Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:19 AM GMT

PDB ID	:	3OGK
Title	:	Structure of COI1-ASK1 in complex with coronatine and an incomplete JAZ1 degron
Authors	:	Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.; Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.
Deposited on	:	2010-08-16
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

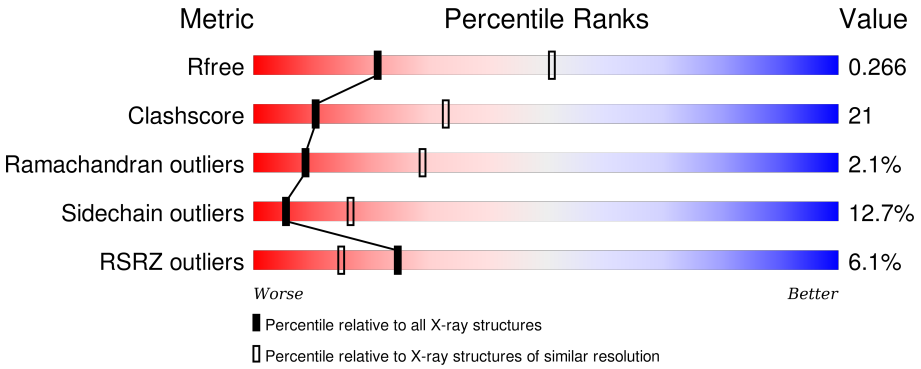
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	160	6% 56% 31% • 9%
1	C	160	18% 54% 30% 6% 9%
1	E	160	3% 58% 29% • 9%
1	G	160	4% 58% 28% 5% 9%
1	I	160	12% 49% 36% 5% 9%

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Mol	Chain	Length	Quality of chain
1	K	160	13% 56% 31% 9%
1	M	160	14% 57% 29% 5% 9%
1	O	160	28% 59% 29% 9%
2	B	592	2% 59% 28% 8%
2	D	592	3% 57% 30% 8%
2	F	592	4% 55% 33% 8%
2	H	592	% 40% 41% 13% 5%
2	J	592	3% 56% 31% 8%
2	L	592	3% 55% 33% 8%
2	N	592	7% 55% 33% 7%
2	P	592	6% 55% 34% 7%
3	Q	22	50% 9% 41%
3	R	22	32% 50% 9% 41%
3	S	22	14% 45% 14% 41%
3	U	22	9% 50% 9% 41%
3	V	22	23% 45% 14% 41%
3	W	22	23% 50% 9% 41%
3	X	22	18% 50% 9% 41%

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
4	OGK	B	1100	X	-	-	-
4	OGK	D	1100	X	-	-	-
4	OGK	H	1100	X	-	-	-
4	OGK	L	1100	X	-	X	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	-	X	-
5	PO4	D	1103	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	F	1101	-	X	-	-
5	PO4	H	1101	-	X	X	-
5	PO4	H	1102	-	-	-	X
5	PO4	H	1103	-	X	X	-
5	PO4	H	1104	-	-	-	X
5	PO4	J	1103	-	-	X	X
5	PO4	N	1103	-	-	X	-
5	PO4	N	1104	-	-	-	X
5	PO4	P	1103	-	-	X	-
5	PO4	P	1104	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46526 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	C	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	E	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	G	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	I	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	K	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	M	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	O	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			

- Molecule 2 is a protein called Coronatine-insensitive protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	D	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	F	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	L	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

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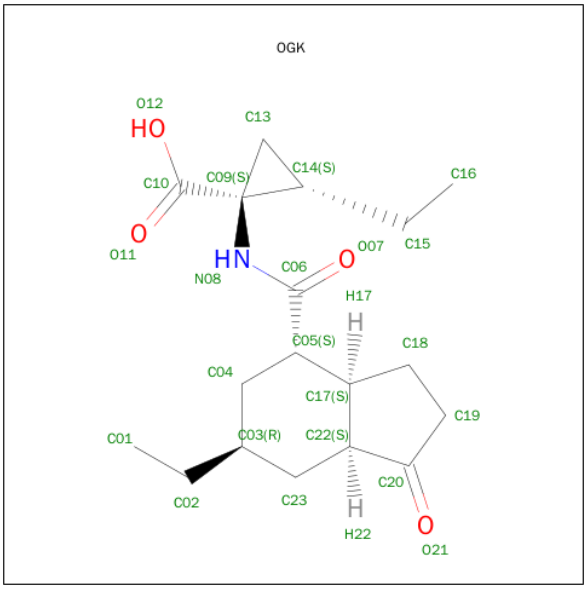
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	P	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

- Molecule 3 is a protein called JAZ1 incomplete degron peptide.

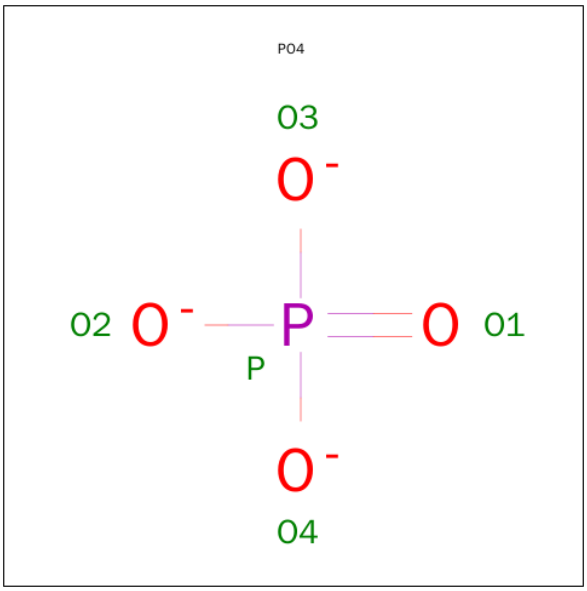
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	R	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	S	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	U	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	V	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	W	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	X	13	Total	C	N	O	0	0	0
			119	74	29	16			

- Molecule 4 is (1S,2S)-2-ETHYL-1-({[(3AS,4S,6R,7AS)-6-ETHYL-1-OXOOCTAHYDRO-1H-INDEN-4-YL]CARBONYL}AMINO)CYCLOPROPANECARBOXYLIC ACID (three-letter code: OGK) (formula: $C_{18}H_{27}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 23 18 1 4	0	0
4	D	1	Total C N O 23 18 1 4	0	0
4	F	1	Total C N O 23 18 1 4	0	0
4	H	1	Total C N O 23 18 1 4	0	0
4	J	1	Total C N O 23 18 1 4	0	0
4	L	1	Total C N O 23 18 1 4	0	0
4	N	1	Total C N O 23 18 1 4	0	0
4	P	1	Total C N O 23 18 1 4	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0

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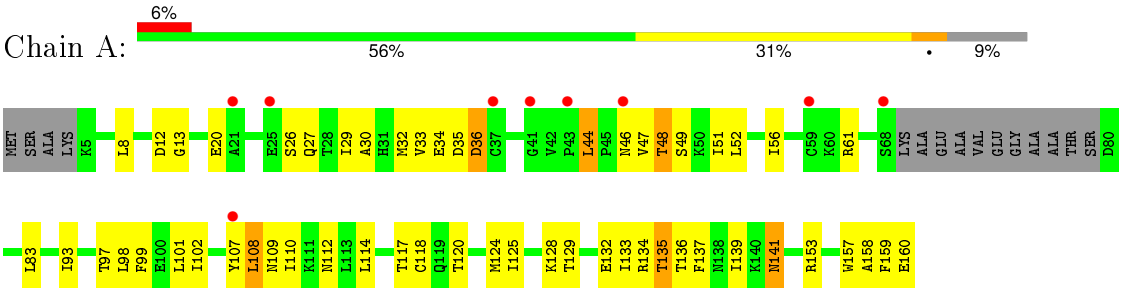
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0

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.

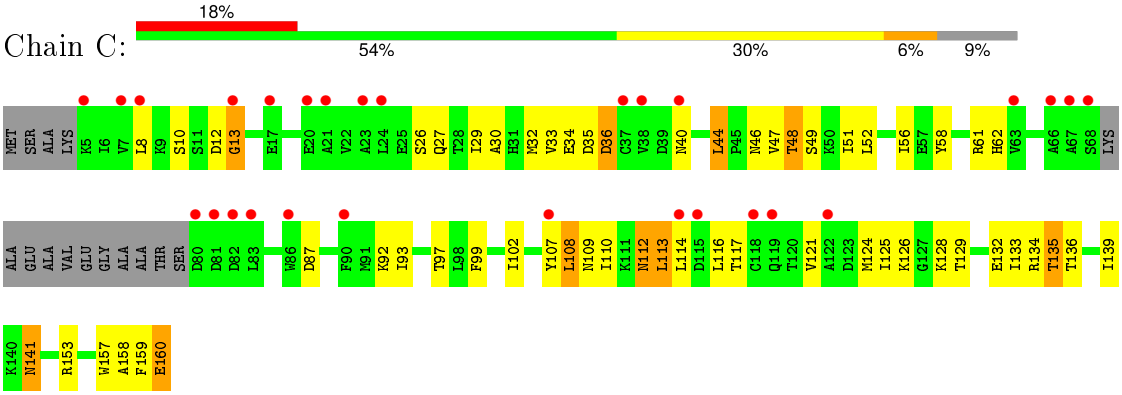
- Molecule 1: SKP1-like protein 1A

Chain A:



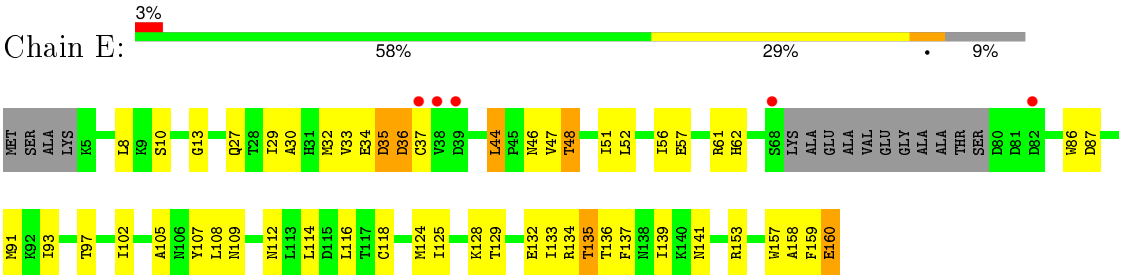
- Molecule 1: SKP1-like protein 1A

Chain C:



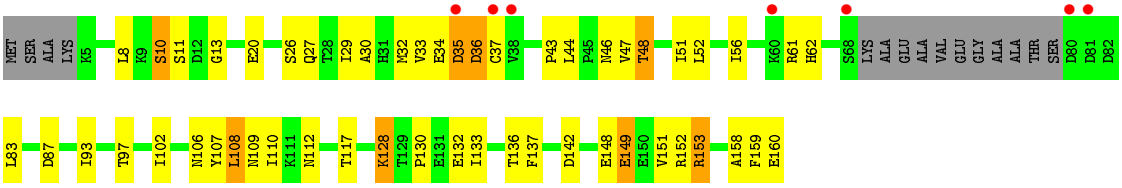
- Molecule 1: SKP1-like protein 1A

Chain E:



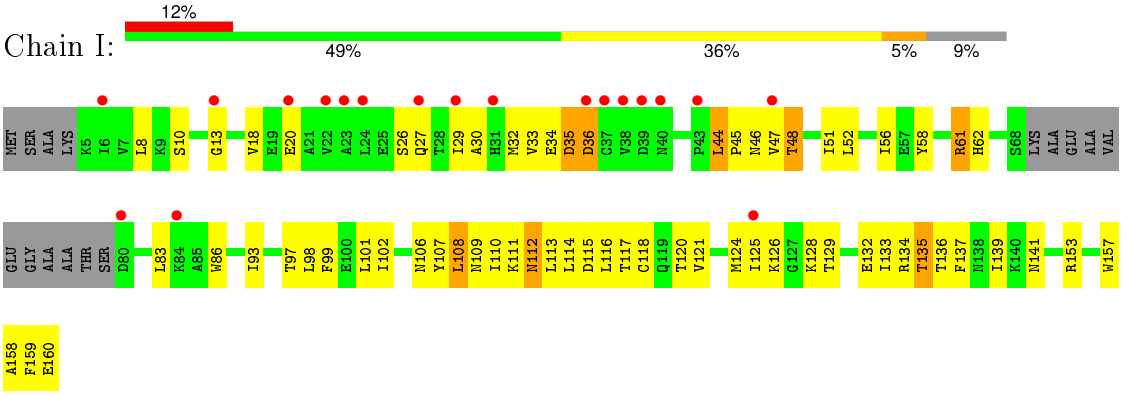
- Molecule 1: SKP1-like protein 1A

Chain G:



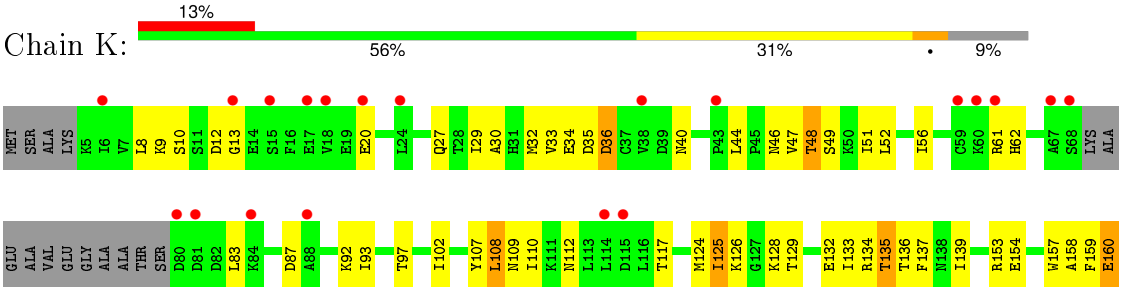
• Molecule 1: SKP1-like protein 1A

Chain I:



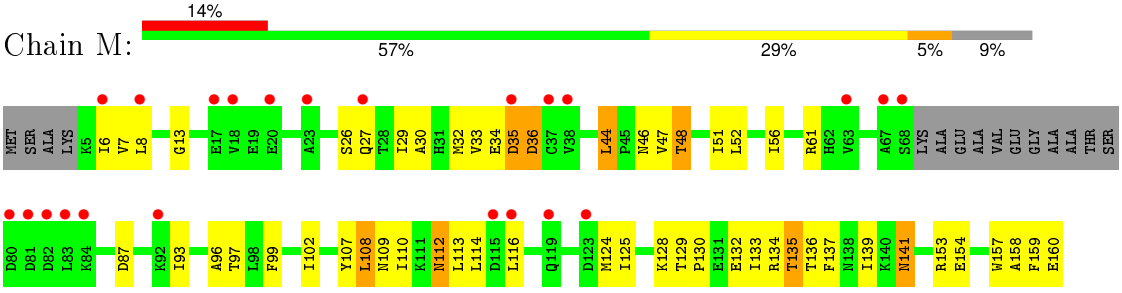
• Molecule 1: SKP1-like protein 1A

Chain K:



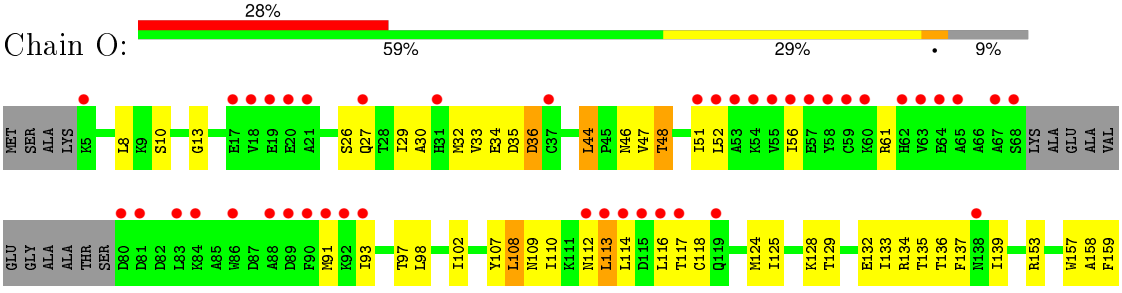
• Molecule 1: SKP1-like protein 1A

Chain M:



• Molecule 1: SKP1-like protein 1A

Chain O:



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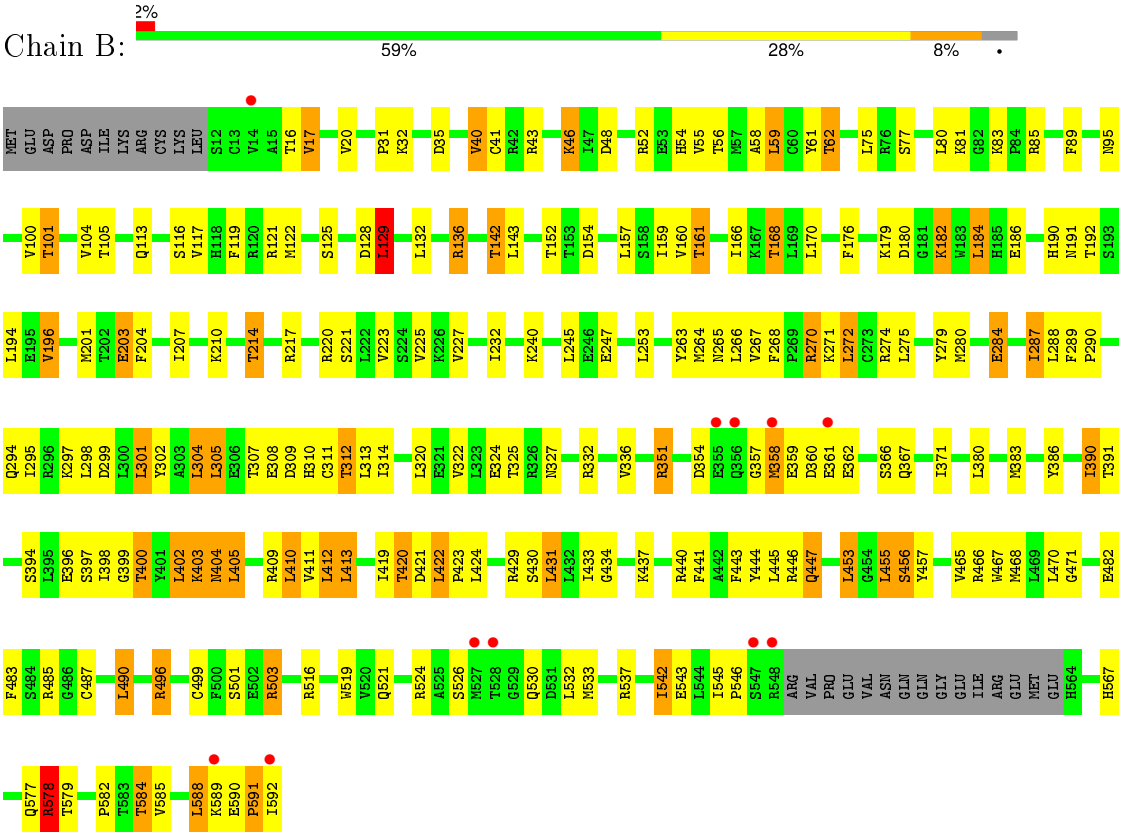
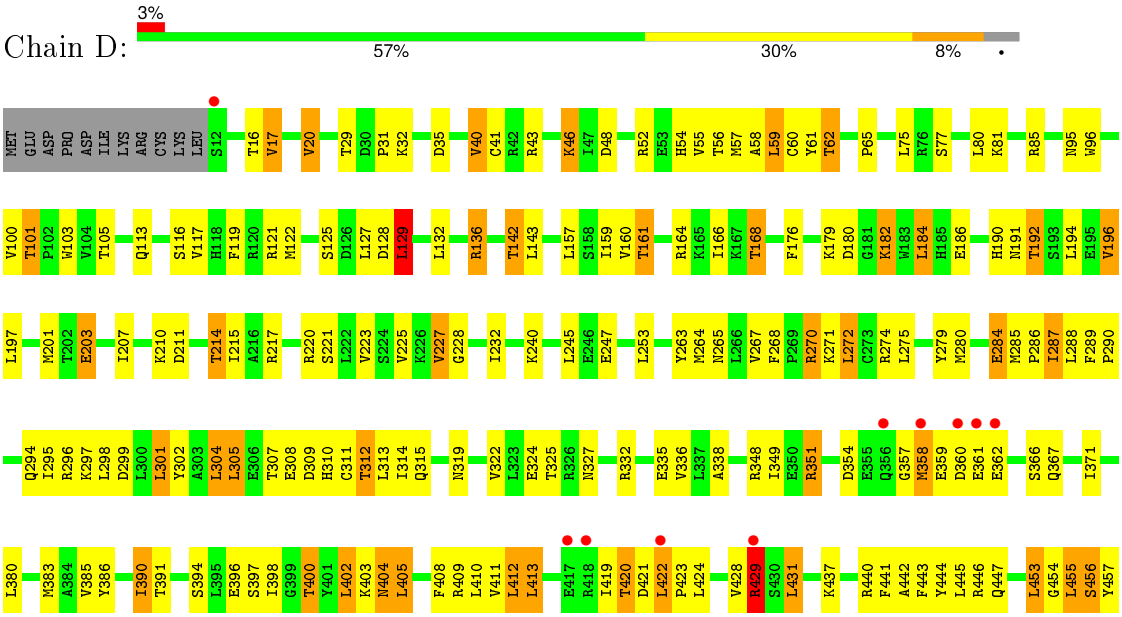
- Molecule 2: Coronatine-insensitive protein 1

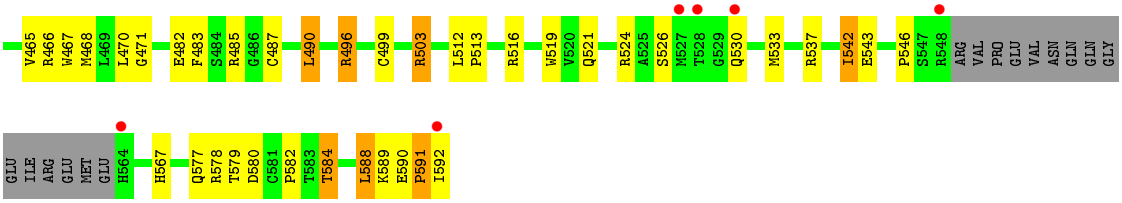
Chain B:



- Molecule 2: Coronatine-insensitive protein 1

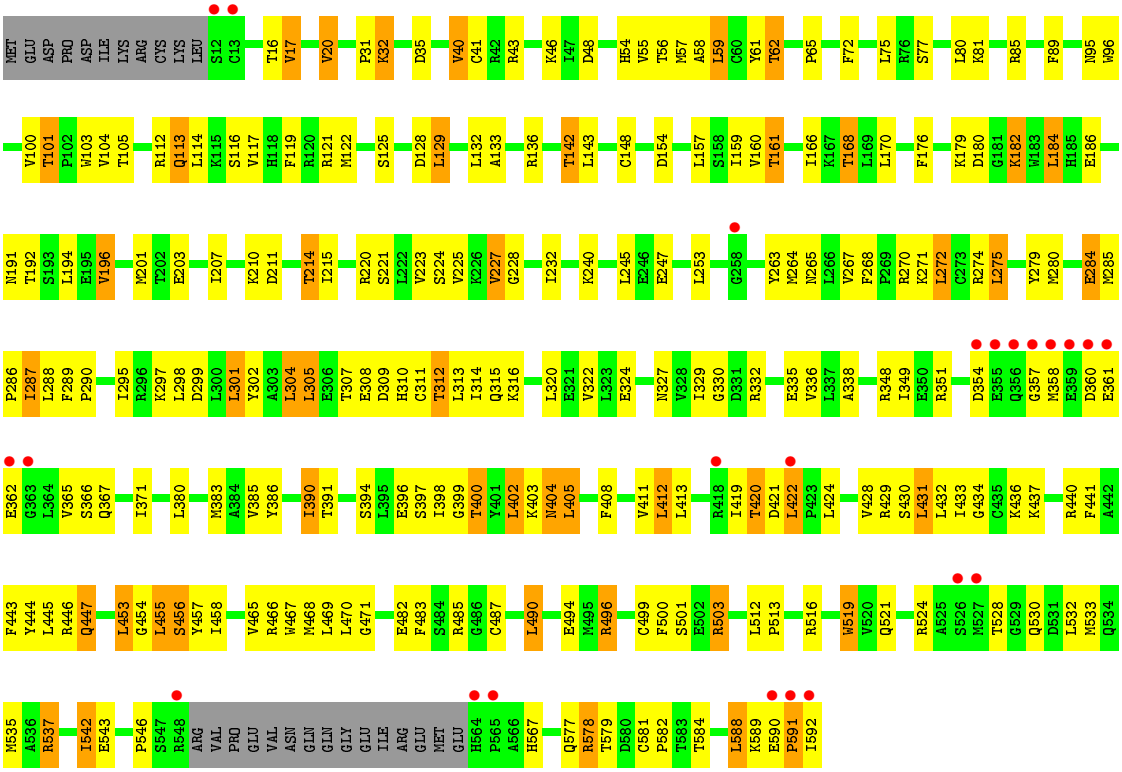
Chain D:





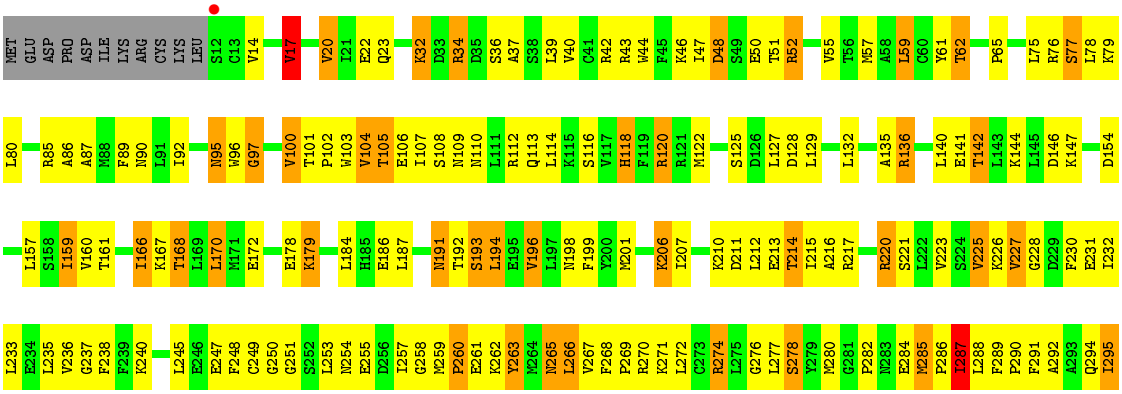
• Molecule 2: Coronatine-insensitive protein 1

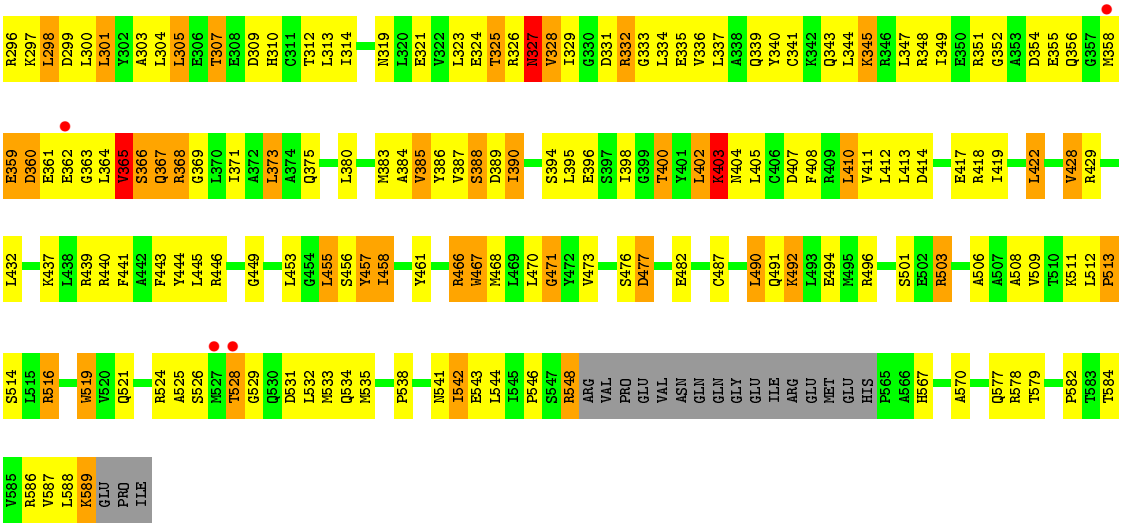
Chain F:



