	701	5TL	O4-S-CAU	3.35	111.18	107.41
2	B	701	5TL	CAU-S-N1	3.36	112.54	108.33
2	H	701	5TL	CAU-S-N1	3.40	112.59	108.33
2	B	701	5TL	CAQ-CAV-NAW	3.43	123.14	118.08
2	D	701	5TL	CAU-S-N1	3.43	112.64	108.33
2	F	701	5TL	CAQ-CAV-NAW	3.44	123.15	118.08
4	A	706	GLC	C1-C2-C3	3.46	113.74	109.55
2	L	701	5TL	CAU-S-N1	3.46	112.67	108.33
5	L	703	PDX	C1-C2-C3	3.48	114.69	109.48
2	H	701	5TL	CAQ-CAV-NAW	3.51	123.25	118.08
2	D	701	5TL	CAQ-CAV-NAW	3.57	123.35	118.08
2	G	701	5TL	CAQ-CAV-NAW	3.57	123.35	118.08
2	K	701	5TL	CAQ-CAV-NAW	3.65	123.46	118.08
2	L	701	5TL	CAQ-CAV-NAW	3.65	123.47	118.08
2	J	701	5TL	CAQ-CAV-NAW	3.66	123.48	118.08
2	C	701	5TL	CAQ-CAV-NAW	3.70	123.53	118.08
4	J	702	GLC	C1-C2-C3	3.74	114.09	109.55
2	I	701	5TL	CAQ-CAV-NAW	3.83	123.72	118.08
2	E	701	5TL	O4-S-CAU	3.85	111.74	107.41
2	D	701	5TL	CAR-CAQ-CAV	3.96	124.80	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	5TL	CAR-CAQ-CAV	3.97	124.81	121.61
2	J	701	5TL	CAU-S-N1	3.99	113.33	108.33
2	B	701	5TL	CAR-CAQ-CAV	4.09	124.90	121.61
2	I	701	5TL	CAR-CAQ-CAV	4.10	124.91	121.61
2	E	701	5TL	CAQ-CAV-NAW	4.15	124.21	118.08
2	F	701	5TL	CAT-CAU-S	4.22	125.96	119.75
2	L	701	5TL	CAR-CAQ-CAV	4.24	125.03	121.61
2	F	701	5TL	CAI-CAJ-CAL	4.29	126.34	118.48
2	A	701	5TL	CAI-CAJ-CAL	4.33	126.42	118.48
2	H	701	5TL	CAR-CAQ-CAV	4.33	125.10	121.61
2	F	701	5TL	CAU-S-N1	4.34	113.77	108.33
2	J	701	5TL	CAR-CAQ-CAV	4.35	125.11	121.61
2	J	701	5TL	CAI-CAJ-CAL	4.36	126.47	118.48
2	G	701	5TL	O4-S-CAU	4.37	112.33	107.41
2	B	701	5TL	CAI-CAJ-CAL	4.39	126.53	118.48
2	L	701	5TL	CAI-CAJ-CAL	4.40	126.54	118.48
2	J	701	5TL	O4-S-CAU	4.40	112.36	107.41
2	K	701	5TL	CAI-CAJ-CAL	4.40	126.55	118.48
2	I	701	5TL	CAI-CAJ-CAL	4.42	126.59	118.48
2	E	701	5TL	CAI-CAJ-CAL	4.44	126.63	118.48
2	D	701	5TL	CAI-CAJ-CAL	4.44	126.63	118.48
2	E	701	5TL	CAR-CAQ-CAV	4.45	125.19	121.61
2	C	701	5TL	CAI-CAJ-CAL	4.47	126.67	118.48
2	H	701	5TL	CAI-CAJ-CAL	4.53	126.78	118.48
2	B	701	5TL	O4-S-CAU	4.53	112.52	107.41
2	K	701	5TL	O4-S-CAU	4.55	112.53	107.41
2	L	701	5TL	O4-S-CAU	4.59	112.58	107.41
2	H	701	5TL	O4-S-CAU	4.59	112.58	107.41
2	A	701	5TL	O4-S-CAU	4.63	112.62	107.41
2	C	701	5TL	CAR-CAQ-CAV	4.66	125.36	121.61
2	I	701	5TL	O4-S-CAU	4.69	112.69	107.41
2	K	701	5TL	CAR-CAQ-CAV	4.70	125.39	121.61
2	G	701	5TL	CAR-CAQ-CAV	4.72	125.41	121.61
2	G	701	5TL	CAI-CAJ-CAL	4.77	127.23	118.48
2	C	701	5TL	O4-S-CAU	4.93	112.97	107.41
2	D	701	5TL	O4-S-CAU	5.17	113.23	107.41
2	L	701	5TL	CAN-CAU-CAT	5.61	127.84	120.42
3	L	707	5LS	O2-C2-C1	5.66	115.86	107.62
2	B	701	5TL	CAN-CAU-CAT	5.82	128.11	120.42
2	H	701	5TL	CAN-CAU-CAT	5.86	128.17	120.42
2	F	701	5TL	CAN-CAU-CAT	5.90	128.22	120.42
2	D	701	5TL	CAN-CAU-CAT	5.92	128.25	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	701	5TL	CAN-CAU-CAT	6.00	128.35	120.42
2	A	701	5TL	CAN-CAU-CAT	6.03	128.40	120.42
2	J	701	5TL	CAN-CAU-CAT	6.06	128.44	120.42
2	C	701	5TL	CAN-CAU-CAT	6.11	128.50	120.42
2	G	701	5TL	CAN-CAU-CAT	6.16	128.56	120.42
2	E	701	5TL	CAN-CAU-CAT	6.21	128.63	120.42
2	K	701	5TL	CAN-CAU-CAT	6.59	129.13	120.42
2	B	701	5TL	CAM-CAL-CAS	13.04	143.03	117.56
2	G	701	5TL	CAM-CAL-CAS	13.08	143.12	117.56
2	I	701	5TL	CAM-CAL-CAS	13.09	143.13	117.56
2	C	701	5TL	CAM-CAL-CAS	13.11	143.16	117.56
2	F	701	5TL	CAM-CAL-CAS	13.13	143.21	117.56
2	A	701	5TL	CAM-CAL-CAS	13.14	143.23	117.56
2	E	701	5TL	CAM-CAL-CAS	13.21	143.37	117.56
2	H	701	5TL	CAM-CAL-CAS	13.25	143.45	117.56
2	K	701	5TL	CAM-CAL-CAS	13.26	143.47	117.56
2	L	701	5TL	CAM-CAL-CAS	13.41	143.76	117.56
2	J	701	5TL	CAM-CAL-CAS	13.48	143.88	117.56
2	D	701	5TL	CAM-CAL-CAS	13.54	144.01	117.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

43 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	5TL	3	0
3	A	705	5LS	1	0
4	A	706	GLC	1	0
2	B	701	5TL	2	0
5	B	703	PDX	1	0
4	B	705	GLC	3	0
5	B	706	PDX	1	0
3	B	707	5LS	2	0
2	C	701	5TL	4	0
3	C	702	5LS	1	0
5	C	704	PDX	1	0
4	C	706	GLC	3	0
9	C	708	5TM	1	0
10	C	709	Z4K	2	0
7	C	710	5TK	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	711	5TH	1	0
2	D	701	5TL	2	0
3	D	705	5LS	1	0
6	D	710	5TJ	1	0
2	E	701	5TL	3	0
4	E	703	GLC	1	0
4	E	706	GLC	2	0
2	F	701	5TL	6	0
4	F	703	GLC	1	0
4	F	706	GLC	1	0
2	G	701	5TL	5	0
4	G	706	GLC	1	0
2	H	701	5TL	2	0
4	H	703	GLC	1	0
3	H	705	5LS	1	0
2	I	701	5TL	6	0
4	I	706	GLC	4	0
2	J	701	5TL	2	0
4	J	702	GLC	1	0
3	J	704	5LS	2	0
4	J	705	GLC	6	0
5	J	706	PDX	4	0
2	K	701	5TL	3	0
5	K	707	PDX	1	0
2	L	701	5TL	2	0
4	L	705	GLC	2	0
5	L	706	PDX	2	0
4	L	708	GLC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	655/655 (100%)	0.06	24 (3%)	45	36	124, 249, 346, 440	0
1	B	655/655 (100%)	0.22	42 (6%)	23	16	166, 260, 355, 433	0
1	C	655/655 (100%)	0.07	22 (3%)	49	39	148, 254, 349, 435	0
1	D	655/655 (100%)	0.19	48 (7%)	18	14	164, 262, 366, 442	0