• Molecule 2: Coronatine-insensitive protein 1

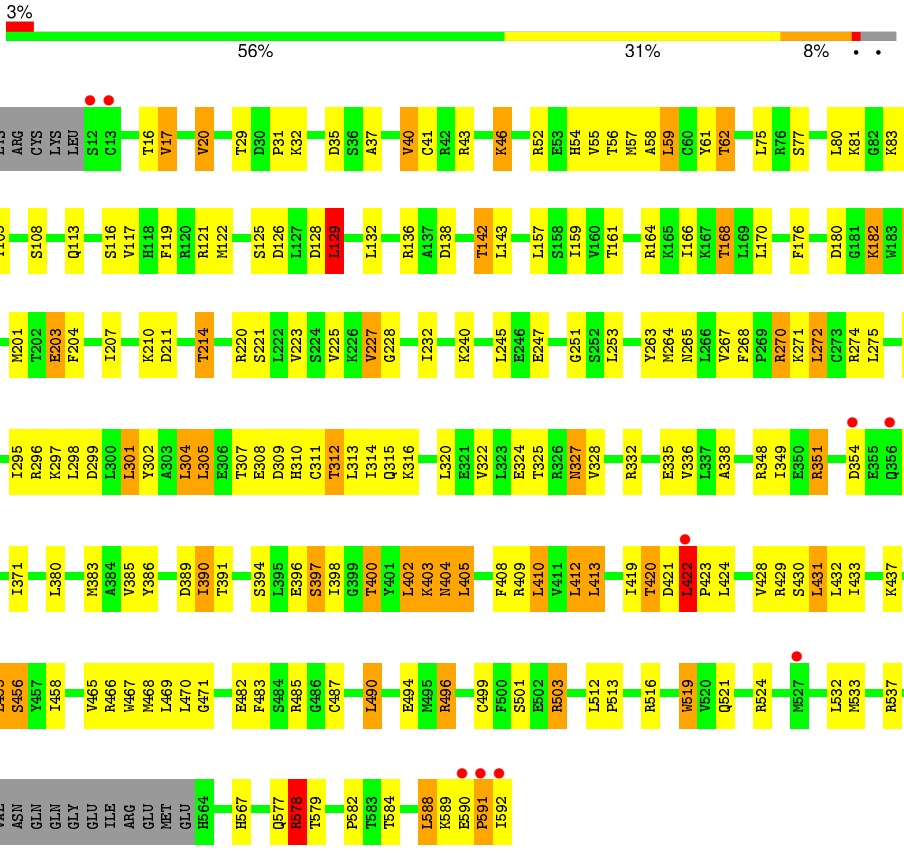
Chain H:





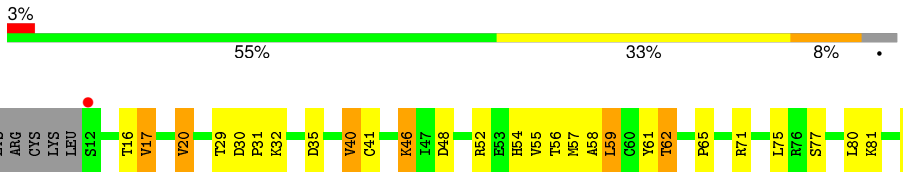
• Molecule 2: Coronatine-insensitive protein 1

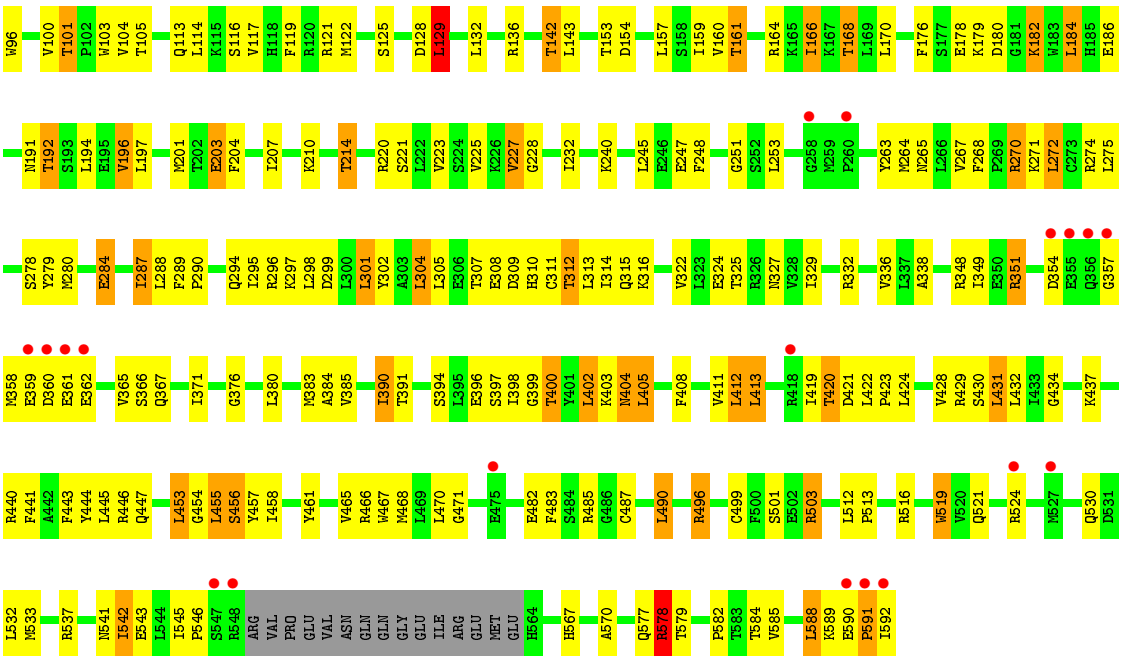
Chain J:



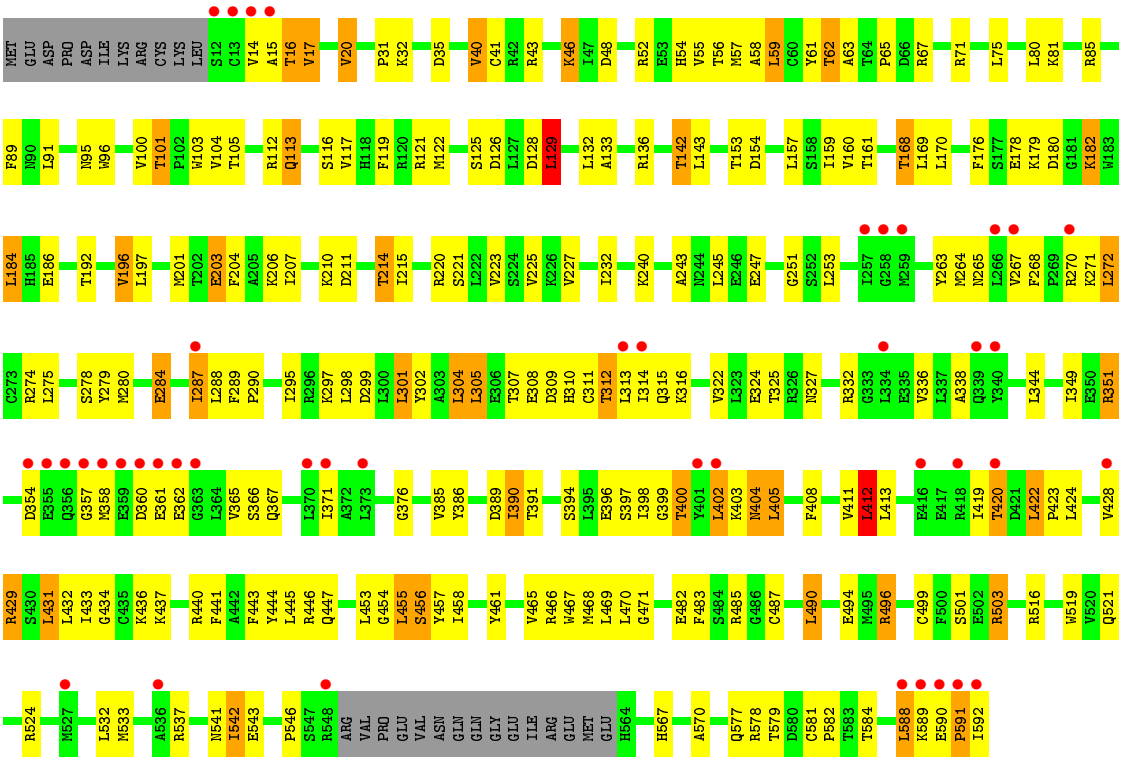
• Molecule 2: Coronatine-insensitive protein 1

Chain L:

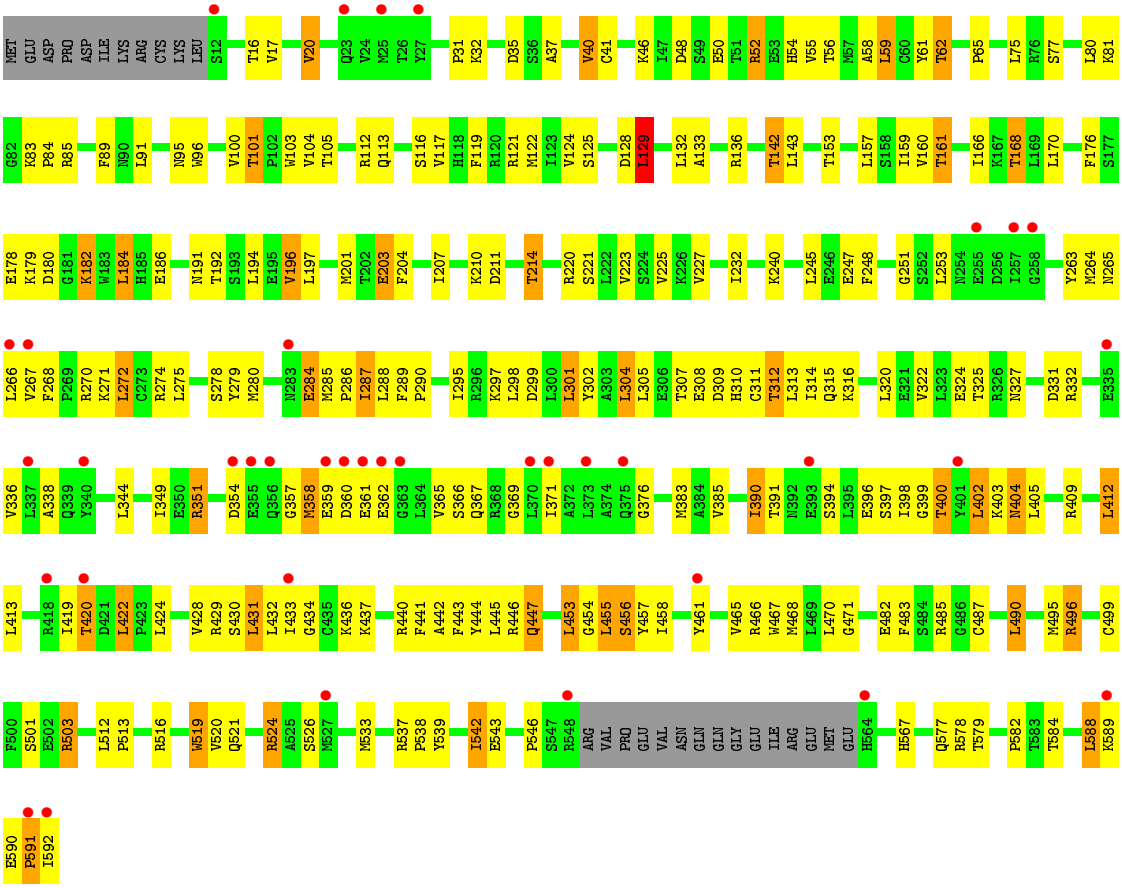




• Molecule 2: Coronatine-insensitive protein 1



• Molecule 2: Coronatine-insensitive protein 1

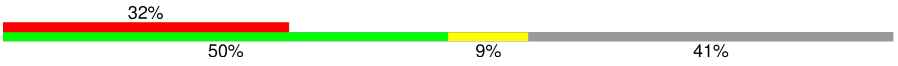


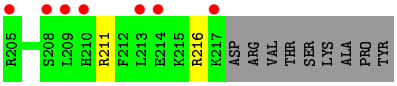
- Molecule 3: JAZ1 incomplete degron peptide

Chain Q:

- Molecule 3: JAZ1 incomplete degron peptide

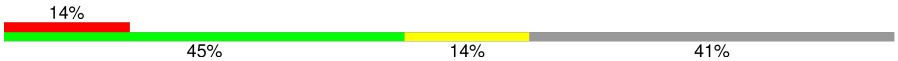
Chain R:

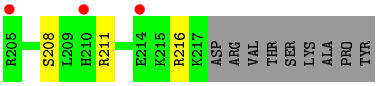




- Molecule 3: JAZ1 incomplete degron peptide

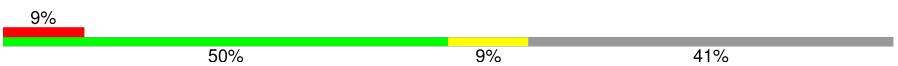
Chain S:

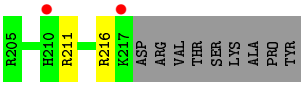




- Molecule 3: JAZ1 incomplete degron peptide

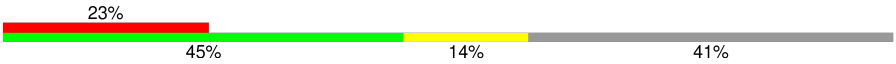
Chain U:

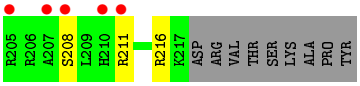




• Molecule 3: JAZ1 incomplete degron peptide

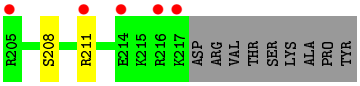
Chain V:





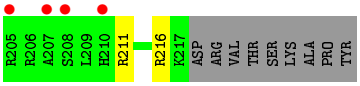
• Molecule 3: JAZ1 incomplete degron peptide

Chain W:



• Molecule 3: JAZ1 incomplete degron peptide

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.85Å 221.46Å 148.47Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.63-2.80) 93.7 (49.63-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.225 , 0.268 0.224 , 0.266	Depositor DCC
R_{free} test set	9332 reflections (5.61%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 186238 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46526	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, OGK

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	0.53	0/1168	0.61	0/1579
1	C	0.59	2/1168 (0.2%)	0.65	0/1579
1	E	0.62	0/1168	0.66	0/1579
1	G	0.64	0/1168	0.69	0/1579
1	I	0.54	1/1168 (0.1%)	0.61	0/1579
1	K	0.50	0/1168	0.62	0/1579
1	M	0.55	0/1168	0.63	0/1579
1	O	0.60	0/1168	0.63	0/1579
2	B	0.70	0/4603	0.79	4/6212 (0.1%)
2	D	0.67	1/4603 (0.0%)	0.79	2/6212 (0.0%)
2	F	0.63	1/4603 (0.0%)	0.78	1/6212 (0.0%)
2	H	0.77	0/4566	0.99	11/6161 (0.2%)
2	J	0.62	0/4603	0.78	4/6212 (0.1%)
2	L	0.59	0/4603	0.77	3/6212 (0.0%)
2	N	0.68	0/4603	0.79	3/6212 (0.0%)
2	P	0.64	0/4603	0.77	1/6212 (0.0%)
3	Q	0.36	0/120	0.62	0/155
3	R	0.42	0/120	0.64	0/155
3	S	0.40	0/120	0.58	0/155
3	U	0.41	0/120	0.61	0/155
3	V	0.46	0/120	0.57	0/155
3	W	0.44	0/120	0.60	0/155
3	X	0.43	0/120	0.59	0/155
All	All	0.64	5/46971 (0.0%)	0.78	29/63362 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	60	CYS	CB-SG	-6.18	1.71	1.82
2	F	148	CYS	CB-SG	-5.77	1.72	1.81
1	C	114	LEU	N-CA	5.58	1.57	1.46
1	I	118	CYS	CB-SG	-5.14	1.73	1.81
1	C	113	LEU	C-N	5.06	1.45	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	129	LEU	CA-CB-CG	10.65	139.79	115.30
2	B	129	LEU	CA-CB-CG	10.24	138.86	115.30
2	D	129	LEU	CA-CB-CG	9.72	137.66	115.30
2	N	129	LEU	CA-CB-CG	9.63	137.46	115.30
2	P	129	LEU	CA-CB-CG	9.35	136.81	115.30
2	L	129	LEU	CA-CB-CG	8.58	135.04	115.30
2	J	129	LEU	CA-CB-CG	8.01	133.73	115.30
2	H	170	LEU	CB-CG-CD1	-7.45	98.33	111.00
2	D	429	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	J	578	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	J	129	LEU	CB-CG-CD1	-6.12	100.60	111.00
2	H	449	GLY	N-CA-C	6.10	128.34	113.10
2	B	578	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	H	17	VAL	CB-CA-C	-5.95	100.10	111.40
2	H	477	ASP	CB-CG-OD1	5.83	123.55	118.30
2	H	410	LEU	CA-CB-CG	5.56	128.08	115.30
2	H	524	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	N	129	LEU	CB-CG-CD1	-5.51	101.63	111.00
2	H	366	SER	N-CA-C	-5.47	96.23	111.00
2	L	129	LEU	CB-CG-CD1	-5.40	101.82	111.00
2	H	458	ILE	CB-CA-C	-5.40	100.80	111.60
2	H	457	TYR	CB-CG-CD2	5.36	124.22	121.00
2	L	578	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	B	410	LEU	CA-CB-CG	5.31	127.52	115.30
2	N	412	LEU	CA-CB-CG	5.27	127.43	115.30
2	J	410	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	129	LEU	CB-CG-CD1	-5.11	102.31	111.00
2	H	97	GLY	C-N-CA	-5.08	111.64	122.30
2	H	365	VAL	CB-CA-C	-5.07	101.76	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	365	VAL	Peptide

5.2 Too-close contacts (i)

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	1152	0	1122	42	0
1	C	1152	0	1122	58	0
1	E	1152	0	1122	46	0
1	G	1152	0	1122	51	0
1	I	1152	0	1122	55	2
1	K	1152	0	1122	49	0
1	M	1152	0	1122	63	0
1	O	1152	0	1122	44	0
2	B	4521	0	4564	169	0
2	D	4521	0	4564	197	2
2	F	4521	0	4564	194	0
2	H	4486	0	4534	354	0
2	J	4521	0	4564	190	0
2	L	4521	0	4564	195	0
2	N	4521	0	4564	219	0
2	P	4521	0	4564	190	0
3	Q	119	0	131	2	0
3	R	119	0	131	2	0
3	S	119	0	131	3	0
3	U	119	0	131	2	0
3	V	119	0	131	4	0
3	W	119	0	131	2	0
3	X	119	0	131	2	0
4	B	23	0	26	6	0
4	D	23	0	26	2	0
4	F	23	0	27	8	0
4	H	23	0	26	8	0
4	J	23	0	27	7	0
4	L	23	0	27	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	23	0	27	7	0
4	P	23	0	27	7	0
5	B	20	0	0	3	0
5	D	20	0	0	3	0
5	F	20	0	0	2	0
5	H	20	0	0	6	0
5	J	20	0	0	2	0
5	L	20	0	0	1	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46526	0	46588	1980	2

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 21.