1	E	655/655 (100%)	0.12	23 (3%)	48	38	132, 252, 350, 465	0
1	F	655/655 (100%)	0.21	45 (6%)	20	15	164, 262, 370, 469	0
1	G	655/655 (100%)	0.04	21 (3%)	51	40	67, 249, 345, 479	0
1	H	655/655 (100%)	0.29	52 (7%)	15	12	149, 261, 356, 419	0
1	I	655/655 (100%)	0.16	38 (5%)	26	20	130, 257, 355, 440	0
1	J	655/655 (100%)	0.26	55 (8%)	14	11	162, 264, 366, 440	0
1	K	655/655 (100%)	0.21	43 (6%)	22	16	128, 252, 347, 450	0
1	L	655/655 (100%)	0.20	41 (6%)	23	17	165, 263, 370, 484	0
All	All	7860/7860 (100%)	0.17	454 (5%)	26	20	67, 257, 357, 484	0

All (454) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	78	ASP	12.8
1	J	7	PRO	9.7
1	K	504	SER	7.9
1	D	180	GLU	7.8
1	L	89	ASP	7.6
1	F	38	ASP	7.3
1	G	376	VAL	6.9
1	D	9	PHE	6.9
1	L	553	GLN	6.5
1	F	76	ALA	6.5
1	H	550	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	H	504	SER	6.1
1	E	504	SER	5.9
1	D	10	GLY	5.9
1	L	550	GLY	5.9
1	J	577	ASP	5.9
1	B	550	GLY	5.8
1	F	79	VAL	5.7
1	L	549	TYR	5.7
1	B	504	SER	5.7
1	F	77	CYS	5.5
1	J	575	PRO	5.5
1	E	553	GLN	5.4
1	E	500	TYR	5.4
1	J	553	GLN	5.3
1	D	8	GLU	5.3
1	J	576	SER	5.3
1	L	296	LYS	5.2
1	C	515	GLU	5.2
1	H	636	ASP	5.2
1	K	550	GLY	5.2
1	B	376	VAL	5.1
1	F	551	ARG	5.0
1	L	9	PHE	5.0
1	D	659	THR	5.0
1	G	288	GLY	4.9
1	K	503	SER	4.9
1	C	657	ALA	4.9
1	C	660	GLN	4.9
1	F	84	ASN	4.9
1	K	502	ILE	4.8
1	D	660	GLN	4.8
1	G	550	GLY	4.8
1	J	550	GLY	4.7
1	F	15	TRP	4.7
1	A	515	GLU	4.7
1	A	289	GLY	4.7
1	F	550	GLY	4.7
1	D	52	THR	4.7
1	H	506	LYS	4.7
1	F	549	TYR	4.6
1	J	506	LYS	4.6
1	I	521	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	8	GLU	4.5
1	B	636	ASP	4.5
1	C	659	THR	4.5
1	D	11	ALA	4.5
1	C	328	LEU	4.4
1	J	656	ILE	4.4
1	A	659	THR	4.4
1	I	375	GLY	4.4
1	H	515	GLU	4.4
1	E	506	LYS	4.4
1	C	311	LYS	4.3
1	J	9	PHE	4.3
1	J	660	GLN	4.3
1	F	89	ASP	4.3
1	I	376	VAL	4.3
1	I	500	TYR	4.3
1	B	377	ARG	4.3
1	J	369	SER	4.2
1	D	657	ALA	4.2
1	K	505	GLU	4.2
1	A	550	GLY	4.2
1	E	55	ARG	4.2
1	C	500	TYR	4.1
1	H	549	TYR	4.1
1	K	500	TYR	4.1
1	J	657	ALA	4.1
1	D	656	ILE	4.0
1	G	175	GLY	4.0
1	K	506	LYS	3.9
1	B	199	THR	3.9
1	L	504	SER	3.9
1	A	553	GLN	3.9
1	F	39	LEU	3.8
1	A	9	PHE	3.8
1	H	198	TYR	3.8
1	I	38	ASP	3.8
1	A	288	GLY	3.8
1	D	55	ARG	3.8
1	H	282	TRP	3.8
1	H	580	TYR	3.8
1	K	527	ILE	3.7
1	L	297	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	551	ARG	3.7
1	K	175	GLY	3.7
1	C	38	ASP	3.7
1	K	92	LEU	3.7
1	D	189	ALA	3.7
1	I	311	LYS	3.7
1	F	553	GLN	3.7
1	E	550	GLY	3.7
1	L	39	LEU	3.6
1	B	549	TYR	3.6
1	C	658	CYS	3.6
1	B	24	GLY	3.6
1	C	376	VAL	3.6
1	B	375	GLY	3.6
1	K	347	ILE	3.6
1	L	15	TRP	3.6
1	D	190	PRO	3.6
1	J	653	LEU	3.6
1	J	368	ALA	3.6
1	L	371	CYS	3.5
1	L	80	PRO	3.5
1	F	502	ILE	3.5
1	H	654	LEU	3.5
1	E	499	THR	3.5
1	H	89	ASP	3.5
1	F	80	PRO	3.4
1	C	379	CYS	3.4
1	I	660	GLN	3.4
1	J	92	LEU	3.4
1	L	502	ILE	3.4
1	C	394	TYR	3.4
1	J	507	MET	3.4
1	K	501	GLY	3.4
1	I	40	LYS	3.4
1	H	505	GLU	3.4
1	B	502	ILE	3.4
1	A	290	PRO	3.4
1	D	191	GLU	3.4
1	E	501	GLY	3.4
1	I	15	TRP	3.4
1	D	553	GLN	3.4
1	G	502	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	174	GLN	3.3
1	A	18	ARG	3.3
1	K	553	GLN	3.3
1	K	499	THR	3.3
1	F	176	GLU	3.3
1	D	504	SER	3.3
1	G	260	GLN	3.3
1	F	296	LYS	3.3
1	I	39	LEU	3.3
1	F	171	ASP	3.3
1	D	12	GLY	3.3
1	I	659	THR	3.3
1	H	553	GLN	3.2
1	J	36	GLU	3.2
1	H	653	LEU	3.2
1	E	503	SER	3.2
1	E	524	VAL	3.2
1	F	33	GLN	3.2
1	L	40	LYS	3.2
1	J	260	GLN	3.2
1	K	89	ASP	3.2
1	D	197	PRO	3.2
1	H	502	ILE	3.2
1	F	23	THR	3.2
1	B	506	LYS	3.2
1	A	175	GLY	3.2
1	I	517	LYS	3.2
1	C	656	ILE	3.1
1	E	175	GLY	3.1
1	D	50	LEU	3.1
1	I	515	GLU	3.1
1	J	574	ARG	3.1
1	J	374	ASP	3.1
1	H	632	ILE	3.1
1	L	180	GLU	3.1
1	I	328	LEU	3.1
1	C	517	LYS	3.0
1	J	90	VAL	3.0
1	L	575	PRO	3.0
1	I	297	GLN	3.0
1	J	371	CYS	3.0
1	K	529	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	658	CYS	3.0
1	J	86	LEU	3.0
1	A	660	GLN	3.0
1	B	6	ASP	3.0
1	D	88	HIS	3.0
1	G	659	THR	3.0
1	H	199	THR	3.0
1	H	372	VAL	3.0
1	I	654	LEU	3.0
1	J	91	PRO	3.0
1	L	8	GLU	3.0
1	J	87	ILE	3.0
1	G	553	GLN	3.0
1	H	174	GLN	3.0
1	F	375	GLY	3.0
1	K	485	LYS	3.0
1	D	260	GLN	3.0
1	B	289	GLY	2.9
1	J	379	CYS	2.9
1	H	503	SER	2.9
1	G	286	GLN	2.9
1	G	377	ARG	2.9
1	E	242	ILE	2.9
1	F	552	ARG	2.9
1	J	10	GLY	2.9
1	K	242	ILE	2.9
1	F	376	VAL	2.9
1	C	524	VAL	2.9
1	D	658	CYS	2.9
1	B	171	ASP	2.9
1	L	639	VAL	2.8
1	F	194	GLU	2.8
1	I	523	GLU	2.8
1	G	289	GLY	2.8
1	H	177	LEU	2.8
1	F	40	LYS	2.8
1	A	6	ASP	2.8
1	K	378	GLY	2.8
1	J	377	ARG	2.8
1	I	636	ASP	2.8
1	B	553	GLN	2.8
1	I	657	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	505	GLU	2.8
1	F	24	GLY	2.8
1	K	93	LEU	2.8
1	J	502	ILE	2.8
1	F	653	LEU	2.8
1	I	379	CYS	2.8
1	C	377	ARG	2.8
1	E	7	PRO	2.8
1	A	376	VAL	2.8
1	G	7	PRO	2.7
1	G	89	ASP	2.7
1	H	9	PHE	2.7
1	B	191	GLU	2.7
1	A	504	SER	2.7
1	A	612	LEU	2.7
1	C	312	ILE	2.7
1	D	496	GLU	2.7
1	B	400	SER	2.7
1	D	632	ILE	2.7