All (1980) 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:H:168:THR:HB	2:H:196:VAL:HG13	1.34	1.08
2:H:305:LEU:HD23	2:H:305:LEU:H	1.24	1.01
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.43	1.00
2:H:364:LEU:HB3	2:H:365:VAL:HG22	1.41	1.00
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.47	0.97
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.43	0.96
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.48	0.95
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.65	0.95
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.46	0.95
1:M:102:ILE:HG21	2:N:20:VAL:CG2	1.97	0.94
2:H:503:ARG:HE	2:H:503:ARG:H	1.15	0.94
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.49	0.94
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.48	0.93
2:H:533:MET:CE	2:H:588:LEU:HD13	1.98	0.93
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.50	0.93
2:H:323:LEU:HD12	2:H:324:GLU:N	1.83	0.93
2:H:533:MET:HE2	2:H:588:LEU:HD13	1.52	0.92
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.50	0.91
2:H:161:THR:HG22	2:H:186:GLU:HG2	1.52	0.91
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.52	0.91
2:N:203:GLU:OE1	3:W:211:ARG:HD3	1.71	0.90
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.71	0.90
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:364:LEU:HD13	2:H:388:SER:H	1.34	0.89
2:J:307:THR:HG21	2:J:362:GLU:HB2	1.54	0.89
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.55	0.88
2:N:307:THR:HG21	2:N:362:GLU:HB2	1.56	0.88
2:B:157:LEU:O	2:B:161:THR:HG23	1.73	0.88
2:H:390:ILE:CD1	2:H:412:LEU:HD21	2.05	0.87
2:L:307:THR:HG21	2:L:362:GLU:HB2	1.54	0.87
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.56	0.87
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.56	0.87
2:F:307:THR:HG21	2:F:362:GLU:HB2	1.54	0.87
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.55	0.86
2:D:80:LEU:HB2	2:D:122:MET:HE2	1.57	0.86
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.55	0.86
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.58	0.86
5:H:1101:PO4:O1	5:H:1103:PO4:O4	1.92	0.85
2:H:364:LEU:HD22	2:H:387:VAL:HA	1.57	0.85
2:F:157:LEU:O	2:F:161:THR:HG23	1.77	0.84
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.77	0.84
2:D:307:THR:HG21	2:D:362:GLU:HB2	1.58	0.84
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.57	0.84
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.57	0.84
2:B:307:THR:HG21	2:B:362:GLU:HB2	1.60	0.84
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.59	0.84
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.56	0.84
1:C:40:ASN:HB3	1:K:13:GLY:O	1.77	0.84
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.78	0.83
2:B:412:LEU:HD12	2:B:412:LEU:O	1.79	0.83
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.44	0.83
2:P:157:LEU:O	2:P:161:THR:HG23	1.79	0.83
2:J:412:LEU:O	2:J:412:LEU:HD12	1.78	0.82
2:L:412:LEU:O	2:L:412:LEU:HD12	1.79	0.82
2:P:307:THR:HG21	2:P:362:GLU:HB2	1.61	0.82
2:B:592:ILE:H	2:B:592:ILE:HD12	1.44	0.82
2:L:157:LEU:O	2:L:161:THR:HG23	1.79	0.82
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.62	0.82
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.60	0.82
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.78	0.82
2:F:89:PHE:CE2	4:F:1100:OGK:H04A	2.14	0.82
1:C:113:LEU:O	1:C:117:THR:HG23	1.80	0.82
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.61	0.81
2:P:412:LEU:HD12	2:P:412:LEU:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:LEU:HD12	2:N:412:LEU:O	1.80	0.81
1:I:48:THR:HG22	1:I:51:ILE:H	1.46	0.81
2:J:80:LEU:HB2	2:J:122:MET:CE	2.11	0.81
2:L:101:THR:HG22	2:L:128:ASP:OD1	1.80	0.81
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.61	0.81
2:F:592:ILE:H	2:F:592:ILE:HD12	1.46	0.81
2:H:37:ALA:O	2:H:40:VAL:HG13	1.81	0.81
2:D:412:LEU:HD12	2:D:412:LEU:O	1.81	0.80
2:L:592:ILE:HD12	2:L:592:ILE:H	1.46	0.80
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.63	0.80
2:N:85:ARG:NH2	4:N:1100:OGK:O07	2.15	0.80
2:H:364:LEU:CB	2:H:365:VAL:HG22	2.11	0.80
2:D:157:LEU:O	2:D:161:THR:HG23	1.81	0.80
1:M:102:ILE:CD1	2:N:20:VAL:HG21	2.13	0.80
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.82	0.80
1:K:158:ALA:HA	2:L:62:THR:HG21	1.64	0.80
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.63	0.79
1:C:160:GLU:OE2	1:C:160:GLU:HA	1.80	0.79
2:F:80:LEU:HB2	2:F:122:MET:HE2	1.62	0.79
1:M:112:ASN:C	1:M:114:LEU:H	1.84	0.79
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.45	0.79
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.64	0.79
2:J:157:LEU:O	2:J:161:THR:HG23	1.81	0.79
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.63	0.79
2:P:592:ILE:H	2:P:592:ILE:HD12	1.47	0.79
2:H:444:TYR:HA	2:H:471:GLY:CA	2.13	0.79
2:N:89:PHE:CE2	4:N:1100:OGK:H04A	2.18	0.79
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.48	0.79
2:F:412:LEU:O	2:F:412:LEU:HD12	1.81	0.79
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.63	0.79
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.65	0.79
2:P:116:SER:HB2	2:P:142:THR:HG23	1.65	0.79
1:C:48:THR:HG22	1:C:51:ILE:H	1.46	0.79
2:D:80:LEU:HB2	2:D:122:MET:CE	2.13	0.78
2:N:157:LEU:O	2:N:161:THR:HG23	1.83	0.78
2:D:592:ILE:H	2:D:592:ILE:HD12	1.47	0.78
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.18	0.78
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.48	0.78
1:K:48:THR:HG22	1:K:51:ILE:H	1.47	0.78
2:J:592:ILE:H	2:J:592:ILE:HD12	1.48	0.78
2:H:364:LEU:HD13	2:H:388:SER:N	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.65	0.78
2:B:396:GLU:O	2:B:400:THR:HG22	1.84	0.78
2:F:142:THR:HB	2:F:168:THR:HG23	1.66	0.78
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.65	0.78
2:H:251:GLY:O	2:H:278:SER:HB2	1.83	0.78
2:H:274:ARG:HG2	2:H:297:LYS:HD2	1.66	0.78
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.66	0.78
1:E:48:THR:HG22	1:E:51:ILE:H	1.48	0.77
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.49	0.77
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.66	0.77
2:B:398:ILE:HG23	2:B:402:LEU:HD11	1.66	0.77
2:H:331:ASP:OD2	2:H:366:SER:HB2	1.83	0.77
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.49	0.77
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.20	0.77
2:P:168:THR:HB	2:P:196:VAL:HG13	1.67	0.77
2:L:397:SER:HA	2:L:400:THR:CG2	2.15	0.77
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.19	0.77
1:O:158:ALA:HA	2:P:62:THR:HG21	1.66	0.77
2:N:592:ILE:H	2:N:592:ILE:HD12	1.49	0.76
2:J:533:MET:CE	2:J:588:LEU:HD13	2.15	0.76
2:H:396:GLU:O	2:H:400:THR:HG23	1.84	0.76
1:O:91:MET:SD	1:O:117:THR:HG22	2.25	0.76
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.67	0.76
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.65	0.76
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.66	0.76
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.68	0.76
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.64	0.76
2:P:89:PHE:CE2	4:P:1100:OGK:H04A	2.20	0.76
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.68	0.76
2:H:85:ARG:NH2	4:H:1100:OGK:O07	2.18	0.75
2:L:240:LYS:HG3	2:L:267:VAL:HG21	1.68	0.75
1:G:48:THR:HG22	1:G:51:ILE:H	1.51	0.75
2:L:80:LEU:HB2	2:L:122:MET:CE	2.17	0.75
2:H:428:VAL:HG13	2:H:443:PHE:CZ	2.22	0.75
1:I:158:ALA:HA	2:J:62:THR:HG21	1.69	0.75
2:H:501:SER:HB2	2:H:503:ARG:CZ	2.17	0.75
2:H:390:ILE:HD11	2:H:412:LEU:HD21	1.66	0.74
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.21	0.74
2:B:116:SER:HB2	2:B:142:THR:HG23	1.70	0.74
1:I:160:GLU:HA	1:I:160:GLU:OE2	1.87	0.74
1:C:102:ILE:HG21	2:D:20:VAL:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.68	0.74
1:O:48:THR:HG22	1:O:51:ILE:H	1.51	0.74
2:N:240:LYS:HG3	2:N:267:VAL:HG21	1.69	0.74
2:D:533:MET:CE	2:D:588:LEU:HD13	2.18	0.74
2:L:203:GLU:OE1	3:V:211:ARG:HD3	1.87	0.74
2:D:240:LYS:HG3	2:D:267:VAL:HG21	1.70	0.74
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.67	0.74
2:N:367:GLN:HG2	2:N:391:THR:HB	1.68	0.74
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.53	0.73
2:P:396:GLU:O	2:P:400:THR:HG22	1.88	0.73
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.70	0.73
1:M:48:THR:HG22	1:M:51:ILE:H	1.52	0.73
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.22	0.73
1:E:158:ALA:HA	2:F:62:THR:HG21	1.69	0.73
2:N:116:SER:HB2	2:N:142:THR:HG23	1.70	0.73
2:H:120:ARG:NH2	5:H:1103:PO4:P	2.62	0.73
2:P:240:LYS:HG3	2:P:267:VAL:HG21	1.70	0.73
2:H:118:HIS:HE1	2:H:146:ASP:OD2	1.72	0.73
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.23	0.73
2:D:367:GLN:HG2	2:D:391:THR:HB	1.70	0.73
2:L:367:GLN:HG2	2:L:391:THR:HB	1.71	0.73
2:H:351:ARG:HG2	2:H:352:GLY:N	2.04	0.73
2:F:80:LEU:HB2	2:F:122:MET:CE	2.18	0.72
2:B:533:MET:CE	2:B:588:LEU:HD13	2.19	0.72
1:G:128:LYS:HB2	1:G:133:ILE:HD13	1.71	0.72
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.69	0.72
2:F:397:SER:HA	2:F:400:THR:CG2	2.20	0.72
2:N:397:SER:HA	2:N:400:THR:CG2	2.20	0.72
2:H:528:THR:HG23	2:H:586:ARG:NH2	2.04	0.72
1:A:48:THR:HG22	1:A:51:ILE:H	1.53	0.72
2:J:240:LYS:HG3	2:J:267:VAL:HG21	1.70	0.72
2:H:168:THR:CB	2:H:196:VAL:HG13	2.16	0.72
1:M:129:THR:O	1:M:133:ILE:HG12	1.89	0.72
2:P:367:GLN:HG2	2:P:391:THR:HB	1.71	0.72
2:H:332:ARG:HG2	2:H:332:ARG:HH11	1.55	0.72
2:F:240:LYS:HG3	2:F:267:VAL:HG21	1.70	0.72
1:E:160:GLU:HA	1:E:160:GLU:OE2	1.90	0.72
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.24	0.72
2:J:397:SER:HA	2:J:400:THR:CG2	2.20	0.71
2:P:307:THR:HG22	2:P:360:ASP:OD2	1.90	0.71
2:P:367:GLN:O	2:P:371:ILE:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.24	0.71
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.25	0.71
2:B:397:SER:HA	2:B:400:THR:CG2	2.21	0.71
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.71	0.71
2:J:161:THR:HG22	2:J:186:GLU:HG2	1.73	0.71
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.59	0.71
2:P:397:SER:HA	2:P:400:THR:CG2	2.21	0.71
1:C:158:ALA:HA	2:D:62:THR:HG21	1.70	0.71
2:B:240:LYS:HG3	2:B:267:VAL:HG21	1.72	0.71
1:E:91:MET:HG2	1:E:116:LEU:HD21	1.73	0.71
2:L:89:PHE:CE2	4:L:1100:OGK:H04A	2.25	0.71
1:A:160:GLU:OE2	1:A:160:GLU:HA	1.90	0.71
2:H:328:VAL:HG13	2:H:359:GLU:HG2	1.71	0.71
1:O:160:GLU:HA	1:O:160:GLU:OE2	1.88	0.71
2:N:168:THR:HB	2:N:196:VAL:HG13	1.72	0.70
2:D:397:SER:HA	2:D:400:THR:CG2	2.21	0.70
2:P:80:LEU:HB2	2:P:122:MET:CE	2.21	0.70
2:J:367:GLN:HG2	2:J:391:THR:HB	1.71	0.70
1:C:112:ASN:O	1:C:116:LEU:HB3	1.91	0.70
2:P:279:TYR:HA	2:P:304:LEU:HD22	1.72	0.70
2:P:310:HIS:O	2:P:314:ILE:HG12	1.90	0.70
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.72	0.70
2:H:386:TYR:HD2	2:H:413:LEU:HD21	1.55	0.70
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.25	0.70
2:J:397:SER:HA	2:J:400:THR:HG22	1.74	0.70
2:N:80:LEU:HB2	2:N:122:MET:CE	2.20	0.70
1:G:160:GLU:OE1	1:G:160:GLU:HA	1.92	0.70
2:H:154:ASP:OD1	2:H:179:LYS:HE2	1.92	0.70
1:A:158:ALA:HA	2:B:62:THR:HG21	1.73	0.70
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.73	0.70
2:N:533:MET:CE	2:N:588:LEU:HD13	2.20	0.70
2:N:310:HIS:O	2:N:314:ILE:HG12	1.91	0.70
1:M:158:ALA:HA	2:N:62:THR:HG21	1.73	0.70
2:L:397:SER:HA	2:L:400:THR:HG22	1.73	0.70
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.57	0.70
2:L:116:SER:HB2	2:L:142:THR:HG23	1.74	0.70
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.72	0.70
2:B:404:ASN:HA	2:B:437:LYS:HD2	1.73	0.70
2:B:279:TYR:HA	2:B:304:LEU:HD22	1.74	0.70
2:F:310:HIS:O	2:F:314:ILE:HG12	1.92	0.70
2:N:397:SER:HA	2:N:400:THR:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:337:LEU:HD11	2:H:344:LEU:HD22	1.72	0.69
2:L:80:LEU:HB2	2:L:122:MET:HE2	1.72	0.69
2:H:310:HIS:O	2:H:314:ILE:HG12	1.92	0.69
1:C:158:ALA:HA	2:D:62:THR:CG2	2.22	0.69
2:D:310:HIS:O	2:D:314:ILE:HG12	1.92	0.69
2:F:367:GLN:HG2	2:F:391:THR:HB	1.74	0.69
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.26	0.69
2:H:274:ARG:HG2	2:H:297:LYS:CD	2.23	0.69
2:B:310:HIS:O	2:B:314:ILE:HG12	1.93	0.69
2:H:362:GLU:C	2:H:364:LEU:H	1.96	0.69
1:K:158:ALA:HA	2:L:62:THR:CG2	2.21	0.69
1:E:48:THR:CG2	1:E:51:ILE:H	2.05	0.69
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.57	0.69
2:H:96:TRP:O	2:H:578:ARG:NH2	2.26	0.69
1:K:160:GLU:HG3	2:L:31:PRO:HB3	1.74	0.69
1:I:48:THR:CG2	1:I:51:ILE:H	2.06	0.69
1:A:160:GLU:HG3	2:B:31:PRO:HB3	1.75	0.69
2:F:533:MET:CE	2:F:588:LEU:HD13	2.23	0.69
2:L:533:MET:CE	2:L:588:LEU:HD13	2.23	0.69
1:E:160:GLU:HG3	2:F:31:PRO:HB3	1.75	0.69
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.74	0.68
2:B:307:THR:HG22	2:B:360:ASP:OD2	1.93	0.68
2:H:528:THR:HG23	2:H:586:ARG:HH22	1.57	0.68
2:F:116:SER:HB2	2:F:142:THR:HG23	1.74	0.68
2:H:95:ASN:O	2:H:582:PRO:HG3	1.93	0.68
2:H:327:ASN:C	2:H:329:ILE:H	1.96	0.68
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.27	0.68
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.26	0.68
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.74	0.68
2:N:431:LEU:HD12	2:N:431:LEU:O	1.93	0.68
1:M:124:MET:O	1:M:128:LYS:HE2	1.93	0.68
2:H:141:GLU:HG2	2:H:167:LYS:HD3	1.75	0.68
2:P:142:THR:HB	2:P:168:THR:HG23	1.74	0.68
1:I:124:MET:O	1:I:128:LYS:HE2	1.94	0.68
1:C:48:THR:CG2	1:C:51:ILE:H	2.06	0.68
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.75	0.68
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.29	0.68
1:G:30:ALA:O	1:G:33:VAL:HG22	1.94	0.68
1:G:102:ILE:HG21	2:H:20:VAL:HG22	1.75	0.68
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.75	0.68
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.74	0.68
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.74	0.68
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.75	0.68
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.74	0.67
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.76	0.67
2:H:221:SER:O	2:H:223:VAL:HG13	1.95	0.67
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.24	0.67
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.75	0.67
2:H:584:THR:HG22	2:H:584:THR:O	1.94	0.67
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.30	0.67
2:J:307:THR:HG22	2:J:360:ASP:OD2	1.94	0.67
1:M:48:THR:CG2	1:M:51:ILE:H	2.07	0.67
2:L:367:GLN:O	2:L:371:ILE:HG22	1.94	0.67
1:O:160:GLU:HG3	2:P:31:PRO:HB3	1.76	0.67
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.76	0.67
2:B:367:GLN:HG2	2:B:391:THR:HB	1.74	0.67
2:N:161:THR:HG22	2:N:186:GLU:HG2	1.77	0.67
2:H:366:SER:HB3	2:H:368:ARG:HG2	1.76	0.67
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.77	0.67
2:D:367:GLN:O	2:D:371:ILE:HG22	1.95	0.67
1:I:101:LEU:HB3	1:I:117:THR:HG21	1.76	0.67
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.77	0.67
2:H:198:ASN:ND2	2:H:226:LYS:HD2	2.10	0.67
2:D:210:LYS:O	2:D:214:THR:HG22	1.96	0.66
2:F:85:ARG:NH2	4:F:1100:OGK:O07	2.25	0.66
2:P:80:LEU:HB2	2:P:122:MET:HE2	1.77	0.66
2:H:307:THR:HB	2:H:328:VAL:O	1.95	0.66
2:D:307:THR:HG22	2:D:360:ASP:OD2	1.96	0.66
2:J:310:HIS:O	2:J:314:ILE:HG12	1.94	0.66
2:J:168:THR:HB	2:J:196:VAL:HG13	1.78	0.66
2:N:58:ALA:HA	2:N:81:LYS:HD2	1.77	0.66
2:J:263:TYR:O	2:J:265:ASN:N	2.29	0.66
2:B:58:ALA:HA	2:B:81:LYS:HD2	1.77	0.66
2:F:263:TYR:O	2:F:265:ASN:N	2.29	0.66
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.77	0.66
2:D:58:ALA:HA	2:D:81:LYS:HD2	1.77	0.66
1:C:113:LEU:O	1:C:117:THR:CG2	2.44	0.66
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.28	0.66
2:B:80:LEU:HB2	2:B:122:MET:HE2	1.78	0.66
2:H:59:LEU:O	2:H:62:THR:HB	1.95	0.66
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:299:ASP:OD2	2:N:301:LEU:HB2	1.96	0.66
1:G:128:LYS:HB2	1:G:133:ILE:CD1	2.26	0.66
2:H:544:LEU:O	2:H:546:PRO:HD3	1.96	0.66
1:I:160:GLU:HG3	2:J:31:PRO:HB3	1.77	0.66
2:N:221:SER:O	2:N:223:VAL:HG23	1.94	0.66
1:I:111:LYS:O	1:I:115:ASP:HB2	1.96	0.66
1:M:160:GLU:HG3	2:N:31:PRO:HB3	1.78	0.66
2:P:519:TRP:HE1	4:P:1100:OGK:H01	1.59	0.65
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.77	0.65
2:P:221:SER:O	2:P:223:VAL:HG23	1.95	0.65
2:F:279:TYR:HA	2:F:304:LEU:HD22	1.78	0.65
1:O:158:ALA:HA	2:P:62:THR:CG2	2.26	0.65
2:B:80:LEU:HB2	2:B:122:MET:CE	2.25	0.65
2:H:212:LEU:HD23	2:H:235:LEU:HD22	1.78	0.65
2:H:301:LEU:HD23	2:H:324:GLU:HB3	1.78	0.65
2:J:367:GLN:O	2:J:371:ILE:HG22	1.96	0.65
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.42	0.65
2:H:125:SER:HB3	2:H:127:LEU:N	2.11	0.65
2:D:279:TYR:HA	2:D:304:LEU:HD22	1.79	0.65
1:I:30:ALA:O	1:I:33:VAL:HG22	1.94	0.65
2:J:164:ARG:HD2	2:N:112:ARG:CG	2.24	0.65
2:N:307:THR:HG22	2:N:360:ASP:OD2	1.97	0.65
2:P:443:PHE:HE2	2:P:445:LEU:HD11	1.62	0.65
2:P:58:ALA:HA	2:P:81:LYS:HD2	1.78	0.65
2:L:210:LYS:O	2:L:214:THR:HG22	1.96	0.65
2:D:397:SER:HA	2:D:400:THR:HG22	1.79	0.65
2:L:58:ALA:HA	2:L:81:LYS:HD2	1.79	0.65
2:L:431:LEU:HD12	2:L:431:LEU:O	1.96	0.65
2:H:533:MET:CE	2:H:588:LEU:HB3	2.26	0.65
1:C:160:GLU:HG3	2:D:31:PRO:HB3	1.79	0.65
2:B:367:GLN:O	2:B:371:ILE:HG22	1.96	0.65
2:L:279:TYR:HA	2:L:304:LEU:HD22	1.77	0.65
1:O:113:LEU:HG	1:O:113:LEU:O	1.97	0.65
2:L:396:GLU:O	2:L:400:THR:HG22	1.97	0.65
1:M:158:ALA:HA	2:N:62:THR:CG2	2.27	0.65
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.30	0.65
1:E:158:ALA:HA	2:F:62:THR:CG2	2.27	0.65
2:F:397:SER:HA	2:F:400:THR:HG22	1.79	0.65
1:I:106:ASN:N	1:I:114:LEU:HD13	2.12	0.65
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.78	0.65
2:H:361:GLU:O	2:H:362:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:468:MET:CE	2:H:470:LEU:HD21	2.26	0.64
1:K:48:THR:CG2	1:K:51:ILE:H	2.10	0.64
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.78	0.64
2:L:168:THR:HB	2:L:196:VAL:HG13	1.79	0.64
2:N:279:TYR:HA	2:N:304:LEU:HD22	1.79	0.64
2:D:263:TYR:O	2:D:265:ASN:N	2.30	0.64
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.80	0.64
2:H:503:ARG:H	2:H:503:ARG:NE	1.92	0.64
2:H:337:LEU:O	2:H:341:CYS:HB2	1.97	0.64
2:F:396:GLU:O	2:F:400:THR:HG22	1.98	0.64
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.78	0.64
1:C:13:GLY:HA3	1:K:9:LYS:HZ2	1.63	0.64
2:B:168:THR:HB	2:B:196:VAL:HG13	1.79	0.64
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.78	0.64
2:B:89:PHE:CE2	4:B:1100:OGK:H04A	2.33	0.64
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.31	0.64
2:H:327:ASN:C	2:H:329:ILE:N	2.48	0.64
1:I:158:ALA:HA	2:J:62:THR:CG2	2.27	0.64
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.33	0.64
2:D:201:MET:HE1	2:D:302:TYR:CE2	2.32	0.64
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.80	0.64
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.80	0.64
1:M:30:ALA:O	1:M:33:VAL:HG22	1.97	0.64
2:P:89:PHE:CD2	4:P:1100:OGK:H04A	2.31	0.64
2:N:80:LEU:HB2	2:N:122:MET:HE2	1.79	0.64
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.63	0.64
2:L:307:THR:HG22	2:L:360:ASP:OD2	1.97	0.64
2:H:332:ARG:O	2:H:336:VAL:HG23	1.98	0.64
1:O:124:MET:O	1:O:128:LYS:HE2	1.97	0.64
2:F:284:GLU:O	2:F:287:ILE:HD13	1.98	0.64
2:H:303:ALA:HB1	2:H:305:LEU:CD2	2.28	0.63
2:J:279:TYR:HA	2:J:304:LEU:HD22	1.80	0.63
2:N:268:PHE:HE1	2:N:287:ILE:HG13	1.61	0.63
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.80	0.63
4:P:1100:OGK:H18A	4:P:1100:OGK:HN08	1.63	0.63
2:F:268:PHE:HE1	2:F:287:ILE:HG13	1.62	0.63
2:D:386:TYR:CE1	4:D:1100:OGK:H15A	2.33	0.63
2:F:519:TRP:HE1	4:F:1100:OGK:H01	1.63	0.63
2:P:210:LYS:O	2:P:214:THR:HG22	1.99	0.63
2:J:210:LYS:O	2:J:214:THR:HG22	1.98	0.63
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LYS:O	2:B:214:THR:HG22	1.97	0.63
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.80	0.63
2:J:95:ASN:O	2:J:582:PRO:HG3	1.98	0.63
2:F:307:THR:HG22	2:F:360:ASP:OD2	1.97	0.63
2:H:211:ASP:O	2:H:215:ILE:HG13	1.99	0.63
2:H:329:ILE:HG12	2:H:333:GLY:HA3	1.81	0.63
2:H:542:ILE:HG13	2:H:588:LEU:HB2	1.80	0.63
2:N:396:GLU:O	2:N:400:THR:HG22	1.99	0.63
2:H:34:ARG:NH1	2:H:48:ASP:OD1	2.32	0.63
2:D:101:THR:HG21	2:N:179:LYS:NZ	2.14	0.63
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.81	0.63
1:M:112:ASN:C	1:M:114:LEU:N	2.52	0.63
1:G:48:THR:CG2	1:G:51:ILE:H	2.10	0.63
1:E:30:ALA:O	1:E:33:VAL:HG22	1.98	0.63
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.33	0.63
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.81	0.63
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.34	0.63
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.81	0.63
2:H:191:ASN:HD21	2:H:194:LEU:H	1.45	0.63
2:B:409:ARG:HB2	4:B:1100:OGK:H16B	1.81	0.63
2:D:116:SER:HB2	2:D:142:THR:HG23	1.80	0.63
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.81	0.62
2:J:116:SER:HB2	2:J:142:THR:HG23	1.80	0.62
2:H:125:SER:HB3	2:H:127:LEU:H	1.64	0.62
2:J:299:ASP:OD2	2:J:301:LEU:HB2	1.98	0.62
1:O:48:THR:CG2	1:O:51:ILE:H	2.12	0.62
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.82	0.62
1:I:52:LEU:O	1:I:56:ILE:HG13	2.00	0.62
1:G:149:GLU:OE1	1:G:153:ARG:NE	2.32	0.62
2:P:431:LEU:O	2:P:431:LEU:HD12	1.99	0.62
2:H:361:GLU:HA	2:H:364:LEU:HD12	1.80	0.62
2:H:366:SER:CB	2:H:368:ARG:HG2	2.29	0.62
2:D:40:VAL:O	2:D:41:CYS:HB3	2.00	0.62
2:J:456:SER:HB2	2:J:482:GLU:HB3	1.80	0.62
2:H:305:LEU:CD2	2:H:305:LEU:H	2.06	0.62
2:F:267:VAL:HG23	2:F:267:VAL:O	2.00	0.62
1:E:160:GLU:CG	2:F:31:PRO:HB3	2.29	0.62
1:K:160:GLU:OE2	1:K:160:GLU:HA	1.98	0.62
2:D:203:GLU:OE1	3:R:211:ARG:HD3	1.99	0.62
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.82	0.62
2:N:367:GLN:O	2:N:371:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:40:VAL:O	2:J:41:CYS:HB3	2.00	0.62
2:P:299:ASP:OD2	2:P:301:LEU:HB2	2.00	0.62
2:F:404:ASN:HA	2:F:437:LYS:HD2	1.82	0.62
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.80	0.62
2:L:201:MET:HE1	2:L:302:TYR:CE2	2.34	0.62
2:H:327:ASN:HA	2:H:329:ILE:HG22	1.82	0.61
2:N:59:LEU:O	2:N:62:THR:HB	1.99	0.61
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.65	0.61
2:H:366:SER:C	2:H:368:ARG:N	2.52	0.61
2:P:519:TRP:NE1	4:P:1100:OGK:H01	2.15	0.61
2:N:443:PHE:HE2	2:N:445:LEU:HD11	1.66	0.61
2:P:404:ASN:HA	2:P:437:LYS:HD2	1.82	0.61
2:L:310:HIS:O	2:L:314:ILE:HG12	2.00	0.61
2:P:263:TYR:O	2:P:265:ASN:N	2.33	0.61
2:D:456:SER:HB2	2:D:482:GLU:HB3	1.81	0.61
1:K:102:ILE:HG12	1:K:117:THR:HB	1.81	0.61
1:I:160:GLU:CG	2:J:31:PRO:HB3	2.31	0.61
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.83	0.61
1:K:30:ALA:O	1:K:33:VAL:HG22	1.99	0.61
2:F:40:VAL:O	2:F:41:CYS:HB3	1.99	0.61
2:F:168:THR:HB	2:F:196:VAL:HG13	1.81	0.61
4:L:1100:OGK:HN08	4:L:1100:OGK:H18A	1.65	0.61
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.82	0.61
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.36	0.61
2:P:533:MET:CE	2:P:588:LEU:HD13	2.30	0.61
1:O:129:THR:O	1:O:133:ILE:HG12	2.01	0.61
1:M:99:PHE:HD2	2:N:15:ALA:O	1.84	0.61
2:H:160:VAL:HG11	2:H:187:LEU:HG	1.82	0.61
2:D:95:ASN:O	2:D:582:PRO:HG3	2.00	0.61
2:D:96:TRP:O	2:D:578:ARG:NH2	2.26	0.61
2:D:190:HIS:HB3	2:H:112:ARG:HD2	1.83	0.61
1:G:159:PHE:O	1:G:160:GLU:HB2	1.99	0.61
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.78	0.61
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.46	0.61
2:P:390:ILE:HD13	2:P:424:LEU:HD11	1.83	0.61
1:M:48:THR:HG22	1:M:51:ILE:HB	1.83	0.61
2:D:164:ARG:HD2	2:H:112:ARG:HD3	1.83	0.61
2:N:95:ASN:O	2:N:582:PRO:HG3	2.01	0.61
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.81	0.61
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.98	0.61
2:D:54:HIS:HD2	2:D:77:SER:OG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:ALA:HA	2:J:81:LYS:HD2	1.82	0.61
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.82	0.61
2:N:456:SER:HB2	2:N:482:GLU:HB3	1.81	0.61
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.83	0.61
1:O:30:ALA:O	1:O:33:VAL:HG22	1.99	0.61
2:J:390:ILE:HD11	2:J:412:LEU:HD23	1.82	0.60
2:N:431:LEU:HD12	2:N:431:LEU:C	2.20	0.60
2:L:263:TYR:O	2:L:265:ASN:N	2.33	0.60
2:B:268:PHE:HE1	2:B:287:ILE:HG13	1.66	0.60
2:H:127:LEU:HD22	2:J:126:ASP:HB3	1.82	0.60
2:H:286:PRO:O	2:H:288:LEU:N	2.34	0.60
2:P:284:GLU:O	2:P:287:ILE:HD13	2.00	0.60
2:B:142:THR:HB	2:B:168:THR:HG23	1.82	0.60
2:H:144:LYS:HG2	2:H:170:LEU:HD13	1.83	0.60
2:H:327:ASN:HD22	2:H:364:LEU:HD21	1.65	0.60
2:H:161:THR:HG22	2:H:186:GLU:CG	2.28	0.60
2:N:89:PHE:CD2	4:N:1100:OGK:H04A	2.35	0.60
1:M:160:GLU:CG	2:N:31:PRO:HB3	2.32	0.60
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.82	0.60
1:G:151:VAL:HG12	2:H:39:LEU:HD21	1.83	0.60
2:H:542:ILE:HD12	2:H:542:ILE:C	2.22	0.60
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.82	0.60
1:C:30:ALA:O	1:C:33:VAL:HG22	2.02	0.60
2:H:386:TYR:CE1	4:H:1100:OGK:H15A	2.36	0.60
2:N:142:THR:HB	2:N:168:THR:HG23	1.83	0.60
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.83	0.60
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.83	0.60
1:K:129:THR:O	1:K:133:ILE:HG12	2.02	0.60
1:C:13:GLY:HA3	1:K:9:LYS:NZ	2.17	0.60
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.83	0.60
2:H:390:ILE:HD13	2:H:412:LEU:HD21	1.82	0.60
4:H:1100:OGK:HN08	4:H:1100:OGK:H18A	1.67	0.60
2:F:85:ARG:HD2	5:F:1101:PO4:O2	2.02	0.60
1:A:48:THR:CG2	1:A:51:ILE:H	2.15	0.60
2:B:263:TYR:O	2:B:265:ASN:N	2.33	0.60
2:F:58:ALA:HA	2:F:81:LYS:HD2	1.82	0.60
2:L:95:ASN:O	2:L:582:PRO:HG3	2.01	0.60
2:H:503:ARG:HE	2:H:503:ARG:N	1.94	0.60
2:L:268:PHE:HE1	2:L:287:ILE:HG13	1.66	0.60
2:L:359:GLU:HG2	3:V:216:ARG:HH22	1.67	0.60
2:F:299:ASP:OD2	2:F:301:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:201:MET:HE1	2:N:302:TYR:CE2	2.37	0.60
2:H:304:LEU:O	2:H:304:LEU:HD13	2.02	0.60
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.84	0.59
2:D:396:GLU:O	2:D:400:THR:HG22	2.01	0.59
2:D:168:THR:HB	2:D:196:VAL:HG13	1.82	0.59
2:N:225:VAL:HG13	2:N:245:LEU:HD11	1.83	0.59
2:B:456:SER:HB2	2:B:482:GLU:HB3	1.83	0.59
2:B:267:VAL:O	2:B:267:VAL:HG23	2.02	0.59
1:O:91:MET:HG2	1:O:116:LEU:HD21	1.83	0.59
2:H:170:LEU:HD23	2:H:172:GLU:H	1.66	0.59
2:P:268:PHE:HE1	2:P:287:ILE:HG13	1.66	0.59
2:D:284:GLU:O	2:D:287:ILE:HD13	2.02	0.59
2:L:456:SER:HB2	2:L:482:GLU:HB3	1.85	0.59
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.37	0.59
2:H:212:LEU:HD22	2:H:230:PHE:CE1	2.38	0.59
2:H:458:ILE:HG21	2:H:468:MET:HE1	1.85	0.59
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.85	0.59
2:D:267:VAL:HG23	2:D:267:VAL:O	2.02	0.59
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.84	0.59
2:D:390:ILE:HD11	2:D:412:LEU:HD23	1.85	0.59
2:P:397:SER:HA	2:P:400:THR:HG22	1.84	0.59
2:H:225:VAL:O	2:H:248:PHE:HA	2.03	0.59
2:J:201:MET:HE1	2:J:302:TYR:CZ	2.38	0.59
1:E:124:MET:O	1:E:128:LYS:HE2	2.02	0.59
2:H:284:GLU:O	2:H:287:ILE:HG23	2.03	0.59
1:K:160:GLU:CG	2:L:31:PRO:HB3	2.32	0.59
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.84	0.59
1:I:129:THR:O	1:I:133:ILE:HG12	2.03	0.59
2:J:267:VAL:O	2:J:267:VAL:HG23	2.03	0.59
1:O:160:GLU:CG	2:P:31:PRO:HB3	2.32	0.59
1:M:160:GLU:HA	1:M:160:GLU:OE2	2.00	0.59
2:J:201:MET:HE1	2:J:302:TYR:CE2	2.37	0.59
2:B:299:ASP:OD2	2:B:301:LEU:HB2	2.02	0.59
1:C:102:ILE:HG21	2:D:20:VAL:HG21	1.84	0.59
2:J:221:SER:O	2:J:223:VAL:HG23	2.03	0.59
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.85	0.59
1:C:124:MET:O	1:C:128:LYS:HE2	2.02	0.58
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.85	0.58
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.67	0.58
2:N:398:ILE:CG2	2:N:402:LEU:HD11	2.31	0.58
4:N:1100:OGK:H18A	4:N:1100:OGK:HN08	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:THR:HG21	2:F:179:LYS:NZ	2.17	0.58
2:J:396:GLU:O	2:J:400:THR:HG22	2.03	0.58
2:F:143:LEU:CD2	2:F:159:ILE:HD13	2.33	0.58
2:N:210:LYS:O	2:N:214:THR:HG22	2.03	0.58
2:B:40:VAL:O	2:B:41:CYS:HB3	2.03	0.58
2:L:40:VAL:O	2:L:41:CYS:HB3	2.02	0.58
1:A:30:ALA:O	1:A:33:VAL:HG22	2.03	0.58
1:O:102:ILE:HD12	2:P:20:VAL:HG21	1.84	0.58
2:P:203:GLU:OE1	3:X:211:ARG:HD3	2.03	0.58
2:B:190:HIS:CG	2:P:112:ARG:HH11	2.22	0.58
2:J:80:LEU:HB2	2:J:122:MET:HE2	1.83	0.58
2:P:267:VAL:O	2:P:267:VAL:HG23	2.04	0.58
1:E:107:TYR:CD1	2:L:270:ARG:O	2.57	0.58
2:L:267:VAL:HG23	2:L:267:VAL:O	2.03	0.58
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.85	0.58
2:D:546:PRO:HD2	2:D:584:THR:O	2.03	0.58
2:H:349:ILE:HD12	2:H:385:VAL:CG2	2.33	0.58
2:H:366:SER:C	2:H:368:ARG:H	2.07	0.58
2:H:118:HIS:CE1	2:H:146:ASP:OD2	2.55	0.58
1:A:158:ALA:HA	2:B:62:THR:CG2	2.32	0.58
2:F:367:GLN:O	2:F:371:ILE:HG22	2.04	0.58
1:I:102:ILE:HG13	1:I:117:THR:HB	1.84	0.58
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.84	0.58
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.85	0.58
2:N:404:ASN:CB	2:N:437:LYS:HD2	2.34	0.58
1:I:102:ILE:CG1	1:I:117:THR:HB	2.34	0.58
2:D:348:ARG:HH22	4:D:1100:OGK:C10	2.17	0.58
2:J:295:ILE:HG21	2:J:298:LEU:HD13	1.84	0.58
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.86	0.58
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.85	0.58
2:H:386:TYR:CD2	2:H:413:LEU:HD21	2.38	0.58
2:H:305:LEU:HD23	2:H:305:LEU:N	2.07	0.58
1:M:99:PHE:CD2	2:N:16:THR:C	2.78	0.58
2:J:284:GLU:O	2:J:287:ILE:HD13	2.03	0.58
2:F:456:SER:HB2	2:F:482:GLU:HB3	1.84	0.58
2:H:328:VAL:HG13	2:H:359:GLU:CG	2.34	0.57
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.38	0.57
2:D:580:ASP:HA	2:N:206:LYS:HE3	1.86	0.57
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.39	0.57
1:E:48:THR:HG22	1:E:51:ILE:HB	1.86	0.57
2:H:292:ALA:HA	2:H:295:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:263:TYR:O	2:N:265:ASN:N	2.37	0.57
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.34	0.57
2:N:85:ARG:HD2	5:N:1101:PO4:O2	2.04	0.57
2:L:384:ALA:HB1	4:L:1100:OGK:H16	1.87	0.57
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.86	0.57
1:I:26:SER:OG	1:I:108:LEU:HB3	2.04	0.57
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.69	0.57
2:L:359:GLU:HG2	3:V:216:ARG:NH2	2.19	0.57
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.38	0.57
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.39	0.57
1:C:102:ILE:HG21	2:D:20:VAL:HG22	1.85	0.57
2:N:267:VAL:HG23	2:N:267:VAL:O	2.05	0.57
1:I:98:LEU:HD21	1:I:120:THR:HG22	1.87	0.57
2:P:304:LEU:HD11	3:X:216:ARG:HG3	1.87	0.57
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.88	0.57
2:J:348:ARG:HH22	4:J:1100:OGK:C10	2.16	0.57
2:H:351:ARG:HG2	2:H:352:GLY:H	1.70	0.57
2:B:390:ILE:HD11	2:B:412:LEU:HD23	1.86	0.57
2:N:143:LEU:CD2	2:N:159:ILE:HD13	2.34	0.57
2:B:284:GLU:O	2:B:287:ILE:HD13	2.04	0.57
2:D:268:PHE:HE1	2:D:287:ILE:HG13	1.68	0.57
2:F:201:MET:HE1	2:F:302:TYR:CZ	2.39	0.57
2:H:299:ASP:OD2	2:H:301:LEU:HB2	2.05	0.57
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.78	0.57
2:J:404:ASN:HA	2:J:437:LYS:HD2	1.87	0.57
2:L:142:THR:HB	2:L:168:THR:HG23	1.85	0.57
2:H:86:ALA:HA	4:H:1100:OGK:H27	1.87	0.56
1:G:130:PRO:HD3	2:H:36:SER:HB3	1.87	0.56
2:F:390:ILE:HD13	2:F:424:LEU:HD11	1.87	0.56
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.86	0.56
2:J:543:GLU:OE2	2:J:578:ARG:HD3	2.04	0.56
2:D:142:THR:HB	2:D:168:THR:HG23	1.85	0.56
2:F:221:SER:O	2:F:223:VAL:HG23	2.04	0.56
2:H:310:HIS:NE2	2:H:328:VAL:HG23	2.21	0.56
1:E:129:THR:O	1:E:133:ILE:HG12	2.04	0.56
2:J:142:THR:HB	2:J:168:THR:HG23	1.86	0.56
2:F:263:TYR:C	2:F:265:ASN:H	2.09	0.56
2:H:345:LYS:NZ	2:H:345:LYS:HB3	2.21	0.56
2:L:80:LEU:HD12	2:L:122:MET:HE1	1.86	0.56
2:L:297:LYS:HG3	2:L:322:VAL:HB	1.88	0.56
2:H:87:ALA:C	2:H:89:PHE:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:275:LEU:HD11	2:F:288:LEU:CD2	2.36	0.56
2:H:587:VAL:HG12	2:H:589:LYS:HD3	1.87	0.56
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.06	0.56
2:H:533:MET:HE3	2:H:588:LEU:HB3	1.86	0.56
2:H:323:LEU:C	2:H:323:LEU:HD12	2.22	0.56
2:N:309:ASP:HA	2:N:312:THR:HG23	1.88	0.56
2:F:431:LEU:HD12	2:F:431:LEU:O	2.06	0.56
2:J:268:PHE:HE1	2:J:287:ILE:HG13	1.70	0.56
1:G:142:ASP:OD2	2:H:42:ARG:HG3	2.06	0.56
1:K:52:LEU:O	1:K:56:ILE:HG13	2.06	0.56
2:D:404:ASN:HA	2:D:437:LYS:HD2	1.88	0.56
2:P:398:ILE:CG2	2:P:402:LEU:HD11	2.36	0.56
2:B:221:SER:O	2:B:223:VAL:HG23	2.05	0.56
2:L:295:ILE:HG21	2:L:298:LEU:HD13	1.88	0.56
1:K:124:MET:O	1:K:128:LYS:HE2	2.05	0.56
2:L:390:ILE:HD11	2:L:412:LEU:HD23	1.87	0.56
2:L:380:LEU:HD13	2:L:383:MET:HE2	1.88	0.56
2:P:201:MET:HE1	2:P:302:TYR:CE2	2.41	0.55
2:P:263:TYR:C	2:P:265:ASN:H	2.10	0.55
2:F:191:ASN:HD21	2:F:194:LEU:H	1.54	0.55
2:H:367:GLN:CD	2:H:367:GLN:H	2.09	0.55
1:M:102:ILE:HB	2:N:20:VAL:HG21	1.88	0.55
2:H:332:ARG:CG	2:H:332:ARG:HH11	2.18	0.55
2:P:143:LEU:CD2	2:P:159:ILE:HD13	2.35	0.55
2:N:468:MET:HE1	2:N:483:PHE:CE1	2.42	0.55
2:B:397:SER:HA	2:B:400:THR:HG22	1.87	0.55
2:N:275:LEU:HD11	2:N:288:LEU:CD2	2.37	0.55
2:H:298:LEU:CD2	2:H:300:LEU:HD21	2.36	0.55
2:H:541:ASN:O	2:H:570:ALA:HA	2.06	0.55
2:F:80:LEU:HD12	2:F:122:MET:HE1	1.88	0.55
2:B:386:TYR:CE1	4:B:1100:OGK:H15A	2.42	0.55
2:B:59:LEU:O	2:B:62:THR:HB	2.07	0.55
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.71	0.55
2:P:95:ASN:O	2:P:582:PRO:HG3	2.07	0.55
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.89	0.55
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.88	0.55
2:H:471:GLY:O	2:H:496:ARG:O	2.25	0.55
2:B:380:LEU:HD13	2:B:383:MET:HE2	1.89	0.55
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.89	0.55
2:H:323:LEU:HD12	2:H:324:GLU:H	1.68	0.55
2:H:543:GLU:OE2	2:H:578:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:292:ALA:C	2:H:294:GLN:H	2.09	0.55
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.89	0.55
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.34	0.55
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.42	0.55
2:N:201:MET:HE1	2:N:302:TYR:CZ	2.42	0.55
2:B:191:ASN:HD21	2:B:194:LEU:H	1.54	0.55
2:H:467:TRP:HZ3	2:H:494:GLU:OE1	1.91	0.54
1:A:160:GLU:CG	2:B:31:PRO:HB3	2.35	0.54
1:M:159:PHE:O	1:M:160:GLU:CB	2.54	0.54
2:P:40:VAL:O	2:P:41:CYS:HB3	2.06	0.54
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.90	0.54
2:F:210:LYS:O	2:F:214:THR:HG22	2.07	0.54
2:B:289:PHE:N	2:B:290:PRO:CD	2.71	0.54
2:D:431:LEU:HD12	2:D:431:LEU:O	2.08	0.54
1:M:112:ASN:O	1:M:114:LEU:N	2.36	0.54
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.37	0.54
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.88	0.54
2:J:121:ARG:HH22	5:J:1103:PO4:P	2.30	0.54
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.90	0.54
2:F:201:MET:HE1	2:F:302:TYR:CE2	2.42	0.54
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.89	0.54
2:H:325:THR:OG1	2:H:326:ARG:N	2.36	0.54
2:H:120:ARG:HH22	5:H:1103:PO4:P	2.29	0.54
2:N:390:ILE:HD13	2:N:424:LEU:HD11	1.88	0.54
1:C:160:GLU:CG	2:D:31:PRO:HB3	2.37	0.54
1:O:91:MET:CG	1:O:116:LEU:HD21	2.37	0.54
2:N:468:MET:HE1	2:N:483:PHE:HE1	1.72	0.54
2:D:263:TYR:C	2:D:265:ASN:H	2.10	0.54
4:J:1100:OGK:HN08	4:J:1100:OGK:H18A	1.72	0.54
1:C:13:GLY:CA	1:K:9:LYS:NZ	2.70	0.54
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.87	0.54
2:N:429:ARG:O	2:N:433:ILE:HG13	2.07	0.54
2:H:365:VAL:HG13	2:H:387:VAL:CG2	2.38	0.54
2:H:519:TRP:HH2	2:H:567:HIS:CE1	2.25	0.54
2:L:543:GLU:OE2	2:L:578:ARG:HD3	2.06	0.54
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.90	0.54
2:N:386:TYR:CE1	4:N:1100:OGK:H15A	2.42	0.54
2:P:59:LEU:O	2:P:62:THR:HB	2.08	0.54
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.88	0.54
1:E:107:TYR:HD1	2:L:270:ARG:O	1.90	0.54
2:H:213:GLU:CD	2:H:237:GLY:HA3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:PHE:HZ	1:I:137:PHE:HE1	1.53	0.54
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.90	0.54
2:N:96:TRP:O	2:N:578:ARG:NH2	2.30	0.54
2:L:546:PRO:HD2	2:L:584:THR:O	2.07	0.54
2:B:543:GLU:OE2	2:B:578:ARG:HD3	2.08	0.54
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.89	0.54
2:L:404:ASN:HA	2:L:437:LYS:HD2	1.89	0.54
2:N:338:ALA:O	2:N:376:GLY:HA3	2.08	0.54
1:K:126:LYS:HZ1	2:L:29:THR:H	1.55	0.54
2:L:590:GLU:CB	2:L:591:PRO:HD2	2.36	0.54
2:D:443:PHE:HE2	2:D:445:LEU:HD11	1.72	0.54
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.38	0.54
2:F:59:LEU:O	2:F:62:THR:HB	2.08	0.54
2:H:259:MET:C	2:H:261:GLU:H	2.11	0.54
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.90	0.54
2:F:309:ASP:HA	2:F:312:THR:HG23	1.90	0.54
2:N:390:ILE:HD11	2:N:412:LEU:HD23	1.90	0.53
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.73	0.53
2:H:227:VAL:HG13	2:H:228:GLY:N	2.22	0.53
2:J:431:LEU:HD12	2:J:431:LEU:O	2.07	0.53
2:N:367:GLN:HG2	2:N:391:THR:CB	2.38	0.53
2:L:225:VAL:HG13	2:L:245:LEU:HD11	1.90	0.53
2:H:245:LEU:HB3	2:H:269:PRO:HG2	1.89	0.53
2:J:546:PRO:HD2	2:J:584:THR:O	2.07	0.53
2:H:351:ARG:HD2	2:H:359:GLU:O	2.08	0.53
2:H:89:PHE:CE2	4:H:1100:OGK:H04A	2.43	0.53
2:J:263:TYR:C	2:J:265:ASN:H	2.11	0.53
2:P:577:GLN:HE22	2:P:589:LYS:HG2	1.73	0.53
2:F:386:TYR:CE1	4:F:1100:OGK:H15A	2.43	0.53
2:F:543:GLU:OE2	2:F:578:ARG:HD3	2.08	0.53
2:N:469:LEU:HA	2:N:494:GLU:O	2.09	0.53
2:H:303:ALA:HB1	2:H:305:LEU:HD23	1.91	0.53
2:P:301:LEU:CD2	2:P:324:GLU:HB3	2.38	0.53
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.38	0.53
2:N:577:GLN:HE22	2:N:589:LYS:HG2	1.73	0.53
2:H:303:ALA:HB1	2:H:305:LEU:HD21	1.89	0.53
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.90	0.53
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.90	0.53
2:D:543:GLU:OE2	2:D:578:ARG:HD3	2.09	0.53
1:E:102:ILE:HG21	2:F:20:VAL:HG22	1.90	0.53
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:ASN:O	2:F:582:PRO:HG3	2.09	0.53
2:D:590:GLU:CB	2:D:591:PRO:HD2	2.35	0.53
2:H:253:LEU:HD13	2:H:284:GLU:HG3	1.91	0.53
2:J:367:GLN:HG2	2:J:391:THR:CB	2.37	0.53
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.42	0.53
2:L:431:LEU:HD12	2:L:431:LEU:C	2.28	0.53
2:H:289:PHE:HB2	2:H:290:PRO:HD3	1.90	0.53
2:F:247:GLU:HA	2:F:274:ARG:O	2.08	0.53
2:H:249:CYS:HA	2:H:276:GLY:O	2.09	0.53
2:H:101:THR:HB	2:H:102:PRO:HD3	1.89	0.53
2:L:348:ARG:HH22	4:L:1100:OGK:C10	2.21	0.53
2:N:404:ASN:CA	2:N:437:LYS:HD2	2.37	0.53
2:N:284:GLU:O	2:N:287:ILE:HD13	2.08	0.53
2:B:95:ASN:O	2:B:582:PRO:HG3	2.09	0.53
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.90	0.53
2:J:117:VAL:HG11	2:J:119:PHE:CZ	2.43	0.53
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.82	0.53
2:P:429:ARG:O	2:P:433:ILE:HG13	2.09	0.53
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.39	0.53
2:F:390:ILE:HD11	2:F:412:LEU:HD23	1.91	0.53
1:M:48:THR:HG22	1:M:51:ILE:CB	2.39	0.53
2:F:577:GLN:HE22	2:F:589:LYS:HG2	1.74	0.53
2:N:180:ASP:OD1	2:N:182:LYS:HG3	2.09	0.53
1:G:52:LEU:O	1:G:56:ILE:HG13	2.09	0.53
2:B:203:GLU:OE1	3:Q:211:ARG:HD3	2.08	0.53
2:J:59:LEU:O	2:J:62:THR:HB	2.08	0.53
2:P:367:GLN:HG2	2:P:391:THR:CB	2.39	0.53
2:L:154:ASP:OD2	2:L:179:LYS:NZ	2.41	0.53
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.74	0.53
1:G:106:ASN:OD1	2:H:23:GLN:OE1	2.27	0.53
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.74	0.52
2:N:590:GLU:CB	2:N:591:PRO:HD2	2.36	0.52
1:E:91:MET:CG	1:E:116:LEU:HD21	2.39	0.52
2:B:59:LEU:HD22	2:B:61:TYR:H	1.74	0.52
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.44	0.52
2:L:284:GLU:O	2:L:287:ILE:HD13	2.09	0.52
2:P:121:ARG:HH22	5:P:1103:PO4:P	2.33	0.52
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.90	0.52
1:O:159:PHE:O	1:O:160:GLU:CB	2.57	0.52
1:C:12:ASP:O	1:K:40:ASN:CB	2.57	0.52
2:J:471:GLY:O	2:J:496:ARG:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:THR:CG2	2:F:128:ASP:OD1	2.54	0.52
2:D:270:ARG:O	1:G:107:TYR:CD1	2.63	0.52
2:H:61:TYR:CD2	2:H:578:ARG:HG2	2.44	0.52
2:P:431:LEU:C	2:P:431:LEU:HD12	2.29	0.52
2:H:178:GLU:OE1	2:H:206:LYS:HB3	2.10	0.52
2:D:101:THR:CG2	2:N:179:LYS:HZ1	2.21	0.52
2:F:125:SER:N	2:F:128:ASP:OD2	2.43	0.52
2:L:59:LEU:O	2:L:62:THR:HB	2.09	0.52
2:J:443:PHE:HE2	2:J:445:LEU:HD11	1.73	0.52
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.91	0.52
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.92	0.52
1:M:27:GLN:HB2	1:M:109:ASN:HB3	1.90	0.52
2:F:295:ILE:HG21	2:F:298:LEU:HD13	1.90	0.52
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.73	0.52
2:H:207:ILE:HD12	2:H:230:PHE:HZ	1.74	0.52
2:D:221:SER:O	2:D:223:VAL:HG23	2.10	0.52
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.10	0.52
2:N:301:LEU:CD2	2:N:324:GLU:HB3	2.40	0.52
1:E:30:ALA:C	1:E:32:MET:H	2.13	0.52
2:F:380:LEU:HD13	2:F:383:MET:HE2	1.91	0.52
2:N:125:SER:N	2:N:128:ASP:OD2	2.43	0.52
2:N:284:GLU:O	2:N:287:ILE:HG23	2.10	0.52
1:C:102:ILE:HD11	1:C:121:VAL:HG21	1.92	0.52
2:F:443:PHE:HE2	2:F:445:LEU:HD11	1.73	0.52
2:N:311:CYS:O	2:N:315:GLN:HB2	2.10	0.52
2:H:286:PRO:C	2:H:288:LEU:H	2.12	0.52
2:B:263:TYR:C	2:B:265:ASN:H	2.13	0.52
2:B:275:LEU:HD11	2:B:288:LEU:CD2	2.39	0.52
1:I:126:LYS:HZ3	2:J:29:THR:H	1.57	0.52
2:P:180:ASP:OD1	2:P:182:LYS:HG3	2.10	0.52
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.91	0.52
1:C:99:PHE:CE2	2:D:17:VAL:HG22	2.44	0.52
2:D:80:LEU:HD12	2:D:122:MET:HE1	1.91	0.52
2:B:101:THR:CG2	2:F:179:LYS:HZ1	2.23	0.52
2:P:159:ILE:HG13	2:P:160:VAL:N	2.25	0.52
1:E:134:ARG:HB2	1:E:139:ILE:O	2.09	0.52
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.92	0.52
2:D:431:LEU:HD12	2:D:431:LEU:C	2.30	0.52
2:D:296:ARG:CZ	1:G:37:CYS:SG	2.98	0.52
2:B:225:VAL:HG13	2:B:245:LEU:HD11	1.91	0.52
2:P:309:ASP:HA	2:P:312:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:THR:O	1:C:133:ILE:HG12	2.10	0.51
2:H:157:LEU:O	2:H:161:THR:HG23	2.10	0.51
2:L:390:ILE:HD13	2:L:424:LEU:HD11	1.92	0.51
2:F:419:ILE:HG21	2:F:422:LEU:HD13	1.92	0.51
2:D:201:MET:HE1	2:D:302:TYR:CZ	2.45	0.51
2:L:263:TYR:C	2:L:265:ASN:H	2.12	0.51
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.45	0.51
2:H:390:ILE:HD13	2:H:390:ILE:N	2.26	0.51
2:L:367:GLN:HG2	2:L:391:THR:CB	2.39	0.51
2:H:136:ARG:HB3	2:H:140:LEU:HB2	1.93	0.51
2:H:267:VAL:O	2:H:267:VAL:HG23	2.10	0.51
1:C:102:ILE:CG2	2:D:20:VAL:CG2	2.86	0.51
2:D:59:LEU:O	2:D:62:THR:HB	2.09	0.51
2:P:311:CYS:O	2:P:315:GLN:HB2	2.10	0.51
2:B:289:PHE:N	2:B:290:PRO:HD2	2.25	0.51
2:H:178:GLU:CD	2:H:206:LYS:HB3	2.31	0.51
2:D:143:LEU:CD2	2:D:159:ILE:HD13	2.41	0.51
1:G:137:PHE:HB3	2:H:17:VAL:HG21	1.92	0.51
2:D:299:ASP:OD2	2:D:301:LEU:HB2	2.09	0.51
2:N:289:PHE:N	2:N:290:PRO:HD2	2.26	0.51
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.75	0.51
2:H:371:ILE:HG22	2:H:375:GLN:HE21	1.74	0.51
2:D:191:ASN:HD21	2:D:194:LEU:H	1.58	0.51
1:C:135:THR:HG22	1:C:136:THR:N	2.24	0.51
1:M:26:SER:OG	1:M:108:LEU:HB3	2.10	0.51
2:H:533:MET:HE1	2:H:588:LEU:HB3	1.91	0.51
2:H:212:LEU:HD22	2:H:230:PHE:HE1	1.75	0.51
2:J:386:TYR:CE1	4:J:1100:OGK:H15A	2.46	0.51
2:D:296:ARG:NE	1:G:37:CYS:SG	2.84	0.51
2:L:180:ASP:OD1	2:L:182:LYS:HG3	2.09	0.51
1:A:46:ASN:HB2	1:A:107:TYR:CZ	2.46	0.51
2:L:308:GLU:HG3	2:L:332:ARG:NH2	2.26	0.51
2:J:519:TRP:HE1	4:J:1100:OGK:H01	1.76	0.51
2:B:295:ILE:HG21	2:B:298:LEU:HD13	1.91	0.51
4:N:1100:OGK:C18	4:N:1100:OGK:HN08	2.23	0.51
2:H:470:LEU:HD13	2:H:473:VAL:HG21	1.93	0.51
2:P:295:ILE:HG21	2:P:298:LEU:HD13	1.93	0.51
1:C:126:LYS:HZ3	2:D:29:THR:H	1.58	0.51
2:L:191:ASN:HD21	2:L:194:LEU:H	1.57	0.51
2:B:577:GLN:HE22	2:B:589:LYS:HG2	1.75	0.51
2:B:294:GLN:NE2	1:O:107:TYR:OH	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.75	0.51
2:H:365:VAL:CG1	2:H:387:VAL:HG21	2.40	0.51
2:J:444:TYR:HA	2:J:471:GLY:CA	2.33	0.51
2:L:59:LEU:HD22	2:L:61:TYR:H	1.76	0.51
1:C:48:THR:HG22	1:C:51:ILE:N	2.21	0.51
2:B:404:ASN:CB	2:B:437:LYS:HD2	2.40	0.51
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.92	0.51
2:B:201:MET:HE1	2:B:302:TYR:CE2	2.46	0.51
2:L:453:LEU:HD11	2:L:457:TYR:OH	2.11	0.51
2:D:361:GLU:HG3	2:D:361:GLU:O	2.09	0.51
2:J:390:ILE:HD13	2:J:424:LEU:HD11	1.92	0.51
2:P:275:LEU:HD11	2:P:288:LEU:CD2	2.41	0.51
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.92	0.51
2:D:180:ASP:OD1	2:D:182:LYS:HG3	2.11	0.51
2:P:124:VAL:HG11	2:P:129:LEU:HD13	1.93	0.51
2:L:398:ILE:CG2	2:L:402:LEU:HD11	2.37	0.51
2:P:590:GLU:CB	2:P:591:PRO:HD2	2.38	0.51
1:I:159:PHE:O	1:I:160:GLU:CB	2.59	0.51
2:D:367:GLN:HG2	2:D:391:THR:CB	2.37	0.51
2:J:380:LEU:HD13	2:J:383:MET:HE2	1.93	0.51
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.93	0.51
1:M:134:ARG:HB2	1:M:139:ILE:O	2.10	0.51
2:P:390:ILE:HD11	2:P:412:LEU:HD23	1.93	0.50
1:E:48:THR:HG22	1:E:51:ILE:CB	2.41	0.50
2:H:335:GLU:OE2	2:H:368:ARG:NH1	2.44	0.50
2:F:59:LEU:HD22	2:F:61:TYR:H	1.76	0.50
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.92	0.50
1:C:13:GLY:CA	1:K:9:LYS:HZ3	2.24	0.50
2:F:301:LEU:CD2	2:F:324:GLU:HB3	2.41	0.50
1:C:12:ASP:O	1:K:40:ASN:ND2	2.43	0.50
2:F:546:PRO:HD2	2:F:584:THR:O	2.11	0.50
2:J:309:ASP:HA	2:J:312:THR:HG23	1.92	0.50
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.60	0.50
2:H:366:SER:CB	2:H:368:ARG:H	2.24	0.50
2:F:482:GLU:O	2:F:485:ARG:HG2	2.10	0.50
1:C:52:LEU:O	1:C:56:ILE:HG13	2.11	0.50
2:D:577:GLN:HE22	2:D:589:LYS:HG2	1.75	0.50
2:N:170:LEU:HD23	2:N:170:LEU:C	2.30	0.50
2:J:311:CYS:CB	2:J:336:VAL:HG21	2.41	0.50
2:B:404:ASN:CA	2:B:437:LYS:HD2	2.40	0.50
1:E:37:CYS:SG	2:L:296:ARG:CZ	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:VAL:HG23	2:H:122:MET:HE2	1.93	0.50
2:D:380:LEU:HD13	2:D:383:MET:HE2	1.93	0.50
2:D:225:VAL:HG13	2:D:245:LEU:HD11	1.92	0.50
2:P:274:ARG:HG2	2:P:297:LYS:HE3	1.93	0.50
2:H:233:LEU:O	2:H:236:VAL:HG23	2.12	0.50
2:N:399:GLY:O	2:N:434:GLY:HA3	2.11	0.50
1:E:52:LEU:O	1:E:56:ILE:HG13	2.11	0.50
1:O:27:GLN:HB2	1:O:109:ASN:HB3	1.93	0.50
2:H:348:ARG:HG3	2:H:384:ALA:HB3	1.93	0.50
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.93	0.50
2:D:295:ILE:HG21	2:D:298:LEU:HD13	1.94	0.50
1:M:44:LEU:O	1:M:44:LEU:HD12	2.11	0.50
2:H:274:ARG:CG	2:H:297:LYS:HB3	2.41	0.50
2:J:301:LEU:CD2	2:J:324:GLU:HB3	2.42	0.50
2:F:431:LEU:C	2:F:431:LEU:HD12	2.32	0.50
2:H:402:LEU:CD1	2:H:405:LEU:HG	2.41	0.50
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.94	0.50
2:F:113:GLN:HE22	2:L:192:THR:CB	2.24	0.50
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.47	0.50
2:B:546:PRO:HD2	2:B:584:THR:O	2.12	0.50
1:O:52:LEU:O	1:O:56:ILE:HG13	2.11	0.50
2:H:168:THR:HA	2:H:196:VAL:O	2.12	0.50
2:F:89:PHE:CD2	4:F:1100:OGK:H04A	2.47	0.50
2:D:304:LEU:HD11	3:R:216:ARG:HG3	1.93	0.50
1:A:124:MET:O	1:A:128:LYS:HE2	2.11	0.50
2:J:192:THR:HG21	2:N:113:GLN:HE22	1.76	0.50
2:D:101:THR:CG2	2:N:179:LYS:NZ	2.75	0.50
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.56	0.50
2:B:101:THR:HG21	2:F:179:LYS:HZ1	1.76	0.50
2:J:367:GLN:HG2	2:J:391:THR:CG2	2.42	0.50
2:H:96:TRP:HA	2:H:582:PRO:HG2	1.93	0.50
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.93	0.50
2:P:125:SER:O	2:P:129:LEU:HD22	2.12	0.50
2:F:154:ASP:OD2	2:F:179:LYS:NZ	2.39	0.50
1:O:91:MET:SD	1:O:117:THR:CG2	2.99	0.50
2:F:404:ASN:CB	2:F:437:LYS:HD2	2.42	0.50