1	K	479	LYS	2.7
1	J	190	PRO	2.7
1	H	479	LYS	2.7
1	I	36	GLU	2.7
1	K	328	LEU	2.7
1	L	653	LEU	2.7
1	B	288	GLY	2.7
1	K	482	PHE	2.7
1	A	656	ILE	2.7
1	I	37	LEU	2.7
1	H	171	ASP	2.7
1	I	369	SER	2.7
1	J	400	SER	2.7
1	L	38	ASP	2.7
1	B	521	TYR	2.7
1	D	177	LEU	2.6
1	L	231	HIS	2.6
1	F	640	MET	2.6
1	H	656	ILE	2.6
1	L	495	SER	2.6
1	D	84	ASN	2.6
1	D	655	LYS	2.6
1	K	377	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	52	THR	2.6
1	I	632	ILE	2.6
1	F	297	GLN	2.6
1	H	50	LEU	2.6
1	B	518	ALA	2.6
1	D	376	VAL	2.6
1	H	518	ALA	2.6
1	I	377	ARG	2.6
1	G	282	TRP	2.6
1	D	523	GLU	2.6
1	K	392	THR	2.6
1	H	325	SER	2.6
1	D	502	ILE	2.6
1	E	502	ILE	2.6
1	B	180	GLU	2.6
1	K	7	PRO	2.6
1	I	6	ASP	2.6
1	E	40	LYS	2.6
1	G	290	PRO	2.6
1	K	554	GLY	2.5
1	G	6	ASP	2.5
1	L	190	PRO	2.5
1	I	502	ILE	2.5
1	H	371	CYS	2.5
1	A	521	TYR	2.5
1	C	518	ALA	2.5
1	F	9	PHE	2.5
1	F	581	SER	2.5
1	H	170	LYS	2.5
1	K	523	GLU	2.5
1	C	36	GLU	2.5
1	K	656	ILE	2.5
1	L	547	SER	2.5
1	L	181	PHE	2.5
1	F	254	PHE	2.5
1	J	338	GLN	2.5
1	L	284	PRO	2.5
1	E	378	GLY	2.5
1	L	656	ILE	2.5
1	L	372	VAL	2.5
1	I	518	ALA	2.5
1	H	575	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	24	GLY	2.5
1	D	254	PHE	2.5
1	B	40	LYS	2.5
1	L	282	TRP	2.5
1	J	35	ARG	2.5
1	J	311	LYS	2.5
1	H	324	ILE	2.4
1	L	194	GLU	2.4
1	H	512	LYS	2.4
1	K	400	SER	2.4
1	J	659	THR	2.4
1	B	635	ALA	2.4
1	C	516	GLU	2.4
1	J	501	GLY	2.4
1	J	15	TRP	2.4
1	A	502	ILE	2.4
1	A	580	TYR	2.4
1	K	524	VAL	2.4
1	B	33	GLN	2.4
1	B	479	LYS	2.4
1	B	476	LEU	2.4
1	G	504	SER	2.4
1	F	636	ASP	2.4
1	K	55	ARG	2.4
1	L	311	LYS	2.4
1	L	55	ARG	2.4
1	I	34	HIS	2.3
1	I	514	MET	2.3
1	D	195	ASN	2.3
1	J	23	THR	2.3
1	J	183	GLY	2.3
1	D	479	LYS	2.3
1	I	14	PRO	2.3
1	C	553	GLN	2.3
1	L	548	PRO	2.3
1	B	285	GLN	2.3
1	F	34	HIS	2.3
1	A	394	TYR	2.3
1	A	657	ALA	2.3
1	J	654	LEU	2.3
1	L	186	GLN	2.3
1	D	7	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	188	LEU	2.3
1	B	170	LYS	2.3
1	D	241	CYS	2.3
1	J	11	ALA	2.3
1	H	191	GLU	2.3
1	J	376	VAL	2.3
1	K	9	PHE	2.3
1	H	574	ARG	2.3
1	I	656	ILE	2.3
1	B	515	GLU	2.3
1	G	577	ASP	2.3
1	A	505	GLU	2.3
1	B	25	GLY	2.3
1	D	240	LYS	2.3
1	F	299	ARG	2.3
1	H	524	VAL	2.3
1	D	377	ARG	2.2
1	D	550	GLY	2.2
1	D	139	LYS	2.2
1	B	503	SER	2.2
1	F	292	ASP	2.2
1	H	376	VAL	2.2
1	L	362	LEU	2.2
1	F	37	LEU	2.2
1	B	89	ASP	2.2
1	H	405	ASP	2.2
1	I	550	GLY	2.2
1	F	607	HIS	2.2
1	J	655	LYS	2.2
1	H	280	LEU	2.2
1	A	286	GLN	2.2
1	H	281	ASN	2.2