1:K:34:GLU:C	1:K:36:ASP:H	2.15	0.50
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.94	0.50
2:H:365:VAL:HG13	2:H:387:VAL:HG21	1.95	0.49
2:H:95:ASN:HD22	2:H:95:ASN:N	2.08	0.49
2:H:144:LYS:HE3	5:H:1104:PO4:O4	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.59	0.49
2:D:247:GLU:HA	2:D:274:ARG:O	2.11	0.49
1:E:44:LEU:O	1:E:44:LEU:HD12	2.12	0.49
1:A:129:THR:O	1:A:133:ILE:HG12	2.12	0.49
2:H:443:PHE:CE2	2:H:445:LEU:HD11	2.47	0.49
2:J:422:LEU:O	2:J:423:PRO:C	2.50	0.49
2:J:240:LYS:CG	2:J:267:VAL:HG21	2.40	0.49
2:H:61:TYR:CE2	2:H:578:ARG:HG2	2.47	0.49
2:L:289:PHE:N	2:L:290:PRO:CD	2.75	0.49
2:H:326:ARG:O	2:H:327:ASN:CB	2.60	0.49
2:J:59:LEU:HD22	2:J:61:TYR:H	1.77	0.49
1:A:134:ARG:HB2	1:A:139:ILE:O	2.12	0.49
2:D:309:ASP:HA	2:D:312:THR:HG23	1.94	0.49
1:M:34:GLU:C	1:M:36:ASP:H	2.16	0.49
2:H:327:ASN:ND2	2:H:364:LEU:HD21	2.27	0.49
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.90	0.49
2:P:404:ASN:CB	2:P:437:LYS:HD2	2.43	0.49
2:N:211:ASP:O	2:N:215:ILE:HG13	2.13	0.49
1:K:27:GLN:HB2	1:K:109:ASN:HB3	1.94	0.49
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.94	0.49
2:P:170:LEU:HD23	2:P:170:LEU:C	2.32	0.49
1:E:34:GLU:C	1:E:36:ASP:H	2.15	0.49
2:B:431:LEU:HD12	2:B:431:LEU:O	2.12	0.49
2:J:275:LEU:HD11	2:J:288:LEU:CD2	2.42	0.49
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.94	0.49
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.95	0.49
2:H:108:SER:OG	2:H:135:ALA:HB2	2.13	0.49
2:H:265:ASN:N	2:H:265:ASN:OD1	2.45	0.49
1:C:48:THR:HG22	1:C:51:ILE:HB	1.94	0.49
2:H:494:GLU:HB3	2:H:519:TRP:HD1	1.76	0.49
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.94	0.49
2:F:304:LEU:HD11	3:S:216:ARG:HG3	1.94	0.49
2:L:275:LEU:HD11	2:L:288:LEU:CD2	2.43	0.49
2:P:225:VAL:HG13	2:P:245:LEU:HD11	1.95	0.49
1:O:134:ARG:HB2	1:O:139:ILE:O	2.13	0.49
2:F:180:ASP:OD1	2:F:182:LYS:HG3	2.13	0.49
1:O:34:GLU:C	1:O:36:ASP:H	2.16	0.49
2:B:154:ASP:OD2	2:B:179:LYS:NZ	2.40	0.49
2:D:121:ARG:HH22	5:D:1103:PO4:P	2.36	0.49
2:B:190:HIS:CG	2:P:112:ARG:NH1	2.80	0.49
2:H:232:ILE:CG2	2:H:266:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.47	0.49
2:N:432:LEU:CD1	2:N:458:ILE:HA	2.43	0.49
2:L:444:TYR:HA	2:L:471:GLY:CA	2.33	0.49
2:N:263:TYR:C	2:N:265:ASN:H	2.14	0.49
1:A:46:ASN:HB2	1:A:107:TYR:CE2	2.48	0.49
2:N:454:GLY:O	2:N:457:TYR:HB2	2.13	0.49
2:D:444:TYR:HA	2:D:471:GLY:CA	2.30	0.49
2:L:471:GLY:O	2:L:496:ARG:O	2.30	0.49
2:J:89:PHE:CE1	4:J:1100:OGK:H17	2.47	0.49
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.95	0.49
2:H:404:ASN:HA	2:H:437:LYS:HD3	1.93	0.49
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.78	0.49
2:L:221:SER:O	2:L:223:VAL:HG23	2.12	0.49
2:J:164:ARG:HD2	2:N:112:ARG:NE	2.28	0.48
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.43	0.48
2:D:275:LEU:HD11	2:D:288:LEU:CD2	2.43	0.48
1:A:34:GLU:C	1:A:36:ASP:H	2.17	0.48
1:K:134:ARG:HB2	1:K:139:ILE:O	2.12	0.48
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.94	0.48
2:J:170:LEU:HD23	2:J:170:LEU:C	2.33	0.48
2:H:519:TRP:HZ3	2:H:567:HIS:HD1	1.51	0.48
2:N:159:ILE:HG13	2:N:160:VAL:N	2.28	0.48
2:F:211:ASP:O	2:F:215:ILE:HG13	2.12	0.48
1:A:52:LEU:O	1:A:56:ILE:HG13	2.12	0.48
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.49	0.48
2:F:419:ILE:CG2	2:F:422:LEU:HD13	2.43	0.48
2:J:311:CYS:O	2:J:315:GLN:HB2	2.14	0.48
2:L:391:THR:HG23	2:L:394:SER:H	1.76	0.48
2:J:391:THR:HG23	2:J:394:SER:H	1.78	0.48
2:L:443:PHE:HE2	2:L:445:LEU:HD11	1.75	0.48
1:K:30:ALA:C	1:K:32:MET:H	2.16	0.48
2:J:289:PHE:N	2:J:290:PRO:HD2	2.28	0.48
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.95	0.48
2:J:203:GLU:OE1	3:U:211:ARG:HD3	2.14	0.48
1:G:27:GLN:HB2	1:G:109:ASN:HB3	1.94	0.48
2:N:501:SER:HA	2:N:524:ARG:HB2	1.94	0.48
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.95	0.48
1:E:135:THR:HG22	1:E:136:THR:N	2.27	0.48
2:H:432:LEU:HB3	2:H:461:TYR:O	2.13	0.48
2:N:295:ILE:HG21	2:N:298:LEU:HD13	1.95	0.48
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:LEU:HD11	3:Q:216:ARG:HG3	1.93	0.48
2:L:201:MET:HE3	3:V:208:SER:HB2	1.95	0.48
2:F:453:LEU:HD11	2:F:457:TYR:OH	2.13	0.48
2:H:89:PHE:CE1	4:H:1100:OGK:H17	2.49	0.48
1:A:125:ILE:HG23	1:A:133:ILE:CD1	2.36	0.48
2:F:240:LYS:CG	2:F:267:VAL:HG21	2.40	0.48
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.43	0.48
1:I:8:LEU:HD22	1:I:29:ILE:HD13	1.95	0.48
2:H:298:LEU:HD21	2:H:300:LEU:HD21	1.94	0.48
2:J:191:ASN:HD21	2:J:194:LEU:H	1.60	0.48
1:C:102:ILE:CG2	2:D:20:VAL:HG21	2.43	0.48
2:B:125:SER:N	2:B:128:ASP:OD2	2.47	0.48
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.48
2:N:391:THR:HG23	2:N:394:SER:H	1.76	0.48
1:A:159:PHE:O	1:A:160:GLU:CB	2.60	0.48
2:B:367:GLN:HG2	2:B:391:THR:CB	2.43	0.48
2:H:125:SER:HB2	2:H:128:ASP:H	1.78	0.48
1:K:46:ASN:HB2	1:K:107:TYR:CE2	2.49	0.48
2:H:490:LEU:O	2:H:514:SER:O	2.30	0.48
2:P:453:LEU:HD11	2:P:457:TYR:OH	2.13	0.48
2:J:247:GLU:HA	2:J:274:ARG:O	2.13	0.48
1:I:27:GLN:HB2	1:I:109:ASN:HB3	1.94	0.48
2:H:327:ASN:C	2:H:327:ASN:OD1	2.51	0.48
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.95	0.48
2:L:125:SER:N	2:L:128:ASP:OD2	2.47	0.48
2:J:398:ILE:CG2	2:J:402:LEU:HD11	2.38	0.48
2:H:212:LEU:HD23	2:H:235:LEU:CD2	2.43	0.48
2:H:191:ASN:ND2	2:H:194:LEU:H	2.11	0.48
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.96	0.48
2:L:274:ARG:HG2	2:L:297:LYS:HE3	1.95	0.48
2:L:247:GLU:HA	2:L:274:ARG:O	2.14	0.48
1:C:8:LEU:HD22	1:C:29:ILE:HD13	1.96	0.48
2:B:180:ASP:OD1	2:B:182:LYS:HG3	2.12	0.48
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.94	0.48
2:B:191:ASN:ND2	2:B:194:LEU:H	2.11	0.48
1:E:48:THR:HG22	1:E:51:ILE:N	2.24	0.48
2:P:391:THR:HG23	2:P:394:SER:H	1.77	0.48
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.96	0.48
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.47	0.48
2:J:577:GLN:HE22	2:J:589:LYS:HG2	1.79	0.48
2:H:394:SER:O	2:H:398:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:577:GLN:HE22	2:L:589:LYS:HG2	1.78	0.48
2:J:429:ARG:O	2:J:433:ILE:HG13	2.14	0.48
2:L:309:ASP:HA	2:L:312:THR:HG23	1.95	0.48
2:D:419:ILE:HD11	2:D:446:ARG:NH2	2.29	0.48
2:F:590:GLU:CB	2:F:591:PRO:HD2	2.40	0.48
2:B:398:ILE:CG2	2:B:402:LEU:HD11	2.40	0.48
2:F:367:GLN:HG2	2:F:391:THR:CB	2.43	0.48
1:K:102:ILE:HG12	1:K:117:THR:CB	2.44	0.48
2:N:247:GLU:HA	2:N:274:ARG:O	2.14	0.48
2:H:487:CYS:HB3	2:H:490:LEU:HB2	1.94	0.48
2:P:454:GLY:O	2:P:457:TYR:HB2	2.13	0.48
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.95	0.48
2:H:373:LEU:HD11	2:H:380:LEU:HD11	1.96	0.48
1:C:159:PHE:O	1:C:160:GLU:CB	2.61	0.47
1:O:48:THR:HG22	1:O:51:ILE:HB	1.96	0.47
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.95	0.47
2:D:201:MET:HE2	2:D:302:TYR:OH	2.14	0.47
1:M:99:PHE:CE2	2:N:17:VAL:N	2.82	0.47
1:A:132:GLU:O	1:A:136:THR:HG23	2.14	0.47
2:N:153:THR:HG23	2:N:178:GLU:HA	1.96	0.47
2:H:526:SER:HB2	2:H:529:GLY:HA3	1.96	0.47
1:C:27:GLN:HB2	1:C:109:ASN:HB3	1.96	0.47
2:J:46:LYS:HE3	2:J:46:LYS:HB2	1.46	0.47
2:H:303:ALA:O	2:H:326:ARG:NH1	2.46	0.47
2:B:471:GLY:O	2:B:496:ARG:O	2.32	0.47
4:P:1100:OGK:H18A	4:P:1100:OGK:N08	2.29	0.47
2:L:96:TRP:O	2:L:578:ARG:NH2	2.36	0.47
2:H:166:ILE:O	2:H:193:SER:HB2	2.14	0.47
2:F:54:HIS:HD2	2:F:77:SER:OG	1.96	0.47
2:B:391:THR:HG23	2:B:394:SER:H	1.79	0.47
2:H:109:ASN:C	2:H:110:ASN:HD22	2.17	0.47
2:L:541:ASN:O	2:L:570:ALA:HA	2.13	0.47
2:F:225:VAL:HG13	2:F:245:LEU:HD11	1.96	0.47
2:F:227:VAL:CG1	2:F:228:GLY:N	2.78	0.47
2:D:125:SER:N	2:D:128:ASP:OD2	2.46	0.47
2:D:270:ARG:O	1:G:107:TYR:HD1	1.97	0.47
2:H:96:TRP:HA	2:H:582:PRO:CG	2.45	0.47
1:G:30:ALA:C	1:G:32:MET:H	2.16	0.47
2:D:201:MET:CE	2:D:302:TYR:CZ	2.98	0.47
2:H:286:PRO:C	2:H:288:LEU:N	2.68	0.47
1:G:34:GLU:C	1:G:36:ASP:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:ARG:O	2:D:336:VAL:HG23	2.14	0.47
2:H:214:THR:HA	2:H:217:ARG:HG2	1.97	0.47
2:P:153:THR:HG23	2:P:178:GLU:HA	1.97	0.47
2:H:168:THR:HB	2:H:196:VAL:CG1	2.24	0.47
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.80	0.47
2:H:104:VAL:HG11	2:H:128:ASP:HB2	1.96	0.47
2:L:201:MET:CE	2:L:302:TYR:CZ	2.98	0.47
1:K:102:ILE:CG1	1:K:117:THR:HB	2.44	0.47
2:N:482:GLU:O	2:N:485:ARG:HG2	2.14	0.47
2:J:431:LEU:HD12	2:J:431:LEU:C	2.35	0.47
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.49	0.47
2:J:389:ASP:OD2	2:J:419:ILE:HG23	2.14	0.47
2:J:469:LEU:HA	2:J:494:GLU:O	2.14	0.47
1:A:102:ILE:HG12	1:A:117:THR:OG1	2.14	0.47
1:G:83:LEU:HD23	1:G:83:LEU:HA	1.78	0.47
2:B:270:ARG:O	1:O:107:TYR:CD1	2.68	0.47
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.95	0.47
2:B:431:LEU:HD12	2:B:431:LEU:C	2.35	0.47
2:H:108:SER:OG	2:H:135:ALA:CB	2.62	0.47
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.49	0.47
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.96	0.47
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.52	0.47
2:B:179:LYS:NZ	2:F:101:THR:HG21	2.29	0.47
2:J:80:LEU:HD12	2:J:122:MET:HE1	1.96	0.47
2:B:590:GLU:CB	2:B:591:PRO:HD2	2.37	0.47
2:F:468:MET:HE1	2:F:483:PHE:CE1	2.50	0.47
2:P:366:SER:HB2	2:P:367:GLN:OE1	2.14	0.47
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.44	0.47
2:J:96:TRP:O	2:J:578:ARG:NH2	2.38	0.47
1:C:30:ALA:C	1:C:32:MET:H	2.17	0.47
2:P:201:MET:HE1	2:P:302:TYR:CZ	2.50	0.47
1:C:99:PHE:CZ	2:D:17:VAL:HG22	2.49	0.47
2:H:347:LEU:CD2	2:H:373:LEU:HD21	2.45	0.47
2:F:446:ARG:HG2	2:F:447:GLN:H	1.79	0.47
1:C:34:GLU:C	1:C:36:ASP:H	2.17	0.47
2:P:46:LYS:HB2	2:P:46:LYS:HE3	1.47	0.47
1:M:132:GLU:O	1:M:136:THR:HG23	2.14	0.47
2:N:422:LEU:O	2:N:423:PRO:C	2.53	0.47
1:K:159:PHE:O	1:K:160:GLU:CB	2.63	0.47
1:G:158:ALA:HA	2:H:62:THR:HG21	1.96	0.47
1:M:30:ALA:C	1:M:32:MET:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:404:ASN:CB	2:J:437:LYS:HD2	2.45	0.47
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.48	0.47
2:B:54:HIS:HD2	2:B:77:SER:OG	1.98	0.47
2:H:403:LYS:O	2:H:404:ASN:OD1	2.32	0.47
2:J:191:ASN:ND2	2:J:194:LEU:H	2.13	0.47
2:J:297:LYS:HG3	2:J:322:VAL:HB	1.96	0.47
1:E:27:GLN:HB2	1:E:109:ASN:HB3	1.96	0.47
2:B:429:ARG:O	2:B:433:ILE:HG13	2.15	0.47
2:H:142:THR:HB	2:H:168:THR:OG1	2.15	0.47
2:N:411:VAL:HG22	2:N:444:TYR:HB3	1.96	0.47
2:L:201:MET:HE2	2:L:302:TYR:OH	2.15	0.47
2:H:199:PHE:CE1	2:H:227:VAL:HG22	2.49	0.47
1:I:135:THR:HG22	1:I:136:THR:N	2.30	0.47
2:L:419:ILE:O	2:L:420:THR:C	2.53	0.47
2:H:120:ARG:NH2	5:H:1103:PO4:O2	2.48	0.47
2:N:101:THR:CG2	2:N:128:ASP:OD1	2.58	0.47
2:H:170:LEU:HA	2:H:198:ASN:O	2.14	0.47
2:B:85:ARG:HD2	5:B:1101:PO4:O2	2.15	0.47
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.50	0.47
2:P:482:GLU:O	2:P:485:ARG:HG2	2.15	0.47
2:F:274:ARG:HG2	2:F:297:LYS:HE3	1.97	0.47
2:F:191:ASN:ND2	2:F:194:LEU:H	2.12	0.47
2:F:113:GLN:NE2	2:L:192:THR:HG21	2.30	0.47
2:F:227:VAL:HG13	2:F:228:GLY:N	2.30	0.47
2:B:217:ARG:NH1	2:P:50:GLU:OE2	2.47	0.47
2:N:40:VAL:O	2:N:41:CYS:HB3	2.14	0.47
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.53	0.47
2:H:548:ARG:HE	2:H:548:ARG:HB3	1.50	0.47
1:A:48:THR:HG22	1:A:51:ILE:HB	1.96	0.46
2:D:211:ASP:O	2:D:215:ILE:HG13	2.15	0.46
2:H:285:MET:N	2:H:286:PRO:CD	2.78	0.46
2:J:54:HIS:HD2	2:J:77:SER:OG	1.98	0.46
2:L:101:THR:CG2	2:L:128:ASP:OD1	2.58	0.46
2:F:366:SER:HB2	2:F:367:GLN:OE1	2.15	0.46
2:N:543:GLU:OE2	2:N:578:ARG:HD3	2.15	0.46
2:F:96:TRP:O	2:F:578:ARG:NH2	2.34	0.46
2:P:191:ASN:HD21	2:P:194:LEU:H	1.63	0.46
2:P:289:PHE:N	2:P:290:PRO:HD2	2.30	0.46
2:D:192:THR:HB	2:H:113:GLN:NE2	2.30	0.46
2:H:327:ASN:HD22	2:H:364:LEU:CD2	2.28	0.46
2:H:533:MET:C	2:H:535:MET:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:429:ARG:HD2	2:H:457:TYR:CD2	2.50	0.46
2:H:440:ARG:CB	2:H:467:TRP:HD1	2.28	0.46
2:N:310:HIS:HE1	2:N:325:THR:OG1	1.99	0.46
2:F:284:GLU:O	2:F:287:ILE:HG23	2.14	0.46
2:F:308:GLU:HG3	2:F:332:ARG:NH2	2.30	0.46
2:H:262:LYS:HD3	2:H:263:TYR:CZ	2.51	0.46
2:L:289:PHE:N	2:L:290:PRO:HD2	2.29	0.46
1:A:101:LEU:HB3	1:A:117:THR:HG21	1.95	0.46
2:J:225:VAL:HG13	2:J:245:LEU:HD11	1.96	0.46
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.97	0.46
2:H:390:ILE:HD12	2:H:410:LEU:CD2	2.38	0.46
1:I:111:LYS:O	1:I:115:ASP:CB	2.62	0.46
2:L:311:CYS:O	2:L:315:GLN:HB2	2.16	0.46
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.50	0.46
2:H:55:VAL:HG23	2:H:75:LEU:HD21	1.97	0.46
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.78	0.46
1:O:132:GLU:O	1:O:136:THR:HG23	2.15	0.46
2:H:414:ASP:HB3	2:H:446:ARG:HH21	1.81	0.46
2:J:335:GLU:O	2:J:338:ALA:HB3	2.15	0.46
2:L:121:ARG:HH22	5:L:1103:PO4:P	2.39	0.46
1:I:34:GLU:C	1:I:36:ASP:H	2.19	0.46
2:H:455:LEU:HA	2:H:455:LEU:HD23	1.65	0.46
2:N:46:LYS:HB2	2:N:46:LYS:HE3	1.47	0.46
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.98	0.46
2:L:310:HIS:HE1	2:L:325:THR:OG1	1.98	0.46
2:D:311:CYS:O	2:D:315:GLN:HB2	2.15	0.46
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.51	0.46
2:P:432:LEU:CD1	2:P:458:ILE:HA	2.46	0.46
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.50	0.46
2:P:409:ARG:HB3	2:P:442:ALA:HB3	1.97	0.46
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.85	0.46
2:H:220:ARG:HA	2:H:220:ARG:HD2	1.67	0.46
2:B:503:ARG:HB3	2:B:503:ARG:NH1	2.31	0.46
2:H:532:LEU:O	2:H:535:MET:HB3	2.15	0.46
2:L:272:LEU:HA	2:L:272:LEU:HD23	1.71	0.46
2:B:446:ARG:HG2	2:B:447:GLN:H	1.79	0.46
2:F:289:PHE:N	2:F:290:PRO:HD2	2.31	0.46
2:H:32:LYS:HA	2:H:32:LYS:HD3	1.47	0.46
1:G:48:THR:HG22	1:G:51:ILE:HB	1.98	0.46
2:L:85:ARG:NH2	4:L:1100:OGK:O07	2.40	0.46
2:D:402:LEU:O	2:D:402:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:ARG:HG2	2:D:297:LYS:HE3	1.97	0.46
2:L:272:LEU:HD13	2:L:275:LEU:HD13	1.97	0.46
2:J:409:ARG:HB2	4:J:1100:OGK:H16B	1.96	0.46
2:F:429:ARG:O	2:F:433:ILE:HG13	2.16	0.46
2:H:216:ALA:HB2	2:H:238:PHE:CD1	2.50	0.46
2:L:176:PHE:CZ	2:L:204:PHE:CZ	3.04	0.46
2:P:331:ASP:OD1	2:P:369:GLY:N	2.47	0.46
2:L:441:PHE:O	2:L:468:MET:HA	2.15	0.46
2:J:284:GLU:O	2:J:287:ILE:HG23	2.15	0.46
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.51	0.46
1:O:26:SER:OG	1:O:108:LEU:HB3	2.15	0.46
2:B:453:LEU:HD11	2:B:457:TYR:OH	2.16	0.46
2:J:180:ASP:OD1	2:J:182:LYS:HG3	2.15	0.46
1:C:141:ASN:OD1	1:C:141:ASN:C	2.54	0.46
2:H:362:GLU:O	2:H:364:LEU:N	2.49	0.46
2:L:530:GLN:HE21	2:L:592:ILE:HD11	1.81	0.46
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.58	0.46
2:L:197:LEU:O	2:L:225:VAL:HA	2.15	0.46
2:F:454:GLY:O	2:F:457:TYR:HB2	2.16	0.46
2:P:191:ASN:ND2	2:P:194:LEU:H	2.14	0.46
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.50	0.46
2:L:117:VAL:HG11	2:L:119:PHE:CZ	2.51	0.46
2:F:203:GLU:OE1	3:S:211:ARG:HD3	2.16	0.46
1:K:153:ARG:HG2	1:K:157:TRP:CZ3	2.51	0.46
2:N:541:ASN:O	2:N:570:ALA:HA	2.16	0.46
2:J:590:GLU:CB	2:J:591:PRO:HD2	2.38	0.46
2:B:270:ARG:O	1:O:107:TYR:HD1	1.98	0.46
1:I:46:ASN:HB2	1:I:107:TYR:CE2	2.51	0.46
2:H:105:THR:HG22	2:H:106:GLU:N	2.31	0.46
2:H:258:GLY:O	2:H:260:PRO:HD2	2.16	0.46
2:L:65:PRO:HA	2:L:103:TRP:CZ3	2.51	0.46
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.97	0.46
2:N:503:ARG:HB3	2:N:503:ARG:NH1	2.30	0.46
2:H:509:VAL:HG21	2:H:535:MET:SD	2.56	0.45
2:H:440:ARG:HB3	2:H:467:TRP:HD1	1.81	0.45
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.51	0.45
2:H:546:PRO:HD2	2:H:584:THR:O	2.16	0.45
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.96	0.45
2:H:441:PHE:O	2:H:468:MET:HA	2.15	0.45
2:N:16:THR:HG22	2:N:17:VAL:H	1.81	0.45
2:F:311:CYS:O	2:F:315:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:117:VAL:HG11	2:P:119:PHE:CZ	2.50	0.45
2:D:305:LEU:HD23	2:D:305:LEU:O	2.16	0.45
2:H:253:LEU:HD12	2:H:280:MET:HA	1.98	0.45
1:O:98:LEU:HD11	1:O:117:THR:HB	1.98	0.45
2:J:405:LEU:HD13	2:J:408:PHE:HB2	1.96	0.45
2:F:391:THR:HG23	2:F:394:SER:H	1.81	0.45
2:H:291:PHE:O	2:H:294:GLN:HB3	2.16	0.45
2:B:543:GLU:OE2	2:B:578:ARG:CD	2.65	0.45
2:P:197:LEU:O	2:P:225:VAL:HA	2.16	0.45
2:H:334:LEU:HD22	2:H:373:LEU:HD22	1.99	0.45
2:P:338:ALA:O	2:P:376:GLY:HA3	2.16	0.45
2:J:501:SER:HA	2:J:524:ARG:HB2	1.99	0.45
1:O:8:LEU:HD22	1:O:29:ILE:HD13	1.98	0.45
2:N:532:LEU:HD23	2:N:532:LEU:HA	1.72	0.45
1:I:48:THR:HG22	1:I:51:ILE:N	2.23	0.45
2:L:366:SER:HB2	2:L:367:GLN:OE1	2.16	0.45
2:H:519:TRP:CZ3	2:H:567:HIS:ND1	2.71	0.45
2:D:59:LEU:HD22	2:D:61:TYR:H	1.80	0.45
1:I:102:ILE:HG12	1:I:117:THR:CB	2.47	0.45
2:B:247:GLU:HA	2:B:274:ARG:O	2.16	0.45
2:N:274:ARG:HG2	2:N:297:LYS:HE3	1.99	0.45
2:B:419:ILE:O	2:B:420:THR:C	2.53	0.45
1:E:8:LEU:HD22	1:E:29:ILE:HD13	1.98	0.45
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.98	0.45
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.51	0.45
1:K:132:GLU:O	1:K:136:THR:HG23	2.15	0.45
2:B:532:LEU:HA	2:B:532:LEU:HD23	1.76	0.45
2:B:170:LEU:C	2:B:170:LEU:HD23	2.36	0.45
1:M:102:ILE:HD13	2:N:20:VAL:CG2	2.46	0.45
2:N:444:TYR:HA	2:N:471:GLY:CA	2.32	0.45
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.96	0.45
2:P:419:ILE:HG21	2:P:422:LEU:HD13	1.97	0.45
2:F:419:ILE:O	2:F:420:THR:C	2.53	0.45
2:N:441:PHE:O	2:N:468:MET:HA	2.17	0.45
1:G:158:ALA:HB2	2:H:62:THR:HG23	1.98	0.45
2:H:255:GLU:HB3	2:H:263:TYR:HE1	1.81	0.45
2:L:191:ASN:ND2	2:L:194:LEU:H	2.15	0.45
1:A:27:GLN:HB2	1:A:109:ASN:HB3	1.97	0.45
2:P:399:GLY:O	2:P:434:GLY:HA3	2.16	0.45
2:P:361:GLU:O	2:P:361:GLU:HG3	2.15	0.45
1:G:48:THR:HG22	1:G:51:ILE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:259:MET:HB2	2:H:262:LYS:HB2	1.99	0.45
2:P:289:PHE:N	2:P:290:PRO:CD	2.78	0.45
1:A:8:LEU:HD22	1:A:29:ILE:HD13	1.98	0.45
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.98	0.45
2:J:305:LEU:HD23	2:J:305:LEU:O	2.17	0.45
1:A:98:LEU:HD21	1:A:120:THR:CG2	2.43	0.45
1:O:48:THR:HG22	1:O:51:ILE:CB	2.47	0.45
2:N:366:SER:HB2	2:N:367:GLN:OE1	2.17	0.45
2:N:308:GLU:HG3	2:N:332:ARG:NH2	2.32	0.45
2:B:419:ILE:HG21	2:B:422:LEU:HD13	1.98	0.45
1:K:135:THR:HG22	1:K:136:THR:N	2.30	0.45
2:J:270:ARG:HB3	1:M:46:ASN:OD1	2.16	0.45
1:A:26:SER:OG	1:A:108:LEU:HB3	2.16	0.45
2:D:46:LYS:HE3	2:D:46:LYS:HB2	1.49	0.45
2:H:120:ARG:HH11	2:H:147:LYS:HZ3	1.63	0.45
2:P:441:PHE:O	2:P:468:MET:HA	2.17	0.45
2:P:468:MET:HB3	2:P:468:MET:HE3	1.76	0.45
2:N:81:LYS:NZ	5:N:1103:PO4:O3	2.35	0.45
2:D:482:GLU:O	2:D:485:ARG:HG2	2.17	0.45
2:H:291:PHE:N	2:H:291:PHE:CD2	2.84	0.45
2:N:197:LEU:O	2:N:225:VAL:HA	2.16	0.45
1:M:134:ARG:CZ	1:M:141:ASN:HB2	2.47	0.45
2:N:432:LEU:HB3	2:N:461:TYR:O	2.17	0.45
2:N:117:VAL:HG11	2:N:119:PHE:CZ	2.52	0.45
1:A:44:LEU:HD12	1:A:44:LEU:O	2.17	0.45
2:P:344:LEU:HD12	2:P:344:LEU:HA	1.83	0.45
2:B:176:PHE:CZ	2:B:204:PHE:CZ	3.04	0.45
2:J:468:MET:HE1	2:J:483:PHE:CE1	2.51	0.45
2:H:259:MET:O	2:H:261:GLU:N	2.49	0.45
1:I:134:ARG:HB2	1:I:139:ILE:O	2.17	0.45
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.52	0.45
2:L:170:LEU:HD23	2:L:170:LEU:C	2.38	0.45
2:D:136:ARG:HG3	2:D:136:ARG:HH11	1.81	0.45
2:N:32:LYS:HD2	2:N:32:LYS:HA	1.89	0.45
2:H:326:ARG:O	2:H:327:ASN:HB3	2.17	0.45
2:H:363:GLY:O	2:H:364:LEU:C	2.55	0.45
2:H:494:GLU:HB3	2:H:519:TRP:CD1	2.51	0.45
2:H:304:LEU:HD22	2:H:304:LEU:HA	1.79	0.45
2:L:301:LEU:CD2	2:L:324:GLU:HB3	2.47	0.45
2:D:296:ARG:NH1	1:G:35:ASP:OD1	2.45	0.45
2:D:301:LEU:CD2	2:D:324:GLU:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:245:LEU:HD12	2:P:245:LEU:HA	1.86	0.45
1:K:8:LEU:HD22	1:K:29:ILE:HD13	1.98	0.45
2:L:432:LEU:HB3	2:L:461:TYR:O	2.17	0.45
2:H:476:SER:O	2:H:477:ASP:C	2.55	0.45
2:L:367:GLN:HG2	2:L:391:THR:CG2	2.47	0.45
2:L:384:ALA:HB1	4:L:1100:OGK:C16	2.46	0.45
2:N:57:MET:HE2	2:N:62:THR:HG22	1.98	0.45
2:P:272:LEU:HD13	2:P:275:LEU:HD13	1.97	0.45
1:O:102:ILE:HD12	2:P:20:VAL:CG2	2.47	0.45
2:H:349:ILE:HD12	2:H:385:VAL:HG23	1.98	0.45
2:D:404:ASN:CB	2:D:437:LYS:HD2	2.46	0.45
2:D:441:PHE:O	2:D:468:MET:HA	2.17	0.45
1:E:114:LEU:O	1:E:118:CYS:HB2	2.17	0.45
1:E:132:GLU:O	1:E:136:THR:HG23	2.16	0.45
2:H:414:ASP:OD2	2:H:418:ARG:NH2	2.50	0.45
1:O:108:LEU:HD12	1:O:110:ILE:HD11	1.99	0.45
2:N:63:ALA:HB1	2:N:67:ARG:HD2	1.99	0.45
1:C:134:ARG:HB2	1:C:139:ILE:O	2.17	0.45
2:H:339:GLN:HG3	2:H:340:TYR:CD1	2.52	0.45
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.98	0.45
2:D:272:LEU:HD23	2:D:272:LEU:HA	1.72	0.45
1:I:112:ASN:N	1:I:112:ASN:OD1	2.50	0.45
1:I:141:ASN:OD1	1:I:141:ASN:C	2.55	0.45
2:P:503:ARG:HB3	2:P:503:ARG:NH1	2.31	0.45
2:H:85:ARG:NH1	5:H:1101:PO4:O2	2.50	0.44
2:D:390:ILE:HD13	2:D:424:LEU:HD11	1.99	0.44
2:J:57:MET:HE2	2:J:62:THR:HG22	1.98	0.44
1:C:158:ALA:HA	2:D:62:THR:HG23	1.99	0.44
2:B:411:VAL:CG2	4:B:1100:OGK:H14	2.47	0.44
2:B:441:PHE:O	2:B:468:MET:HA	2.17	0.44
4:J:1100:OGK:C18	4:J:1100:OGK:HN08	2.30	0.44
2:L:432:LEU:CD1	2:L:458:ILE:HA	2.47	0.44
2:B:117:VAL:HG11	2:B:119:PHE:CZ	2.52	0.44
1:M:8:LEU:HD22	1:M:29:ILE:HD13	1.98	0.44
2:P:546:PRO:HD2	2:P:584:THR:O	2.17	0.44
2:P:248:PHE:CD2	2:P:248:PHE:C	2.90	0.44
2:D:419:ILE:O	2:D:420:THR:C	2.56	0.44
1:K:48:THR:HG22	1:K:51:ILE:N	2.24	0.44
1:G:48:THR:HG22	1:G:51:ILE:HG12	2.00	0.44
2:D:367:GLN:HG2	2:D:391:THR:CG2	2.46	0.44
2:H:236:VAL:HG12	2:H:240:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:PHE:HB3	2:H:17:VAL:CG2	2.47	0.44
2:P:298:LEU:HB2	2:P:320:LEU:HD11	1.99	0.44
2:H:348:ARG:HA	2:H:384:ALA:O	2.17	0.44
2:J:419:ILE:O	2:J:420:THR:C	2.56	0.44
2:L:501:SER:HA	2:L:524:ARG:HB2	2.00	0.44
2:N:419:ILE:O	2:N:420:THR:C	2.55	0.44
2:L:503:ARG:HB3	2:L:503:ARG:NH1	2.32	0.44
2:D:454:GLY:O	2:D:457:TYR:HB2	2.17	0.44
2:H:443:PHE:O	2:H:471:GLY:N	2.50	0.44
2:D:422:LEU:O	2:D:423:PRO:C	2.54	0.44
2:H:366:SER:HB3	2:H:369:GLY:H	1.81	0.44
2:J:57:MET:CE	2:J:62:THR:HG22	2.48	0.44
2:B:85:ARG:NH2	4:B:1100:OGK:O07	2.39	0.44
2:P:211:ASP:HA	2:P:214:THR:HG23	2.00	0.44
2:P:284:GLU:O	2:P:287:ILE:HG23	2.16	0.44
2:N:201:MET:CE	2:N:302:TYR:CZ	3.00	0.44
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.81	0.44
2:F:501:SER:HA	2:F:524:ARG:HB2	2.00	0.44
2:H:531:ASP:O	2:H:534:GLN:HG2	2.17	0.44
2:B:361:GLU:O	2:B:361:GLU:HG3	2.18	0.44
2:F:444:TYR:HA	2:F:471:GLY:CA	2.36	0.44
1:M:48:THR:HG22	1:M:51:ILE:N	2.28	0.44
2:D:391:THR:HG23	2:D:394:SER:H	1.82	0.44
2:D:310:HIS:HE1	2:D:325:THR:OG1	2.00	0.44
2:B:121:ARG:HH22	5:B:1103:PO4:P	2.40	0.44
1:I:132:GLU:O	1:I:136:THR:HG23	2.17	0.44
1:G:26:SER:OG	1:G:108:LEU:HB3	2.18	0.44
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.99	0.44
2:L:351:ARG:HD3	2:L:413:LEU:HD11	1.98	0.44
2:H:47:ILE:O	2:H:51:THR:HG23	2.17	0.44
2:H:467:TRP:CZ3	2:H:494:GLU:OE1	2.68	0.44
2:P:310:HIS:HE1	2:P:325:THR:OG1	2.01	0.44
2:N:59:LEU:HD22	2:N:61:TYR:H	1.82	0.44
2:J:428:VAL:HG22	2:J:443:PHE:CZ	2.52	0.44
2:B:274:ARG:HG2	2:B:297:LYS:HE3	1.98	0.44
2:L:143:LEU:CD2	2:L:159:ILE:HD13	2.47	0.44
2:N:289:PHE:N	2:N:290:PRO:CD	2.81	0.44
1:C:132:GLU:O	1:C:136:THR:HG23	2.17	0.44
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.99	0.44
2:J:227:VAL:HG13	2:J:228:GLY:N	2.32	0.44
2:F:503:ARG:NH1	2:F:503:ARG:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:546:PRO:HD2	2:N:584:THR:O	2.18	0.44
2:P:383:MET:HB2	2:P:383:MET:HE2	1.82	0.44
2:L:496:ARG:HB2	2:L:521:GLN:HB3	2.00	0.44
2:B:590:GLU:O	2:B:591:PRO:C	2.55	0.44
1:G:128:LYS:HE3	1:G:136:THR:HG21	1.99	0.44
2:D:428:VAL:HG22	2:D:443:PHE:CZ	2.52	0.44
2:B:159:ILE:HG13	2:B:160:VAL:N	2.32	0.44
1:O:113:LEU:CG	1:O:113:LEU:O	2.65	0.44
1:O:30:ALA:C	1:O:32:MET:H	2.21	0.44
2:D:191:ASN:ND2	2:D:194:LEU:HB2	2.32	0.44
1:O:114:LEU:O	1:O:118:CYS:HB2	2.17	0.44
2:B:309:ASP:HA	2:B:312:THR:HG23	1.99	0.44
2:D:85:ARG:HD2	5:D:1101:PO4:O2	2.18	0.44
2:P:512:LEU:HA	2:P:513:PRO:HD2	1.83	0.44
2:N:154:ASP:OD2	2:N:179:LYS:NZ	2.46	0.44
1:C:102:ILE:HG12	1:C:117:THR:HB	1.98	0.44
2:H:194:LEU:HD12	2:H:194:LEU:HA	1.61	0.44
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.48	0.44
2:D:284:GLU:O	2:D:287:ILE:HG23	2.18	0.44
2:B:419:ILE:HD11	2:B:446:ARG:NH2	2.33	0.44
1:M:102:ILE:HD13	2:N:20:VAL:HG22	2.00	0.44
2:D:125:SER:O	2:D:129:LEU:HD22	2.18	0.44
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.33	0.44
1:K:125:ILE:HG23	1:K:133:ILE:CD1	2.38	0.44
2:P:419:ILE:CG2	2:P:422:LEU:HD13	2.48	0.44
2:F:405:LEU:HD13	2:F:408:PHE:HB2	1.99	0.44
2:D:203:GLU:HG2	2:D:203:GLU:H	1.62	0.44
2:P:201:MET:CE	2:P:302:TYR:CZ	3.00	0.44
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.48	0.44
2:F:543:GLU:OE2	2:F:578:ARG:CD	2.66	0.44
2:J:308:GLU:HG3	2:J:332:ARG:NH2	2.32	0.44
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.53	0.44
2:B:545:ILE:HG12	2:B:585:VAL:HG22	2.00	0.44
2:P:251:GLY:O	2:P:278:SER:HB2	2.18	0.44
1:K:83:LEU:HA	1:K:83:LEU:HD23	1.84	0.44
2:J:138:ASP:OD2	2:J:164:ARG:HG3	2.18	0.44
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.47	0.44
2:L:590:GLU:O	2:L:591:PRO:C	2.56	0.44
1:K:48:THR:HG22	1:K:51:ILE:HB	1.99	0.44
2:F:590:GLU:O	2:F:591:PRO:C	2.56	0.44
2:F:428:VAL:HG22	2:F:443:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:ALA:HB2	2:F:159:ILE:HG22	2.00	0.44
2:F:194:LEU:HA	2:F:194:LEU:HD12	1.84	0.44
2:H:367:GLN:N	2:H:367:GLN:CD	2.72	0.44
2:J:192:THR:HG21	2:N:113:GLN:NE2	2.33	0.44
2:J:285:MET:HB3	2:J:286:PRO:HD3	2.00	0.44
1:G:10:SER:OG	1:G:11:SER:N	2.49	0.44
2:D:227:VAL:CG1	2:D:228:GLY:N	2.80	0.44
2:J:327:ASN:HD22	2:J:328:VAL:N	2.16	0.44
2:D:512:LEU:HA	2:D:513:PRO:HD2	1.88	0.44
2:F:32:LYS:HD2	2:F:32:LYS:HA	1.85	0.44
2:B:390:ILE:HD13	2:B:424:LEU:HD11	1.99	0.43
2:J:402:LEU:HD13	2:J:405:LEU:HG	2.00	0.43
2:N:80:LEU:HD12	2:N:122:MET:HE1	2.00	0.43
2:F:159:ILE:HG13	2:F:160:VAL:N	2.32	0.43
2:H:125:SER:CB	2:H:128:ASP:H	2.31	0.43
2:H:468:MET:HE2	2:H:470:LEU:HD21	1.99	0.43
2:D:453:LEU:HD11	2:D:457:TYR:OH	2.18	0.43
2:D:503:ARG:NH1	2:D:503:ARG:HB3	2.33	0.43
2:N:272:LEU:HD23	2:N:272:LEU:HA	1.77	0.43
2:D:184:LEU:HD12	2:D:207:ILE:HB	2.00	0.43
2:H:365:VAL:CG1	2:H:387:VAL:CG2	2.96	0.43
2:D:590:GLU:O	2:D:591:PRO:C	2.56	0.43
2:P:419:ILE:O	2:P:420:THR:C	2.56	0.43
2:L:101:THR:HG21	2:P:179:LYS:NZ	2.34	0.43
2:F:422:LEU:O	2:F:424:LEU:HG	2.18	0.43
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.53	0.43
2:P:80:LEU:HD12	2:P:122:MET:HE1	1.99	0.43
2:H:170:LEU:HD23	2:H:170:LEU:C	2.38	0.43
2:N:301:LEU:HA	2:N:301:LEU:HD13	1.76	0.43
2:F:404:ASN:CA	2:F:437:LYS:HD2	2.48	0.43
2:N:210:LYS:O	2:N:214:THR:CG2	2.66	0.43
2:J:272:LEU:HD13	2:J:275:LEU:HD13	2.00	0.43
2:F:201:MET:CE	2:F:302:TYR:CZ	3.01	0.43
2:P:247:GLU:HA	2:P:274:ARG:O	2.17	0.43
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.06	0.43
1:I:44:LEU:O	1:I:44:LEU:HD12	2.19	0.43
2:H:92:ILE:HD12	2:H:92:ILE:HG23	1.65	0.43
1:I:83:LEU:HD23	1:I:83:LEU:HA	1.80	0.43
1:E:141:ASN:C	1:E:141:ASN:OD1	2.55	0.43
2:D:419:ILE:HG21	2:D:422:LEU:HD13	2.01	0.43
2:D:422:LEU:O	2:D:424:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LEU:HD12	2:B:402:LEU:O	2.19	0.43
2:P:428:VAL:HG22	2:P:443:PHE:CZ	2.53	0.43
2:F:441:PHE:O	2:F:468:MET:HA	2.18	0.43
2:L:519:TRP:HE1	4:L:1100:OGK:H01	1.82	0.43
2:N:289:PHE:HB2	2:N:290:PRO:HD3	1.99	0.43
2:D:191:ASN:ND2	2:D:194:LEU:H	2.16	0.43
2:F:245:LEU:HD12	2:F:245:LEU:HA	1.83	0.43
2:J:227:VAL:CG1	2:J:228:GLY:N	2.81	0.43
2:D:351:ARG:HD3	2:D:413:LEU:HD11	2.00	0.43
2:P:96:TRP:O	2:P:578:ARG:NH2	2.35	0.43
2:L:32:LYS:HD2	2:L:32:LYS:HA	1.85	0.43
2:L:338:ALA:O	2:L:376:GLY:HA3	2.17	0.43
2:D:240:LYS:CG	2:D:267:VAL:HG21	2.45	0.43
2:H:79:LYS:HG3	2:H:118:HIS:CD2	2.54	0.43
2:F:272:LEU:HD13	2:F:275:LEU:HD13	2.01	0.43
2:J:482:GLU:O	2:J:485:ARG:HG2	2.18	0.43
1:A:30:ALA:C	1:A:32:MET:H	2.22	0.43
2:H:298:LEU:HD22	2:H:300:LEU:HD21	2.00	0.43
2:H:404:ASN:HB2	2:H:437:LYS:NZ	2.33	0.43
2:J:419:ILE:HD11	2:J:446:ARG:NH2	2.32	0.43
2:N:389:ASP:OD2	2:N:419:ILE:HG23	2.17	0.43
2:H:77:SER:HB3	2:H:116:SER:HB3	1.99	0.43
2:F:285:MET:HB3	2:F:286:PRO:HD3	2.00	0.43
2:J:432:LEU:CD1	2:J:458:ILE:HA	2.48	0.43
2:H:57:MET:HB2	2:H:80:LEU:HD23	2.00	0.43
2:H:107:ILE:HG12	2:H:114:LEU:CD2	2.48	0.43
2:D:496:ARG:HB2	2:D:521:GLN:HB3	1.99	0.43
2:F:80:LEU:O	2:F:122:MET:HE2	2.18	0.43
2:F:468:MET:HE1	2:F:483:PHE:HE1	1.83	0.43
2:P:240:LYS:CG	2:P:267:VAL:HG21	2.44	0.43
2:F:405:LEU:HA	2:F:405:LEU:HD23	1.88	0.43
1:E:159:PHE:O	1:E:160:GLU:CB	2.66	0.43
2:D:405:LEU:HD13	2:D:408:PHE:HB2	2.01	0.43
1:G:158:ALA:CB	2:H:62:THR:HG23	2.49	0.43
2:L:482:GLU:O	2:L:485:ARG:HG2	2.18	0.43
2:J:272:LEU:HD23	2:J:272:LEU:HA	1.78	0.43
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.53	0.43
2:F:65:PRO:HA	2:F:103:TRP:CZ3	2.53	0.43
2:F:436:LYS:HB3	2:F:436:LYS:HE2	1.84	0.43
2:B:136:ARG:HH11	2:B:136:ARG:HG3	1.82	0.43
2:N:436:LYS:HB3	2:N:436:LYS:HE2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:LEU:HD12	2:F:114:LEU:HA	1.80	0.43
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.99	0.43
2:D:179:LYS:NZ	2:N:101:THR:HG21	2.34	0.43
2:B:412:LEU:HD12	2:B:412:LEU:C	2.37	0.43
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.49	0.43
2:H:274:ARG:HG3	2:H:297:LYS:HB3	2.00	0.43
2:N:468:MET:HE3	2:N:470:LEU:HD21	2.00	0.43
2:L:404:ASN:CB	2:L:437:LYS:HD2	2.49	0.43
2:D:159:ILE:HG13	2:D:160:VAL:N	2.32	0.43
2:H:136:ARG:HG3	2:H:136:ARG:NH1	2.34	0.43
2:F:54:HIS:HE1	2:F:56:THR:OG1	2.00	0.43
2:L:419:ILE:CG2	2:L:422:LEU:HD13	2.48	0.43
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.84	0.43
2:B:399:GLY:O	2:B:434:GLY:HA3	2.18	0.43
2:F:121:ARG:HH22	5:F:1103:PO4:P	2.41	0.43
2:L:227:VAL:HG13	2:L:228:GLY:N	2.33	0.43
2:L:532:LEU:HA	2:L:532:LEU:HD23	1.74	0.43
2:F:361:GLU:HG3	2:F:361:GLU:O	2.18	0.43
2:H:422:LEU:H	2:H:422:LEU:CD1	2.28	0.43
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.49	0.43
2:J:592:ILE:H	2:J:592:ILE:CD1	2.24	0.43
2:H:284:GLU:O	2:H:287:ILE:HD13	2.18	0.43
1:G:160:GLU:CG	2:H:52:ARG:HH21	2.32	0.43
2:P:332:ARG:O	2:P:336:VAL:HG23	2.18	0.43
2:L:454:GLY:O	2:L:457:TYR:HB2	2.19	0.43
1:A:135:THR:HG22	1:A:136:THR:N	2.33	0.43
2:P:538:PRO:O	2:P:539:TYR:HB2	2.18	0.43
2:P:446:ARG:HG2	2:P:447:GLN:H	1.82	0.43
2:L:114:LEU:HD12	2:L:114:LEU:HA	1.78	0.43
2:B:272:LEU:HA	2:B:272:LEU:HD23	1.72	0.43
1:K:133:ILE:HG21	2:L:40:VAL:HG11	2.00	0.43
4:N:1100:OGK:N08	4:N:1100:OGK:C18	2.80	0.43
2:H:247:GLU:HA	2:H:274:ARG:O	2.18	0.43
1:O:98:LEU:HD11	1:O:117:THR:CB	2.48	0.43
2:L:533:MET:CE	2:L:588:LEU:HD22	2.49	0.43
1:M:159:PHE:O	1:M:160:GLU:HB2	2.17	0.43
2:J:468:MET:HE1	2:J:483:PHE:HE1	1.83	0.43
2:H:298:LEU:HD22	2:H:300:LEU:CD2	2.49	0.43
2:H:233:LEU:HD11	2:H:262:LYS:HG2	2.00	0.43
2:F:446:ARG:HG2	2:F:447:GLN:N	2.34	0.43
2:B:422:LEU:O	2:B:423:PRO:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:251:GLY:O	2:L:278:SER:HB2	2.19	0.43
2:P:65:PRO:HA	2:P:103:TRP:CZ3	2.54	0.43
1:C:46:ASN:HB2	1:C:107:TYR:CZ	2.53	0.43
2:L:405:LEU:HD13	2:L:408:PHE:HB2	2.01	0.43
2:P:32:LYS:HA	2:P:32:LYS:HD2	1.86	0.43
2:F:170:LEU:C	2:F:170:LEU:HD23	2.38	0.43
2:P:436:LYS:HB3	2:P:436:LYS:HE2	1.81	0.43
2:L:57:MET:CE	2:L:62:THR:HG22	2.49	0.43
2:L:54:HIS:HD2	2:L:77:SER:OG	2.02	0.43
2:H:213:GLU:OE1	2:H:237:GLY:HA3	2.19	0.43
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.54	0.43
2:D:227:VAL:HG13	2:D:228:GLY:N	2.33	0.43
1:A:12:ASP:OD2	1:A:49:SER:HB2	2.19	0.43
2:N:176:PHE:CZ	2:N:204:PHE:CZ	3.07	0.43
2:H:327:ASN:ND2	2:H:364:LEU:CD2	2.81	0.43
2:N:402:LEU:HD12	2:N:402:LEU:O	2.19	0.43
2:B:530:GLN:HE21	2:B:592:ILE:HD11	1.83	0.43
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.41	0.43
2:P:85:ARG:HD2	5:P:1101:PO4:O2	2.19	0.43
2:F:398:ILE:CG2	2:F:402:LEU:HD11	2.44	0.43
1:A:48:THR:HG22	1:A:51:ILE:CB	2.48	0.43
2:H:519:TRP:CH2	2:H:567:HIS:CE1	3.05	0.43
2:D:211:ASP:HA	2:D:214:THR:HG23	2.01	0.43
1:I:111:LYS:HG2	1:I:115:ASP:OD2	2.19	0.43
2:H:289:PHE:HB2	2:H:290:PRO:CD	2.49	0.43
1:I:44:LEU:HA	1:I:45:PRO:HD3	1.79	0.43
2:D:117:VAL:HG11	2:D:119:PHE:CZ	2.53	0.43
1:G:8:LEU:HD22	1:G:29:ILE:HD13	2.00	0.43
2:J:83:LYS:HA	2:J:84:PRO:HD3	1.88	0.43
2:H:439:ARG:HE	2:H:466:ARG:HH11	1.66	0.43
2:P:125:SER:N	2:P:128:ASP:OD2	2.52	0.42
1:I:48:THR:HG22	1:I:51:ILE:HB	2.01	0.42
2:H:274:ARG:HG2	2:H:297:LYS:HB3	2.01	0.42
4:L:1100:OGK:C18	4:L:1100:OGK:N08	2.81	0.42
2:B:80:LEU:HD12	2:B:122:MET:HE1	2.01	0.42
2:L:159:ILE:HG13	2:L:160:VAL:N	2.32	0.42
2:P:201:MET:HE2	2:P:302:TYR:OH	2.19	0.42
2:H:367:GLN:O	2:H:371:ILE:HB	2.18	0.42
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.49	0.42
2:H:268:PHE:O	2:H:269:PRO:C	2.58	0.42
2:D:308:GLU:HG3	2:D:332:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:CG1	1:A:117:THR:HB	2.49	0.42
2:B:403:LYS:O	2:B:405:LEU:N	2.52	0.42
2:F:535:MET:O	2:F:537:ARG:HG3	2.19	0.42
2:H:362:GLU:C	2:H:364:LEU:N	2.62	0.42
2:H:89:PHE:CD2	4:H:1100:OGK:H04A	2.54	0.42
2:P:422:LEU:O	2:P:424:LEU:HG	2.18	0.42
2:H:332:ARG:NH1	2:H:332:ARG:CG	2.81	0.42
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.19	0.42
2:J:543:GLU:OE2	2:J:578:ARG:CD	2.67	0.42
2:L:201:MET:HE1	2:L:302:TYR:CZ	2.54	0.42
2:P:543:GLU:OE2	2:P:578:ARG:HD3	2.19	0.42
2:H:422:LEU:HD12	2:H:422:LEU:N	2.33	0.42
1:I:58:TYR:CE1	1:I:62:HIS:CE1	3.07	0.42
2:P:501:SER:HA	2:P:524:ARG:HB2	2.00	0.42
1:K:62:HIS:HE1	1:K:87:ASP:OD1	2.03	0.42
2:F:176:PHE:CD2	2:F:176:PHE:C	2.93	0.42
2:H:411:VAL:CG2	4:H:1100:OGK:H14	2.49	0.42
1:K:48:THR:HG22	1:K:51:ILE:CB	2.49	0.42
2:H:366:SER:OG	2:H:368:ARG:HB3	2.19	0.42
2:L:533:MET:HE1	2:L:588:LEU:HD22	2.02	0.42
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.54	0.42
2:B:136:ARG:NH1	2:B:136:ARG:HG3	2.35	0.42
1:C:46:ASN:HB2	1:C:107:TYR:CE2	2.55	0.42
2:J:251:GLY:O	2:J:278:SER:HB2	2.18	0.42
2:H:314:ILE:HG21	2:H:337:LEU:HA	2.02	0.42
2:H:360:ASP:HB2	2:H:361:GLU:H	1.43	0.42
2:H:542:ILE:CG1	2:H:588:LEU:HB2	2.48	0.42
2:H:301:LEU:CD2	2:H:324:GLU:HB3	2.47	0.42
2:J:125:SER:N	2:J:128:ASP:OD2	2.52	0.42
2:D:366:SER:HB2	2:D:367:GLN:OE1	2.20	0.42
2:B:409:ARG:CB	4:B:1100:OGK:H16B	2.47	0.42
2:L:428:VAL:HG22	2:L:443:PHE:CZ	2.54	0.42
2:D:296:ARG:HH22	1:G:35:ASP:HB2	1.83	0.42
2:H:75:LEU:HA	2:H:75:LEU:HD23	1.91	0.42
2:P:503:ARG:H	2:P:503:ARG:HH11	1.66	0.42
2:D:289:PHE:N	2:D:290:PRO:CD	2.82	0.42
2:F:432:LEU:CD1	2:F:458:ILE:HA	2.50	0.42
2:B:358:MET:O	2:B:359:GLU:HB2	2.19	0.42
1:M:6:ILE:HG22	1:M:7:VAL:N	2.34	0.42
1:G:128:LYS:HB3	1:G:132:GLU:HB2	2.01	0.42
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:ASP:HA	2:N:214:THR:HG23	2.01	0.42
2:B:191:ASN:ND2	2:B:194:LEU:HB2	2.35	0.42
2:H:227:VAL:O	2:H:250:GLY:HA3	2.20	0.42
2:L:419:ILE:HD11	2:L:446:ARG:NH2	2.34	0.42
2:D:285:MET:N	2:D:286:PRO:CD	2.82	0.42
2:F:399:GLY:O	2:F:434:GLY:HA3	2.20	0.42
2:D:217:ARG:NH1	2:H:50:GLU:OE2	2.53	0.42
2:J:503:ARG:HB3	2:J:503:ARG:NH1	2.34	0.42
2:D:471:GLY:O	2:D:496:ARG:O	2.37	0.42
2:B:412:LEU:CD1	2:B:412:LEU:C	2.88	0.42
2:F:80:LEU:HB2	2:F:122:MET:HE1	2.01	0.42
2:P:367:GLN:HG2	2:P:391:THR:CG2	2.50	0.42
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.55	0.42
1:M:154:GLU:OE2	2:N:71:ARG:HD3	2.20	0.42
2:D:32:LYS:HA	2:D:32:LYS:HD2	1.83	0.42
2:F:305:LEU:O	2:F:305:LEU:HD23	2.19	0.42
2:H:351:ARG:NH1	2:H:360:ASP:HA	2.33	0.42
2:H:533:MET:CE	2:H:588:LEU:CD1	2.86	0.42
2:N:405:LEU:HD13	2:N:408:PHE:HB2	2.02	0.42
2:N:590:GLU:O	2:N:591:PRO:C	2.58	0.42
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.82	0.42
2:N:75:LEU:HA	2:N:75:LEU:HD23	1.89	0.42
1:G:149:GLU:OE1	1:G:153:ARG:CD	2.67	0.42
2:J:289:PHE:N	2:J:290:PRO:CD	2.82	0.42
2:B:422:LEU:HD12	2:B:422:LEU:HA	1.70	0.42
2:D:289:PHE:N	2:D:290:PRO:HD2	2.34	0.42
1:I:113:LEU:HA	1:I:116:LEU:HB3	2.01	0.42
1:E:62:HIS:HE1	1:E:87:ASP:OD1	2.02	0.42
1:O:44:LEU:O	1:O:44:LEU:HD12	2.19	0.42
1:C:44:LEU:HD12	1:C:44:LEU:O	2.20	0.42
2:N:402:LEU:HD13	2:N:405:LEU:HG	2.00	0.42
2:J:402:LEU:C	2:J:403:LYS:O	2.58	0.42
1:E:158:ALA:CB	2:F:62:THR:HG23	2.50	0.42
1:G:133:ILE:HG21	2:H:44:TRP:CZ3	2.55	0.42
2:L:519:TRP:NE1	4:L:1100:OGK:H01	2.35	0.42
2:J:298:LEU:HB2	2:J:320:LEU:HD11	2.01	0.42
2:H:587:VAL:HG12	2:H:589:LYS:CD	2.49	0.42
2:L:422:LEU:O	2:L:423:PRO:C	2.58	0.42
2:B:501:SER:HA	2:B:524:ARG:HB2	2.02	0.42
2:P:351:ARG:HD3	2:P:413:LEU:HD11	2.01	0.42
2:J:361:GLU:O	2:J:361:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:125:SER:O	2:J:129:LEU:HD22	2.20	0.42
2:N:125:SER:O	2:N:129:LEU:HD22	2.18	0.42
2:F:411:VAL:CG2	4:F:1100:OGK:H14	2.50	0.42
1:I:102:ILE:HG12	1:I:117:THR:HB	2.02	0.42
1:C:13:GLY:HA2	1:K:9:LYS:HZ3	1.85	0.42
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.19	0.42
2:F:298:LEU:HB2	2:F:320:LEU:HD11	2.02	0.42
2:J:274:ARG:HG2	2:J:297:LYS:HE3	2.01	0.42
2:P:432:LEU:HB3	2:P:461:TYR:O	2.19	0.42
2:D:127:LEU:HD22	2:N:126:ASP:HB3	2.01	0.42
2:P:495:MET:O	2:P:520:VAL:HA	2.19	0.42
2:N:251:GLY:O	2:N:278:SER:HB2	2.20	0.42
2:F:469:LEU:HA	2:F:494:GLU:O	2.19	0.42
2:J:253:LEU:HD12	2:J:280:MET:HB2	2.01	0.42
2:P:52:ARG:HD3	2:P:52:ARG:HH11	1.73	0.42
2:J:164:ARG:NE	2:N:112:ARG:CG	2.83	0.42
2:F:196:VAL:HB	2:F:224:SER:HB3	2.01	0.42
1:E:51:ILE:HD12	1:E:51:ILE:HG23	1.84	0.42
2:H:567:HIS:CD2	2:H:567:HIS:N	2.88	0.42
2:J:310:HIS:HE1	2:J:325:THR:OG1	2.01	0.42
1:I:18:VAL:HG11	1:I:56:ILE:HD13	2.01	0.42
2:F:211:ASP:HA	2:F:214:THR:HG23	2.01	0.42
2:N:419:ILE:HD11	2:N:446:ARG:NH2	2.35	0.42
2:L:153:THR:HG23	2:L:178:GLU:HA	2.02	0.42
1:M:96:ALA:HB2	2:N:14:VAL:HG12	2.02	0.42
2:D:319:ASN:ND2	1:G:43:PRO:HG3	2.35	0.42
2:N:184:LEU:HD12	2:N:207:ILE:HB	2.01	0.42
2:N:305:LEU:HD23	2:N:305:LEU:O	2.20	0.42
2:J:164:ARG:CD	2:N:112:ARG:NE	2.83	0.41
2:J:422:LEU:O	2:J:424:LEU:HG	2.20	0.41
2:F:519:TRP:NE1	4:F:1100:OGK:H01	2.32	0.41
2:J:590:GLU:O	2:J:591:PRO:C	2.59	0.41
2:H:277:LEU:HD12	2:H:280:MET:HE3	2.02	0.41
2:H:274:ARG:HG2	2:H:297:LYS:HE3	2.02	0.41
2:J:211:ASP:HA	2:J:214:THR:HG23	2.02	0.41
2:J:96:TRP:HA	2:J:582:PRO:HG2	2.02	0.41
2:J:37:ALA:O	2:J:40:VAL:HG13	2.20	0.41
2:H:405:LEU:HD13	2:H:408:PHE:HB2	2.02	0.41
2:D:75:LEU:HA	2:D:75:LEU:HD23	1.82	0.41
2:P:285:MET:HB3	2:P:286:PRO:HD3	2.01	0.41
2:H:456:SER:HB2	2:H:482:GLU:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:VAL:HG11	2:F:119:PHE:CZ	2.55	0.41
2:J:532:LEU:HA	2:J:532:LEU:HD23	1.77	0.41
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.96	0.41
2:P:471:GLY:O	2:P:496:ARG:O	2.38	0.41
1:I:102:ILE:HG12	1:I:117:THR:OG1	2.20	0.41
2:H:34:ARG:HD2	2:H:34:ARG:HA	1.79	0.41
2:H:288:LEU:HD23	2:H:291:PHE:CZ	2.55	0.41
2:B:263:TYR:HB3	2:B:266:LEU:CD2	2.50	0.41
2:P:308:GLU:HG3	2:P:332:ARG:NH2	2.35	0.41
2:B:301:LEU:CD2	2:B:324:GLU:HB3	2.50	0.41
2:P:37:ALA:O	2:P:40:VAL:HG13	2.21	0.41
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.55	0.41
2:J:296:ARG:HH22	1:M:35:ASP:HB2	1.85	0.41
1:G:148:GLU:HG2	1:G:152:ARG:NH1	2.35	0.41
2:N:351:ARG:HD3	2:N:413:LEU:HD11	2.02	0.41
2:B:305:LEU:O	2:B:305:LEU:HD23	2.20	0.41
2:H:319:ASN:N	2:H:319:ASN:HD22	2.18	0.41
1:I:48:THR:HG22	1:I:51:ILE:CB	2.50	0.41
2:L:468:MET:HE1	2:L:483:PHE:CE1	2.55	0.41
2:D:398:ILE:CG2	2:D:402:LEU:HD11	2.45	0.41
2:B:366:SER:HB2	2:B:367:GLN:OE1	2.20	0.41
2:J:201:MET:CE	2:J:302:TYR:CZ	3.03	0.41
2:F:184:LEU:HD12	2:F:207:ILE:HB	2.03	0.41
1:A:141:ASN:OD1	1:A:141:ASN:C	2.58	0.41
2:N:361:GLU:O	2:N:361:GLU:HG3	2.19	0.41
2:H:314:ILE:HG22	2:H:341:CYS:SG	2.59	0.41
2:H:321:GLU:HA	2:H:344:LEU:HA	2.03	0.41
2:H:364:LEU:CD1	2:H:388:SER:HB2	2.50	0.41
2:B:444:TYR:HA	2:B:471:GLY:CA	2.33	0.41
1:E:51:ILE:HA	1:E:51:ILE:HD13	1.84	0.41
1:O:91:MET:CE	1:O:117:THR:HG22	2.50	0.41
2:N:428:VAL:HG22	2:N:443:PHE:CZ	2.55	0.41
2:N:404:ASN:HB3	2:N:437:LYS:HD2	2.03	0.41
2:D:402:LEU:HD13	2:D:405:LEU:HG	2.01	0.41
1:I:102:ILE:HD11	1:I:121:VAL:CG2	2.51	0.41
1:K:102:ILE:HG21	2:L:20:VAL:HG22	2.02	0.41
2:B:446:ARG:HG2	2:B:447:GLN:N	2.36	0.41
2:L:227:VAL:CG1	2:L:228:GLY:N	2.83	0.41
2:P:176:PHE:CD2	2:P:176:PHE:C	2.94	0.41
2:J:176:PHE:C	2:J:176:PHE:CD2	2.94	0.41
2:P:349:ILE:HG13	2:P:385:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:419:ILE:O	2:H:419:ILE:HD12	2.21	0.41
2:L:361:GLU:HG3	2:L:361:GLU:O	2.20	0.41
2:H:365:VAL:HG13	2:H:387:VAL:HG22	2.02	0.41
2:P:404:ASN:CA	2:P:437:LYS:HD2	2.49	0.41
2:F:581:CYS:HA	2:F:582:PRO:HD3	1.90	0.41
1:M:35:ASP:O	1:M:36:ASP:C	2.59	0.41
2:H:109:ASN:C	2:H:110:ASN:ND2	2.74	0.41
2:D:358:MET:O	2:D:359:GLU:HB2	2.20	0.41
1:E:57:GLU:OE1	1:E:86:TRP:HH2	2.03	0.41
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.85	0.41
2:L:248:PHE:C	2:L:248:PHE:CD2	2.94	0.41
2:L:166:ILE:HG23	2:L:166:ILE:HD13	1.85	0.41
2:L:412:LEU:HD12	2:L:412:LEU:C	2.39	0.41
2:L:125:SER:O	2:L:129:LEU:HD22	2.20	0.41
2:F:530:GLN:HE21	2:F:592:ILE:HD11	1.86	0.41
2:N:57:MET:CE	2:N:62:THR:HG22	2.51	0.41
2:P:468:MET:HE1	2:P:483:PHE:CE1	2.56	0.41
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.85	0.41
2:D:197:LEU:O	2:D:225:VAL:HA	2.20	0.41
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.36	0.41
2:L:419:ILE:HG21	2:L:422:LEU:HD13	2.01	0.41
2:B:453:LEU:HD13	2:B:457:TYR:CZ	2.56	0.41
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.55	0.41
2:H:355:GLU:HB3	2:H:356:GLN:H	1.76	0.41
2:J:351:ARG:HD3	2:J:413:LEU:HD11	2.02	0.41
1:M:52:LEU:O	1:M:56:ILE:HG13	2.21	0.41
2:D:176:PHE:CD2	2:D:176:PHE:C	2.94	0.41
2:F:348:ARG:HH22	4:F:1100:OGK:C10	2.33	0.41
2:N:422:LEU:O	2:N:424:LEU:HG	2.21	0.41
2:N:496:ARG:HB2	2:N:521:GLN:HB3	2.01	0.41
2:P:91:LEU:O	2:P:567:HIS:HE1	2.03	0.41
2:P:85:ARG:NH2	4:P:1100:OGK:O07	2.45	0.41
2:B:310:HIS:HE1	2:B:325:THR:OG1	2.04	0.41
2:L:30:ASP:OD1	2:L:31:PRO:HD2	2.21	0.41
2:N:159:ILE:HD11	2:N:169:LEU:HD13	2.03	0.41
2:J:304:LEU:HD11	3:U:216:ARG:HG3	2.02	0.41
2:H:298:LEU:CD2	2:H:300:LEU:CD2	2.99	0.41
1:G:35:ASP:O	1:G:36:ASP:C	2.59	0.41
1:M:135:THR:HG22	1:M:136:THR:N	2.35	0.41
1:C:26:SER:OG	1:C:108:LEU:HB3	2.20	0.41
2:D:503:ARG:HH11	2:D:503:ARG:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:512:LEU:HA	2:F:513:PRO:HD2	1.87	0.41
1:M:87:ASP:CG	1:M:116:LEU:HD22	2.41	0.41
2:P:358:MET:O	2:P:359:GLU:HB2	2.20	0.41
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.44	0.41
2:L:411:VAL:HG22	2:L:444:TYR:HB3	2.03	0.41
2:D:57:MET:CE	2:D:62:THR:HG22	2.51	0.41
2:N:133:ALA:HB2	2:N:159:ILE:HG22	2.02	0.41
2:P:54:HIS:HD2	2:P:77:SER:OG	2.04	0.41
1:E:35:ASP:O	1:E:36:ASP:C	2.59	0.41
2:J:197:LEU:O	2:J:225:VAL:HA	2.20	0.41
1:C:62:HIS:HE1	1:C:87:ASP:OD1	2.04	0.41
2:H:496:ARG:HG3	2:H:521:GLN:HB3	2.02	0.41
1:C:102:ILE:HD11	1:C:121:VAL:CG2	2.50	0.41
1:K:158:ALA:CB	2:L:62:THR:HG23	2.51	0.41
2:H:274:ARG:HD2	2:H:297:LYS:HE3	2.02	0.41
4:L:1100:OGK:C18	4:L:1100:OGK:HN08	2.30	0.41
2:J:366:SER:HB2	2:J:367:GLN:OE1	2.21	0.41
1:I:30:ALA:C	1:I:32:MET:H	2.22	0.41
2:N:201:MET:HE3	3:W:208:SER:O	2.21	0.41
2:J:298:LEU:HD12	2:J:298:LEU:HA	1.83	0.41
2:B:83:LYS:O	2:B:121:ARG:HD2	2.20	0.41
2:D:136:ARG:HG3	2:D:136:ARG:NH1	2.35	0.41
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.50	0.41
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.09	0.41
2:F:329:ILE:HG23	2:F:330:GLY:N	2.35	0.41
1:K:154:GLU:OE2	2:L:71:ARG:HD3	2.21	0.41
2:H:78:LEU:HD12	2:H:78:LEU:HA	1.66	0.41
2:D:335:GLU:O	2:D:338:ALA:HB3	2.20	0.41
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.43	0.41
1:G:160:GLU:HG3	2:H:52:ARG:HH21	1.86	0.41
2:P:263:TYR:HB3	2:P:266:LEU:CD2	2.51	0.41
1:I:26:SER:OG	1:I:29:ILE:HG13	2.21	0.41
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.55	0.41
2:F:289:PHE:N	2:F:290:PRO:CD	2.83	0.41
2:H:80:LEU:HA	2:H:80:LEU:HD23	1.68	0.41
2:H:114:LEU:HA	2:H:114:LEU:HD12	1.77	0.41
2:J:512:LEU:HA	2:J:513:PRO:HD2	1.92	0.41
2:F:532:LEU:HA	2:F:532:LEU:HD23	1.71	0.41
2:H:428:VAL:HG23	2:H:429:ARG:N	2.36	0.40
2:P:590:GLU:O	2:P:591:PRO:C	2.59	0.40
2:B:125:SER:O	2:B:129:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.43	0.40
2:F:422:LEU:HD12	2:F:422:LEU:HA	1.72	0.40
2:L:89:PHE:CE1	4:L:1100:OGK:H17	2.56	0.40
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.56	0.40
2:J:81:LYS:NZ	5:J:1103:PO4:O3	2.48	0.40
2:H:292:ALA:C	2:H:294:GLN:N	2.73	0.40
2:B:482:GLU:O	2:B:485:ARG:HG2	2.20	0.40
2:L:329:ILE:HG21	2:L:349:ILE:HD12	2.02	0.40
2:J:289:PHE:HB2	2:J:290:PRO:HD3	2.02	0.40
2:J:503:ARG:H	2:J:503:ARG:HH11	1.69	0.40
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.87	0.40
1:A:114:LEU:O	1:A:118:CYS:HB2	2.22	0.40
2:P:390:ILE:CD1	2:P:424:LEU:HD11	2.50	0.40
2:N:91:LEU:O	2:N:567:HIS:HE1	2.04	0.40
2:P:59:LEU:HD22	2:P:61:TYR:H	1.86	0.40
2:H:467:TRP:O	2:H:467:TRP:CD1	2.74	0.40
2:P:133:ALA:HB2	2:P:159:ILE:HG22	2.03	0.40
2:F:263:TYR:C	2:F:265:ASN:N	2.74	0.40
2:F:55:VAL:HG21	2:F:72:PHE:CD1	2.56	0.40
2:H:34:ARG:HB3	2:H:34:ARG:HH11	1.86	0.40
2:D:96:TRP:HA	2:D:582:PRO:HG2	2.02	0.40
2:J:446:ARG:HG2	2:J:447:GLN:H	1.87	0.40
2:P:176:PHE:CZ	2:P:204:PHE:CZ	3.09	0.40
2:F:335:GLU:O	2:F:338:ALA:HB3	2.21	0.40
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.21	0.40
2:D:409:ARG:HB3	2:D:442:ALA:HB3	2.02	0.40
1:G:62:HIS:HE1	1:G:87:ASP:OD1	2.04	0.40
2:H:210:LYS:HD3	2:H:210:LYS:HA	1.87	0.40
2:D:101:THR:HG23	2:N:179:LYS:HZ1	1.86	0.40
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.50	0.40
2:D:530:GLN:HE21	2:D:592:ILE:HD11	1.86	0.40
2:H:274:ARG:HG2	2:H:297:LYS:CE	2.51	0.40
2:B:267:VAL:O	2:B:267:VAL:CG2	2.70	0.40
2:F:201:MET:CE	3:S:208:SER:HB2	2.51	0.40
2:B:298:LEU:HB2	2:B:320:LEU:HD11	2.03	0.40
2:H:159:ILE:HD13	2:H:166:ILE:HD11	2.03	0.40
2:B:308:GLU:HG3	2:B:332:ARG:NH2	2.36	0.40
2:H:354:ASP:OD2	2:H:355:GLU:N	2.54	0.40
2:F:496:ARG:HB2	2:F:521:GLN:HB3	2.02	0.40
2:H:277:LEU:O	2:H:278:SER:C	2.60	0.40
2:N:301:LEU:HD23	2:N:324:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:578:ARG:H	2:D:578:ARG:HG3	1.78	0.40
2:H:349:ILE:HG21	2:H:349:ILE:HD13	1.86	0.40
2:H:383:MET:O	2:H:408:PHE:HA	2.21	0.40
2:H:136:ARG:NE	2:H:136:ARG:HA	2.37	0.40
1:M:130:PRO:O	1:M:134:ARG:HG2	2.22	0.40
2:N:503:ARG:HH11	2:N:503:ARG:H	1.70	0.40
2:H:22:GLU:HG2	2:H:47:ILE:HD11	2.03	0.40
1:K:137:PHE:CD1	2:L:17:VAL:HG21	2.56	0.40
2:F:349:ILE:HG13	2:F:385:VAL:HG22	2.03	0.40
2:H:282:PRO:HB3	2:H:309:ASP:OD2	2.22	0.40
2:J:32:LYS:HD2	2:J:32:LYS:HA	1.82	0.40
2:L:512:LEU:HA	2:L:513:PRO:HD2	1.93	0.40
2:H:508:ALA:O	2:H:509:VAL:C	2.60	0.40
2:L:80:LEU:CD1	2:L:122:MET:HE1	2.51	0.40
2:N:240:LYS:CG	2:N:267:VAL:HG21	2.45	0.40
2:F:57:MET:CE	2:F:62:THR:HG22	2.52	0.40
2:F:402:LEU:HD13	2:F:405:LEU:HG	2.03	0.40
2:H:440:ARG:CB	2:H:467:TRP:CD1	3.02	0.40
2:F:112:ARG:HD3	2:F:112:ARG:HH11	1.76	0.40
2:N:581:CYS:HA	2:N:582:PRO:HD3	1.94	0.40
2:B:301:LEU:HD13	2:B:301:LEU:HA	1.83	0.40
2:B:468:MET:CE	2:B:470:LEU:HD21	2.49	0.40
2:D:468:MET:HE3	2:D:470:LEU:HD21	2.02	0.40
1:A:137:PHE:CD1	2:B:17:VAL:HG21	2.57	0.40
1:O:137:PHE:CD1	2:P:17:VAL:CG2	3.04	0.40
2:J:285:MET:N	2:J:286:PRO:CD	2.85	0.40
2:P:446:ARG:HG2	2:P:447:GLN:N	2.37	0.40
2:L:399:GLY:O	2:L:434:GLY:HA3	2.21	0.40
2:L:545:ILE:HG12	2:L:585:VAL:HG22	2.04	0.40
2:N:344:LEU:HD12	2:N:344:LEU:HA	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:ARG:NH2	1:I:61:ARG:NH1[2_555]	2.03	0.17
2:D:429:ARG:NH1	1:I:86:TRP:CE3[2_555]	2.06	0.14