1	I	33	GLN	2.2
1	H	6	ASP	2.2
1	J	505	GLU	2.2
1	J	335	HIS	2.2
1	A	7	PRO	2.2
1	D	181	PHE	2.2
1	E	35	ARG	2.2
1	K	36	GLU	2.2
1	D	51	SER	2.2
1	E	400	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	640	MET	2.2
1	B	36	GLU	2.2
1	G	521	TYR	2.2
1	B	378	GLY	2.2
1	J	367	PRO	2.2
1	K	33	GLN	2.2
1	E	557	MET	2.2
1	B	632	ILE	2.2
1	F	495	SER	2.2
1	K	653	LEU	2.1
1	D	242	ILE	2.1
1	F	290	PRO	2.1
1	K	660	GLN	2.1
1	I	343	ARG	2.1
1	E	576	SER	2.1
1	J	375	GLY	2.1
1	L	607	HIS	2.1
1	I	639	VAL	2.1
1	B	16	GLU	2.1
1	E	532	ASP	2.1
1	H	7	PRO	2.1
1	G	262	ASN	2.1
1	K	332	GLU	2.1
1	K	530	LEU	2.1
1	D	198	TYR	2.1
1	F	548	PRO	2.1
1	C	37	LEU	2.1
1	H	652	HIS	2.1
1	D	49	GLU	2.1
1	F	498	MET	2.1
1	J	658	CYS	2.1
1	H	242	ILE	2.1
1	F	362	LEU	2.1
1	H	523	GLU	2.1
1	B	7	PRO	2.1
1	J	551	ARG	2.1
1	H	143	ARG	2.1
1	D	170	LYS	2.1
1	J	652	HIS	2.1
1	K	611	LEU	2.1
1	B	284	PRO	2.0
1	D	196	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	92	LEU	2.0
1	L	33	GLN	2.0
1	I	394	TYR	2.0
1	H	476	LEU	2.0
1	B	143	ARG	2.0
1	K	346	GLY	2.0
1	G	261	PRO	2.0
1	H	52	THR	2.0
1	J	349	THR	2.0
1	J	529	TYR	2.0
1	B	86	LEU	2.0
1	L	659	THR	2.0
1	L	291	VAL	2.0
1	E	505	GLU	2.0
1	F	546	LYS	2.0
1	H	240	LYS	2.0
1	J	357	GLU	2.0
1	F	175	GLY	2.0
1	H	180	GLU	2.0
1	B	39	LEU	2.0
1	H	525	GLY	2.0
1	H	526	VAL	2.0
1	K	352	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	5LS	K	702	20/20	0.11	0.99	14.18	363,425,467,471	0
4	GLC	K	703	11/12	0.47	1.14	9.56	360,413,466,537	0
3	5LS	D	702	20/20	0.50	0.65	4.49	340,440,517,518	0
2	5TL	L	701	26/26	0.51	0.77	3.52	158,266,335,350	0
5	PDX	K	707	19/20	0.68	0.50	3.02	257,458,487,488	0
3	5LS	L	704	20/20	0.48	0.49	2.92	358,404,444,460	0
2	5TL	H	701	26/26	0.65	0.51	2.50	226,257,279,282	0
2	5TL	E	701	26/26	0.55	0.59	2.34	127,197,233,277	0
3	5LS	B	707	20/20	0.13	1.10	2.12	410,470,536,552	0
2	5TL	K	701	26/26	0.59	0.57	1.91	131,202,237,288	0
5	PDX	I	704	19/20	0.76	0.32	1.75	247,401,449,453	0
10	Z4K	C	709	15/16	0.81	0.62	1.73	512,546,562,567	0
2	5TL	A	701	26/26	0.72	0.51	1.71	121,206,278,306	0
5	PDX	G	704	19/20	0.72	0.49	1.66	394,475,502,529	0
2	5TL	B	701	26/26	0.48	0.63	1.55	149,237,280,287	0
2	5TL	J	701	26/26	0.54	0.55	1.40	179,264,307,319	0
3	5LS	G	702	20/20	0.66	0.48	1.31	282,367,436,438	0
2	5TL	I	701	26/26	0.68	0.49	1.20	152,242,284,323	0
2	5TL	C	701	26/26	0.73	0.44	1.04	150,234,279,291	0
2	5TL	F	701	26/26	0.61	0.44	0.97	157,307,408,431	0
2	5TL	D	701	26/26	0.73	0.43	0.71	197,297,320,332	0
4	GLC	C	706	11/12	0.64	0.34	0.39	287,335,428,484	0
2	5TL	G	701	26/26	0.78	0.39	0.28	108,200,280,288	0
5	PDX	L	709	19/20	0.20	0.49	0.25	302,421,476,480	0
5	PDX	E	707	19/20	0.58	0.36	0.11	330,398,456,471	0
5	PDX	C	704	19/20	0.81	0.21	-2.04	382,434,463,471	0
3	5LS	K	705	20/20	0.82	0.17	-	347,522,574,579	0
3	5LS	D	705	20/20	0.59	0.18	-	368,431,456,471	0
3	5LS	F	705	20/20	0.68	0.26	-	404,467,489,501	0
5	PDX	G	707	19/20	0.70	0.29	-	241,384,434,436	0
3	5LS	A	702	20/20	0.77	0.56	-	337,376,407,435	0
3	5LS	E	702	20/20	0.60	0.41	-	384,414,438,442	0
3	5LS	F	702	20/20	0.70	0.34	-	348,474,507,510	0
9	5TM	J	708	17/18	0.69	0.54	-	429,491,543,555	0
4	GLC	H	703	11/12	0.69	0.28	-	220,288,388,445	0
9	5TM	G	708	17/18	0.29	0.50	-	462,507,517,524	0
10	Z4K	J	709	15/16	0.51	0.30	-	437,501,519,520	0
9	5TM	C	708	17/18	0.68	0.35	-	479,506,524,529	0
8	5TH	I	711	17/18	0.70	0.43	-	384,477,520,526	0
4	GLC	F	703	11/12	0.45	0.57	-	347,378,409,472	0
3	5LS	L	707	20/20	0.51	0.39	-	442,520,539,550	0
5	PDX	I	707	19/20	0.60	0.51	-	270,404,472,478	0
4	GLC	I	706	11/12	0.87	0.35	-	197,292,365,403	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PDX	L	703	19/20	0.80	0.49	-	291,428,471,474	0
4	GLC	B	702	11/12	0.82	0.27	-	259,379,417,450	0
5	PDX	A	707	19/20	0.67	0.51	-	218,410,475,496	0
3	5LS	A	705	20/20	0.48	0.29	-	320,445,483,493	0
5	PDX	J	706	19/20	0.15	0.70	-	321,419,508,517	0
3	5LS	G	705	20/20	0.87	0.21	-	361,462,493,495	0
7	5TK	I	710	13/14	0.83	0.62	-	409,452,467,476	0
3	5LS	C	702	20/20	0.80	0.40	-	412,438,452,452	0
4	GLC	I	703	11/12	0.83	0.27	-	216,358,388,409	0
4	GLC	J	705	11/12	0.89	0.51	-	329,361,377,405	0
9	5TM	B	708	17/18	0.51	0.77	-	442,503,540,543	0
6	5TJ	A	709	17/18	0.66	0.44	-	394,528,538,539	0
3	5LS	D	708	20/20	0.52	0.41	-	406,436,450,462	0
6	5TJ	D	710	17/18	0.72	0.94	-	487,535,554,557	0
5	PDX	C	707	19/20	0.61	0.44	-	242,541,570,575	0
3	5LS	J	707	20/20	0.52	0.39	-	472,553,561,566	0
6	5TJ	H	708	17/18	0.57	0.74	-	305,465,516,533	0
3	5LS	I	705	20/20	0.82	0.16	-	255,515,567,577	0
4	GLC	C	703	11/12	0.76	0.38	-	358,404,431,439	0
3	5LS	E	705	20/20	0.76	0.17	-	275,459,474,500	0
3	5LS	H	707	20/20	0.66	1.05	-	430,502,561,583	0
5	PDX	H	704	19/20	0.80	0.62	-	266,436,468,474	0
3	5LS	C	705	20/20	0.45	0.29	-	318,398,444,472	0