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	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	4	15
1	C	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	4	15
1	E	141/160 (88%)	117 (83%)	21 (15%)	3 (2%)	9	29
1	G	141/160 (88%)	119 (84%)	18 (13%)	4 (3%)	6	21
1	I	141/160 (88%)	116 (82%)	21 (15%)	4 (3%)	6	21
1	K	141/160 (88%)	118 (84%)	19 (14%)	4 (3%)	6	21
1	M	141/160 (88%)	114 (81%)	22 (16%)	5 (4%)	4	15
1	O	141/160 (88%)	114 (81%)	23 (16%)	4 (3%)	6	21
2	B	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	12	38
2	D	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	11	34
2	F	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	12	38
2	H	558/592 (94%)	475 (85%)	63 (11%)	20 (4%)	4	14
2	J	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	11	34
2	L	562/592 (95%)	508 (90%)	46 (8%)	8 (1%)	14	42
2	N	562/592 (95%)	505 (90%)	49 (9%)	8 (1%)	14	42
2	P	562/592 (95%)	503 (90%)	49 (9%)	10 (2%)	11	34
3	Q	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	R	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	S	11/22 (50%)	9 (82%)	2 (18%)	0	100	100
3	U	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	V	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	W	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	X	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
All	All	5697/6170 (92%)	5022 (88%)	557 (10%)	118 (2%)	9	29

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	LYS
2	B	404	ASN
2	B	420	THR
2	D	271	LYS
2	D	420	THR
2	D	591	PRO
2	F	271	LYS
2	F	420	THR
2	F	591	PRO
2	H	254	ASN
2	H	278	SER
2	H	287	ILE
2	H	365	VAL
2	J	271	LYS
2	J	404	ASN
2	J	420	THR
2	L	271	LYS
2	L	420	THR
2	L	591	PRO
2	N	271	LYS
2	N	420	THR
2	P	271	LYS
2	P	420	THR
2	P	591	PRO
1	A	36	ASP
2	B	357	GLY
2	B	358	MET
2	B	591	PRO
1	C	36	ASP
2	D	357	GLY
2	D	358	MET
2	D	404	ASN
1	E	36	ASP
1	E	108	LEU
2	F	264	MET
2	F	357	GLY
2	F	404	ASN
1	G	36	ASP
1	G	108	LEU
2	H	201	MET
2	H	295	ILE
2	H	367	GLN

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Mol	Chain	Res	Type
2	H	528	THR
1	I	36	ASP
2	J	264	MET
2	J	403	LYS
2	J	591	PRO
1	K	36	ASP
1	K	108	LEU
2	L	357	GLY
2	L	358	MET
2	L	404	ASN
1	M	36	ASP
1	M	108	LEU
2	N	357	GLY
2	N	358	MET
2	N	404	ASN
2	N	591	PRO
1	O	36	ASP
1	O	108	LEU
2	P	357	GLY
2	P	358	MET
2	P	404	ASN
1	A	108	LEU
1	A	141	ASN
2	B	264	MET
2	B	403	LYS
1	C	92	LYS
1	C	108	LEU
2	D	264	MET
2	D	403	LYS
2	F	358	MET
2	H	206	LYS
2	H	260	PRO
2	H	270	ARG
2	H	328	VAL
2	H	525	ALA
1	I	108	LEU
2	J	357	GLY
2	J	358	MET
2	L	264	MET
2	L	403	LYS
1	M	141	ASN
2	N	264	MET