4	GLC	E	703	11/12	0.76	0.42	-	335,392,442,495	0
3	5LS	B	704	20/20	0.40	0.47	-	356,421,481,498	0
3	5LS	H	705	20/20	0.77	0.38	-	402,453,485,501	0
5	PDX	J	703	19/20	0.71	0.34	-	404,488,531,532	0
3	5LS	L	702	20/20	0.72	0.34	-	414,473,550,553	0
7	5TK	C	710	13/14	0.72	0.99	-	498,545,563,567	0
5	PDX	L	706	19/20	0.43	0.65	-	373,474,502,503	0
5	PDX	A	704	19/20	0.51	0.96	-	294,542,568,576	0
5	PDX	D	704	19/20	0.64	0.44	-	395,433,465,466	0
4	GLC	J	702	11/12	0.74	0.33	-	394,429,498,537	0
6	5TJ	I	709	17/18	0.82	0.52	-	385,519,554,575	0
3	5LS	H	702	20/20	0.70	0.23	-	291,429,473,484	0
3	5LS	I	702	20/20	0.81	0.32	-	388,452,499,510	0
4	GLC	A	703	11/12	0.77	0.42	-	366,443,481,495	0
8	5TH	A	711	17/18	0.64	0.29	-	382,454,506,522	0
8	5TH	C	711	17/18	0.42	0.75	-	286,465,514,523	0
3	5LS	J	704	20/20	0.60	0.31	-	308,429,475,496	0
4	GLC	B	705	11/12	0.76	1.04	-	333,423,476,483	0
5	PDX	F	704	19/20	0.50	0.47	-	366,456,485,489	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GLC	E	706	11/12	0.89	0.18	-	275,289,341,375	0
4	GLC	F	706	11/12	0.78	0.55	-	267,377,431,435	0
3	5LS	D	709	20/20	0.33	0.44	-	390,510,562,568	0
7	5TK	A	710	13/14	0.71	0.78	-	377,494,522,528	0
5	PDX	F	707	19/20	0.25	0.54	-	366,469,493,510	0
4	GLC	A	706	11/12	0.76	0.43	-	357,383,424,432	0
10	Z4K	H	710	15/16	0.51	0.28	-	442,503,528,534	0
5	PDX	D	707	19/20	0.44	0.30	-	373,430,480,492	0
5	PDX	K	704	19/20	0.37	0.44	-	442,555,569,571	0
6	5TJ	A	708	17/18	0.48	0.60	-	520,543,568,570	0
5	PDX	B	706	19/20	0.55	0.65	-	309,489,529,530	0
7	5TK	G	709	13/14	0.68	0.64	-	431,547,571,574	0
4	GLC	L	708	11/12	0.83	0.64	-	315,385,428,432	0
5	PDX	E	704	19/20	0.59	0.34	-	120,485,579,583	0
4	GLC	H	706	11/12	0.84	0.38	-	361,408,422,461	0
4	GLC	K	706	11/12	0.76	0.20	-	321,350,440,452	0
4	GLC	L	705	11/12	0.60	0.41	-	330,367,393,433	0
6	5TJ	I	708	17/18	0.60	0.85	-	468,554,566,566	0
4	GLC	G	703	11/12	0.58	0.37	-	370,394,435,475	0
6	5TJ	D	711	17/18	0.44	0.55	-	291,502,575,583	0
4	GLC	G	706	11/12	0.84	0.27	-	263,307,356,360	0
5	PDX	B	703	19/20	0.76	0.34	-	246,460,539,547	0
8	5TH	G	710	17/18	0.40	0.45	-	386,527,562,566	0
4	GLC	D	706	11/12	0.79	0.40	-	380,397,417,446	0
6	5TJ	H	709	17/18	0.50	0.45	-	452,494,530,541	0
4	GLC	D	703	11/12	0.23	0.80	-	419,441,472,478	0
10	Z4K	B	709	15/16	0.46	0.33	-	441,493,519,523	0

6.5 Other polymers (i)

There are no such residues in this entry.