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Mol	Chain	Res	Type
2	N	403	LYS
2	P	264	MET
2	D	524	ARG
2	H	327	ASN
2	H	403	LYS
2	H	471	GLY
1	I	20	GLU
2	P	403	LYS
2	F	403	LYS
2	F	500	PHE
1	G	20	GLU
1	K	20	GLU
1	M	113	LEU
1	O	113	LEU
2	P	524	ARG
1	A	20	GLU
2	B	526	SER
1	C	141	ASN
2	D	526	SER
2	H	14	VAL
1	K	92	LYS
2	P	526	SER
1	E	13	GLY
1	G	13	GLY
2	H	538	PRO
1	I	13	GLY
1	M	13	GLY
2	J	20	VAL
1	A	13	GLY
1	C	13	GLY
2	H	513	PRO
1	O	13	GLY
2	H	97	GLY
2	J	422	LEU

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	128/137 (93%)	121 (94%)	7 (6%)	27 59
1	C	128/137 (93%)	119 (93%)	9 (7%)	19 47
1	E	128/137 (93%)	119 (93%)	9 (7%)	19 47
1	G	128/137 (93%)	118 (92%)	10 (8%)	16 41
1	I	128/137 (93%)	120 (94%)	8 (6%)	22 53
1	K	128/137 (93%)	118 (92%)	10 (8%)	16 41
1	M	128/137 (93%)	121 (94%)	7 (6%)	27 59
1	O	128/137 (93%)	120 (94%)	8 (6%)	22 53
2	B	498/523 (95%)	424 (85%)	74 (15%)	4 11
2	D	498/523 (95%)	428 (86%)	70 (14%)	4 12
2	F	498/523 (95%)	427 (86%)	71 (14%)	4 12
2	H	494/523 (94%)	402 (81%)	92 (19%)	2 6
2	J	498/523 (95%)	426 (86%)	72 (14%)	4 11
2	L	498/523 (95%)	428 (86%)	70 (14%)	4 12
2	N	498/523 (95%)	432 (87%)	66 (13%)	5 14
2	P	498/523 (95%)	433 (87%)	65 (13%)	5 15
3	Q	12/20 (60%)	12 (100%)	0	100 100
3	R	12/20 (60%)	12 (100%)	0	100 100
3	S	12/20 (60%)	12 (100%)	0	100 100
3	U	12/20 (60%)	12 (100%)	0	100 100
3	V	12/20 (60%)	12 (100%)	0	100 100
3	W	12/20 (60%)	12 (100%)	0	100 100
3	X	12/20 (60%)	12 (100%)	0	100 100
All	All	5088/5420 (94%)	4440 (87%)	648 (13%)	5 16

All (648) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	44	LEU
1	A	47	VAL
1	A	48	THR
1	A	61	ARG
1	A	112	ASN
1	A	135	THR

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Mol	Chain	Res	Type
2	B	16	THR
2	B	17	VAL
2	B	20	VAL
2	B	32	LYS
2	B	35	ASP
2	B	40	VAL
2	B	43	ARG
2	B	46	LYS
2	B	48	ASP
2	B	52	ARG
2	B	59	LEU
2	B	62	THR
2	B	100	VAL
2	B	101	THR
2	B	104	VAL
2	B	105	THR
2	B	113	GLN
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	152	THR
2	B	161	THR
2	B	166	ILE
2	B	168	THR
2	B	182	LYS
2	B	184	LEU
2	B	192	THR
2	B	196	VAL
2	B	203	GLU
2	B	214	THR
2	B	220	ARG
2	B	227	VAL
2	B	232	ILE
2	B	270	ARG
2	B	272	LEU
2	B	284	GLU
2	B	287	ILE
2	B	301	LEU
2	B	304	LEU
2	B	305	LEU
2	B	312	THR

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Mol	Chain	Res	Type
2	B	313	LEU
2	B	327	ASN
2	B	351	ARG
2	B	354	ASP
2	B	390	ILE
2	B	400	THR
2	B	402	LEU
2	B	405	LEU
2	B	410	LEU
2	B	412	LEU
2	B	413	LEU
2	B	421	ASP
2	B	422	LEU
2	B	430	SER
2	B	431	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	456	SER
2	B	466	ARG
2	B	490	LEU
2	B	496	ARG
2	B	499	CYS
2	B	503	ARG
2	B	516	ARG
2	B	519	TRP
2	B	537	ARG
2	B	542	ILE
2	B	578	ARG
2	B	579	THR
2	B	584	THR
2	B	588	LEU
1	C	10	SER
1	C	35	ASP
1	C	44	LEU
1	C	47	VAL
1	C	48	THR
1	C	61	ARG
1	C	112	ASN
1	C	135	THR
1	C	160	GLU
2	D	16	THR

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Mol	Chain	Res	Type
2	D	17	VAL
2	D	20	VAL
2	D	35	ASP
2	D	40	VAL
2	D	43	ARG
2	D	46	LYS
2	D	48	ASP
2	D	52	ARG
2	D	59	LEU
2	D	62	THR
2	D	100	VAL
2	D	101	THR
2	D	105	THR
2	D	113	GLN
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	161	THR
2	D	166	ILE
2	D	168	THR
2	D	182	LYS
2	D	184	LEU
2	D	192	THR
2	D	196	VAL
2	D	203	GLU
2	D	214	THR
2	D	220	ARG
2	D	227	VAL
2	D	232	ILE
2	D	270	ARG
2	D	272	LEU
2	D	284	GLU
2	D	287	ILE
2	D	301	LEU
2	D	304	LEU
2	D	305	LEU
2	D	312	THR
2	D	313	LEU
2	D	327	ASN
2	D	351	ARG
2	D	354	ASP

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Mol	Chain	Res	Type
2	D	390	ILE
2	D	400	THR
2	D	402	LEU
2	D	405	LEU
2	D	410	LEU
2	D	412	LEU
2	D	413	LEU
2	D	421	ASP
2	D	422	LEU
2	D	429	ARG
2	D	431	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	456	SER
2	D	466	ARG
2	D	490	LEU
2	D	496	ARG
2	D	499	CYS
2	D	503	ARG
2	D	516	ARG
2	D	519	TRP
2	D	537	ARG
2	D	542	ILE
2	D	579	THR
2	D	584	THR
2	D	588	LEU
1	E	10	SER
1	E	35	ASP
1	E	44	LEU
1	E	47	VAL
1	E	48	THR
1	E	61	ARG
1	E	112	ASN
1	E	135	THR
1	E	160	GLU
2	F	16	THR
2	F	17	VAL
2	F	20	VAL
2	F	32	LYS
2	F	35	ASP
2	F	40	VAL

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Mol	Chain	Res	Type
2	F	43	ARG
2	F	48	ASP
2	F	59	LEU
2	F	62	THR
2	F	100	VAL
2	F	101	THR
2	F	104	VAL
2	F	105	THR
2	F	113	GLN
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	161	THR
2	F	166	ILE
2	F	168	THR
2	F	182	LYS
2	F	184	LEU
2	F	192	THR
2	F	196	VAL
2	F	214	THR
2	F	220	ARG
2	F	227	VAL
2	F	232	ILE
2	F	270	ARG
2	F	272	LEU
2	F	275	LEU
2	F	284	GLU
2	F	287	ILE
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR
2	F	313	LEU
2	F	327	ASN
2	F	351	ARG
2	F	354	ASP
2	F	365	VAL
2	F	390	ILE
2	F	400	THR
2	F	402	LEU
2	F	405	LEU

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Mol	Chain	Res	Type
2	F	412	LEU
2	F	413	LEU
2	F	421	ASP
2	F	422	LEU
2	F	430	SER
2	F	431	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	456	SER
2	F	466	ARG
2	F	490	LEU
2	F	496	ARG
2	F	499	CYS
2	F	503	ARG
2	F	516	ARG
2	F	519	TRP
2	F	528	THR
2	F	537	ARG
2	F	542	ILE
2	F	578	ARG
2	F	579	THR
2	F	588	LEU
1	G	10	SER
1	G	35	ASP
1	G	44	LEU
1	G	47	VAL
1	G	48	THR
1	G	61	ARG
1	G	112	ASN
1	G	128	LYS
1	G	149	GLU
1	G	153	ARG
2	H	17	VAL
2	H	20	VAL
2	H	32	LYS
2	H	34	ARG
2	H	43	ARG
2	H	46	LYS
2	H	48	ASP
2	H	52	ARG
2	H	59	LEU

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Mol	Chain	Res	Type
2	H	62	THR
2	H	76	ARG
2	H	77	SER
2	H	90	ASN
2	H	95	ASN
2	H	100	VAL
2	H	104	VAL
2	H	105	THR
2	H	118	HIS
2	H	120	ARG
2	H	129	LEU
2	H	132	LEU
2	H	136	ARG
2	H	142	THR
2	H	159	ILE
2	H	166	ILE
2	H	168	THR
2	H	179	LYS
2	H	184	LEU
2	H	191	ASN
2	H	192	THR
2	H	193	SER
2	H	194	LEU
2	H	196	VAL
2	H	214	THR
2	H	220	ARG
2	H	225	VAL
2	H	227	VAL
2	H	231	GLU
2	H	257	ILE
2	H	263	TYR
2	H	265	ASN
2	H	266	LEU
2	H	271	LYS
2	H	272	LEU
2	H	274	ARG
2	H	285	MET
2	H	287	ILE
2	H	296	ARG
2	H	298	LEU
2	H	301	LEU
2	H	305	LEU

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Mol	Chain	Res	Type
2	H	307	THR
2	H	312	THR
2	H	313	LEU
2	H	325	THR
2	H	327	ASN
2	H	332	ARG
2	H	343	GLN
2	H	345	LYS
2	H	358	MET
2	H	359	GLU
2	H	360	ASP
2	H	365	VAL
2	H	368	ARG
2	H	373	LEU
2	H	385	VAL
2	H	388	SER
2	H	389	ASP
2	H	390	ILE
2	H	395	LEU
2	H	400	THR
2	H	402	LEU
2	H	403	LYS
2	H	417	GLU
2	H	422	LEU
2	H	428	VAL
2	H	453	LEU
2	H	455	LEU
2	H	466	ARG
2	H	467	TRP
2	H	490	LEU
2	H	491	GLN
2	H	492	LYS
2	H	503	ARG
2	H	511	LYS
2	H	516	ARG
2	H	519	TRP
2	H	542	ILE
2	H	548	ARG
2	H	577	GLN
2	H	579	THR
2	H	589	LYS
1	I	10	SER

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Mol	Chain	Res	Type
1	I	35	ASP
1	I	44	LEU
1	I	47	VAL
1	I	48	THR
1	I	61	ARG
1	I	112	ASN
1	I	135	THR
2	J	16	THR
2	J	17	VAL
2	J	20	VAL
2	J	35	ASP
2	J	40	VAL
2	J	43	ARG
2	J	46	LYS
2	J	52	ARG
2	J	59	LEU
2	J	62	THR
2	J	100	VAL
2	J	101	THR
2	J	104	VAL
2	J	105	THR
2	J	108	SER
2	J	113	GLN
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG
2	J	142	THR
2	J	166	ILE
2	J	168	THR
2	J	182	LYS
2	J	184	LEU
2	J	192	THR
2	J	196	VAL
2	J	203	GLU
2	J	214	THR
2	J	220	ARG
2	J	227	VAL
2	J	232	ILE
2	J	270	ARG
2	J	272	LEU
2	J	284	GLU
2	J	287	ILE

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Mol	Chain	Res	Type
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	313	LEU
2	J	327	ASN
2	J	351	ARG
2	J	354	ASP
2	J	365	VAL
2	J	390	ILE
2	J	397	SER
2	J	400	THR
2	J	402	LEU
2	J	405	LEU
2	J	410	LEU
2	J	412	LEU
2	J	413	LEU
2	J	421	ASP
2	J	422	LEU
2	J	430	SER
2	J	431	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	456	SER
2	J	466	ARG
2	J	490	LEU
2	J	496	ARG
2	J	499	CYS
2	J	503	ARG
2	J	516	ARG
2	J	519	TRP
2	J	537	ARG
2	J	542	ILE
2	J	578	ARG
2	J	579	THR
2	J	588	LEU
1	K	10	SER
1	K	35	ASP
1	K	44	LEU
1	K	47	VAL
1	K	48	THR

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Mol	Chain	Res	Type
1	K	61	ARG
1	K	112	ASN
1	K	125	ILE
1	K	135	THR
1	K	160	GLU
2	L	16	THR
2	L	17	VAL
2	L	20	VAL
2	L	35	ASP
2	L	40	VAL
2	L	46	LYS
2	L	48	ASP
2	L	52	ARG
2	L	59	LEU
2	L	62	THR
2	L	100	VAL
2	L	101	THR
2	L	104	VAL
2	L	105	THR
2	L	113	GLN
2	L	129	LEU
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	161	THR
2	L	166	ILE
2	L	168	THR
2	L	182	LYS
2	L	184	LEU
2	L	192	THR
2	L	196	VAL
2	L	203	GLU
2	L	214	THR
2	L	220	ARG
2	L	227	VAL
2	L	232	ILE
2	L	270	ARG
2	L	272	LEU
2	L	284	GLU
2	L	287	ILE
2	L	301	LEU
2	L	304	LEU

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Mol	Chain	Res	Type
2	L	305	LEU
2	L	312	THR
2	L	313	LEU
2	L	327	ASN
2	L	351	ARG
2	L	354	ASP
2	L	365	VAL
2	L	390	ILE
2	L	400	THR
2	L	402	LEU
2	L	405	LEU
2	L	412	LEU
2	L	413	LEU
2	L	421	ASP
2	L	429	ARG
2	L	430	SER
2	L	431	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	456	SER
2	L	466	ARG
2	L	490	LEU
2	L	496	ARG
2	L	499	CYS
2	L	503	ARG
2	L	516	ARG
2	L	519	TRP
2	L	537	ARG
2	L	542	ILE
2	L	578	ARG
2	L	579	THR
2	L	588	LEU
1	M	35	ASP
1	M	44	LEU
1	M	47	VAL
1	M	48	THR
1	M	61	ARG
1	M	112	ASN
1	M	135	THR
2	N	16	THR
2	N	17	VAL

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Mol	Chain	Res	Type
2	N	20	VAL
2	N	35	ASP
2	N	40	VAL
2	N	43	ARG
2	N	46	LYS
2	N	48	ASP
2	N	52	ARG
2	N	59	LEU
2	N	62	THR
2	N	100	VAL
2	N	101	THR
2	N	104	VAL
2	N	105	THR
2	N	113	GLN
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG
2	N	142	THR
2	N	168	THR
2	N	182	LYS
2	N	184	LEU
2	N	192	THR
2	N	196	VAL
2	N	203	GLU
2	N	214	THR
2	N	220	ARG
2	N	227	VAL
2	N	232	ILE
2	N	270	ARG
2	N	272	LEU
2	N	284	GLU
2	N	287	ILE
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	313	LEU
2	N	327	ASN
2	N	351	ARG
2	N	354	ASP
2	N	365	VAL
2	N	390	ILE

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Mol	Chain	Res	Type
2	N	400	THR
2	N	402	LEU
2	N	405	LEU
2	N	412	LEU
2	N	422	LEU
2	N	429	ARG
2	N	431	LEU
2	N	447	GLN
2	N	453	LEU
2	N	455	LEU
2	N	456	SER
2	N	466	ARG
2	N	490	LEU
2	N	496	ARG
2	N	499	CYS
2	N	503	ARG
2	N	516	ARG
2	N	519	TRP
2	N	537	ARG
2	N	542	ILE
2	N	579	THR
2	N	588	LEU
1	O	10	SER
1	O	35	ASP
1	O	44	LEU
1	O	47	VAL
1	O	48	THR
1	O	61	ARG
1	O	112	ASN
1	O	135	THR
2	P	16	THR
2	P	20	VAL
2	P	35	ASP
2	P	40	VAL
2	P	48	ASP
2	P	52	ARG
2	P	59	LEU
2	P	62	THR
2	P	100	VAL
2	P	101	THR
2	P	104	VAL
2	P	105	THR

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Mol	Chain	Res	Type
2	P	113	GLN
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	161	THR
2	P	166	ILE
2	P	168	THR
2	P	182	LYS
2	P	184	LEU
2	P	192	THR
2	P	196	VAL
2	P	203	GLU
2	P	214	THR
2	P	220	ARG
2	P	227	VAL
2	P	232	ILE
2	P	270	ARG
2	P	272	LEU
2	P	284	GLU
2	P	287	ILE
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	313	LEU
2	P	327	ASN
2	P	351	ARG
2	P	354	ASP
2	P	365	VAL
2	P	390	ILE
2	P	400	THR
2	P	402	LEU
2	P	405	LEU
2	P	412	LEU
2	P	422	LEU
2	P	430	SER
2	P	431	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	456	SER

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Mol	Chain	Res	Type
2	P	466	ARG
2	P	490	LEU
2	P	496	ARG
2	P	499	CYS
2	P	503	ARG
2	P	516	ARG
2	P	519	TRP
2	P	537	ARG
2	P	542	ILE
2	P	579	THR
2	P	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	62	HIS
2	B	54	HIS
2	B	191	ASN
2	B	294	GLN
2	B	310	HIS
2	B	327	ASN
2	B	343	GLN
2	B	460	GLN
2	B	489	ASN
2	B	530	GLN
1	C	31	HIS
1	C	62	HIS
2	D	54	HIS
2	D	109	ASN
2	D	190	HIS
2	D	191	ASN
2	D	254	ASN
2	D	294	GLN
2	D	310	HIS
2	D	319	ASN
2	D	327	ASN
2	D	343	GLN
2	D	489	ASN
2	D	530	GLN
1	E	31	HIS
1	E	62	HIS

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Mol	Chain	Res	Type
2	F	54	HIS
2	F	109	ASN
2	F	113	GLN
2	F	191	ASN
2	F	310	HIS
2	F	327	ASN
2	F	343	GLN
2	F	460	GLN
2	F	489	ASN
2	F	530	GLN
1	G	31	HIS
1	G	62	HIS
2	H	23	GLN
2	H	54	HIS
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	118	HIS
2	H	191	ASN
2	H	315	GLN
2	H	319	ASN
2	H	343	GLN
2	H	375	GLN
2	H	447	GLN
2	H	577	GLN
1	I	31	HIS
1	I	62	HIS
2	J	54	HIS
2	J	109	ASN
2	J	191	ASN
2	J	254	ASN
2	J	294	GLN
2	J	310	HIS
2	J	327	ASN
2	J	343	GLN
2	J	460	GLN
2	J	489	ASN
2	J	530	GLN
1	K	31	HIS
1	K	62	HIS
2	L	54	HIS
2	L	74	ASN

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Mol	Chain	Res	Type
2	L	109	ASN
2	L	191	ASN
2	L	254	ASN
2	L	294	GLN
2	L	310	HIS
2	L	319	ASN
2	L	327	ASN
2	L	343	GLN
2	L	489	ASN
2	L	530	GLN
1	M	31	HIS
1	M	62	HIS
2	N	54	HIS
2	N	109	ASN
2	N	113	GLN
2	N	191	ASN
2	N	254	ASN
2	N	310	HIS
2	N	327	ASN
2	N	343	GLN
2	N	404	ASN
2	N	460	GLN
2	N	489	ASN
2	N	530	GLN
1	O	31	HIS
1	O	62	HIS
2	P	54	HIS
2	P	109	ASN
2	P	191	ASN
2	P	310	HIS
2	P	327	ASN
2	P	343	GLN
2	P	460	GLN
2	P	489	ASN
2	P	530	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

40 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	$\#\|Z\| > 2$
4	OGK	B	1100	-	22,25,25	6.37	9 (40%)	25,38,38	2.72	10 (40%)
5	PO4	B	1101	-	4,4,4	2.95	3 (75%)	6,6,6	0.30	0
5	PO4	B	1102	-	4,4,4	3.05	4 (100%)	6,6,6	0.26	0
5	PO4	B	1103	-	4,4,4	2.74	3 (75%)	6,6,6	0.32	0
5	PO4	B	1104	-	4,4,4	2.87	3 (75%)	6,6,6	0.32	0
4	OGK	D	1100	-	22,25,25	6.33	8 (36%)	25,38,38	3.06	12 (48%)
5	PO4	D	1101	-	4,4,4	3.00	3 (75%)	6,6,6	0.33	0
5	PO4	D	1102	-	4,4,4	3.12	3 (75%)	6,6,6	0.28	0
5	PO4	D	1103	-	4,4,4	2.62	3 (75%)	6,6,6	0.30	0
5	PO4	D	1104	-	4,4,4	2.93	3 (75%)	6,6,6	0.33	0
4	OGK	F	1100	-	22,25,25	6.41	8 (36%)	25,38,38	2.58	13 (52%)
5	PO4	F	1101	-	4,4,4	3.04	4 (100%)	6,6,6	0.35	0
5	PO4	F	1102	-	4,4,4	3.11	3 (75%)	6,6,6	0.27	0
5	PO4	F	1103	-	4,4,4	2.74	3 (75%)	6,6,6	0.28	0
5	PO4	F	1104	-	4,4,4	3.07	3 (75%)	6,6,6	0.31	0
4	OGK	H	1100	-	22,25,25	6.28	8 (36%)	25,38,38	2.69	13 (52%)
5	PO4	H	1101	-	4,4,4	3.10	4 (100%)	6,6,6	0.32	0
5	PO4	H	1102	-	4,4,4	3.25	3 (75%)	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	H	1103	-	4,4,4	3.01	4 (100%)	6,6,6	0.27	0
5	PO4	H	1104	-	4,4,4	2.96	3 (75%)	6,6,6	0.39	0
4	OGK	J	1100	-	22,25,25	6.17	8 (36%)	25,38,38	2.64	12 (48%)
5	PO4	J	1101	-	4,4,4	3.09	3 (75%)	6,6,6	0.29	0
5	PO4	J	1102	-	4,4,4	3.12	3 (75%)	6,6,6	0.28	0
5	PO4	J	1103	-	4,4,4	2.75	3 (75%)	6,6,6	0.29	0
5	PO4	J	1104	-	4,4,4	2.82	3 (75%)	6,6,6	0.27	0
4	OGK	L	1100	-	22,25,25	6.40	9 (40%)	25,38,38	3.23	15 (60%)
5	PO4	L	1101	-	4,4,4	2.89	3 (75%)	6,6,6	0.34	0
5	PO4	L	1102	-	4,4,4	3.02	3 (75%)	6,6,6	0.27	0
5	PO4	L	1103	-	4,4,4	2.99	3 (75%)	6,6,6	0.27	0
5	PO4	L	1104	-	4,4,4	2.89	3 (75%)	6,6,6	0.27	0
4	OGK	N	1100	-	22,25,25	6.34	8 (36%)	25,38,38	2.51	7 (28%)
5	PO4	N	1101	-	4,4,4	3.06	3 (75%)	6,6,6	0.32	0
5	PO4	N	1102	-	4,4,4	2.98	3 (75%)	6,6,6	0.27	0
5	PO4	N	1103	-	4,4,4	2.89	3 (75%)	6,6,6	0.30	0
5	PO4	N	1104	-	4,4,4	3.05	3 (75%)	6,6,6	0.29	0
4	OGK	P	1100	-	22,25,25	6.52	9 (40%)	25,38,38	3.09	11 (44%)
5	PO4	P	1101	-	4,4,4	2.97	3 (75%)	6,6,6	0.30	0
5	PO4	P	1102	-	4,4,4	3.09	3 (75%)	6,6,6	0.28	0
5	PO4	P	1103	-	4,4,4	2.93	3 (75%)	6,6,6	0.29	0
5	PO4	P	1104	-	4,4,4	3.09	3 (75%)	6,6,6	0.30	0

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
4	OGK	B	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
5	PO4	B	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	D	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
5	PO4	D	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1102	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	D	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	F	1100	-	-	0/13/52/52	0/2/3/3
5	PO4	F	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	H	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
5	PO4	H	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	J	1100	-	-	0/13/52/52	0/2/3/3
5	PO4	J	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	L	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
5	PO4	L	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	N	1100	-	-	0/13/52/52	0/2/3/3
5	PO4	N	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	P	1100	-	-	0/13/52/52	0/2/3/3
5	PO4	P	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1104	-	-	0/0/0/0	0/0/0/0

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1100	OGK	C13-C09	-22.54	1.27	1.51
4	P	1100	OGK	C13-C09	-22.22	1.27	1.51
4	L	1100	OGK	C13-C09	-21.98	1.28	1.51
4	F	1100	OGK	C13-C09	-21.73	1.28	1.51
4	H	1100	OGK	C13-C09	-21.66	1.28	1.51
4	B	1100	OGK	C13-C09	-21.56	1.28	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1100	OGK	C13-C09	-21.35	1.28	1.51
4	N	1100	OGK	C13-C09	-21.32	1.28	1.51
4	P	1100	OGK	C09-C14	-17.40	1.34	1.52
4	B	1100	OGK	C09-C14	-17.40	1.34	1.52
4	F	1100	OGK	C09-C14	-17.31	1.34	1.52
4	N	1100	OGK	C09-C14	-17.13	1.34	1.52
4	L	1100	OGK	C09-C14	-16.50	1.35	1.52
4	H	1100	OGK	C09-C14	-16.44	1.35	1.52
4	J	1100	OGK	C09-C14	-16.17	1.35	1.52
4	D	1100	OGK	C09-C14	-16.11	1.35	1.52
4	F	1100	OGK	C13-C14	-6.90	1.32	1.50
4	B	1100	OGK	C13-C14	-6.82	1.32	1.50
4	L	1100	OGK	C13-C14	-6.71	1.32	1.50
4	J	1100	OGK	C13-C14	-6.64	1.32	1.50
4	D	1100	OGK	C13-C14	-6.61	1.32	1.50
4	H	1100	OGK	C13-C14	-6.59	1.32	1.50
4	P	1100	OGK	C13-C14	-6.56	1.33	1.50
4	N	1100	OGK	C13-C14	-6.49	1.33	1.50
4	F	1100	OGK	C18-C17	-3.78	1.43	1.54
4	P	1100	OGK	C18-C17	-3.36	1.44	1.54
4	J	1100	OGK	C18-C17	-3.24	1.44	1.54
4	D	1100	OGK	O07-C06	-3.11	1.17	1.23
4	N	1100	OGK	C18-C17	-3.09	1.45	1.54
4	B	1100	OGK	C18-C17	-3.07	1.45	1.54
4	D	1100	OGK	C18-C17	-3.01	1.45	1.54
4	H	1100	OGK	O07-C06	-3.00	1.17	1.23
4	P	1100	OGK	O07-C06	-2.92	1.17	1.23
4	L	1100	OGK	C18-C17	-2.91	1.45	1.54
4	H	1100	OGK	C18-C17	-2.86	1.46	1.54
4	B	1100	OGK	O07-C06	-2.42	1.18	1.23
4	F	1100	OGK	O07-C06	-2.38	1.18	1.23
4	L	1100	OGK	O07-C06	-2.33	1.18	1.23
4	B	1100	OGK	C04-C05	-2.27	1.50	1.53
4	F	1100	OGK	C04-C05	-2.18	1.50	1.53
5	F	1101	PO4	P-O2	-2.18	1.45	1.53
4	N	1100	OGK	C04-C05	-2.16	1.50	1.53
5	H	1103	PO4	P-O2	-2.10	1.45	1.53
5	B	1102	PO4	P-O2	-2.03	1.46	1.53
4	B	1100	OGK	C22-C17	-2.02	1.49	1.54
5	H	1101	PO4	P-O2	-2.01	1.46	1.53
4	N	1100	OGK	C05-C06	2.13	1.55	1.52
4	P	1100	OGK	C05-C06	2.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1100	OGK	C09-N08	2.24	1.49	1.45
4	J	1100	OGK	C23-C22	2.40	1.57	1.53
4	P	1100	OGK	C09-N08	2.42	1.50	1.45
4	D	1100	OGK	C23-C22	2.43	1.57	1.53
4	F	1100	OGK	C09-N08	2.54	1.50	1.45
5	F	1103	PO4	P-O3	2.58	1.62	1.53
4	D	1100	OGK	C05-C06	2.58	1.56	1.52
5	B	1103	PO4	P-O4	2.68	1.63	1.53
4	H	1100	OGK	C09-N08	2.73	1.50	1.45
5	D	1103	PO4	P-O3	2.77	1.63	1.53
5	D	1101	PO4	P-O1	2.78	1.64	1.52
5	H	1101	PO4	P-O1	2.79	1.64	1.52
5	J	1103	PO4	P-O4	2.79	1.63	1.53
4	B	1100	OGK	C23-C22	2.79	1.58	1.53
5	N	1101	PO4	P-O1	2.79	1.64	1.52
5	B	1104	PO4	P-O1	2.80	1.64	1.52
5	F	1101	PO4	P-O1	2.81	1.64	1.52
5	P	1101	PO4	P-O1	2.82	1.64	1.52
5	D	1103	PO4	P-O4	2.83	1.63	1.53
5	B	1101	PO4	P-O4	2.85	1.63	1.53
5	B	1101	PO4	P-O1	2.90	1.65	1.52
5	D	1104	PO4	P-O1	2.90	1.65	1.52
5	L	1101	PO4	P-O1	2.90	1.65	1.52
5	L	1101	PO4	P-O4	2.94	1.64	1.53
5	F	1104	PO4	P-O4	2.98	1.64	1.53
5	J	1103	PO4	P-O1	3.02	1.65	1.52
5	H	1103	PO4	P-O4	3.03	1.64	1.53
5	L	1103	PO4	P-O4	3.04	1.64	1.53
4	L	1100	OGK	C09-N08	3.04	1.51	1.45
5	D	1103	PO4	P-O1	3.05	1.65	1.52
5	J	1101	PO4	P-O1	3.05	1.65	1.52
5	D	1102	PO4	P-O1	3.06	1.65	1.52
5	J	1104	PO4	P-O4	3.06	1.64	1.53
5	P	1102	PO4	P-O1	3.07	1.65	1.52
5	N	1103	PO4	P-O1	3.07	1.65	1.52
5	F	1101	PO4	P-O4	3.09	1.64	1.53
5	N	1103	PO4	P-O4	3.10	1.64	1.53
5	N	1102	PO4	P-O1	3.10	1.66	1.52
5	L	1102	PO4	P-O1	3.10	1.66	1.52
5	H	1104	PO4	P-O1	3.11	1.66	1.52
5	J	1104	PO4	P-O1	3.12	1.66	1.52
5	B	1102	PO4	P-O1	3.13	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1102	PO4	P-O1	3.15	1.66	1.52
5	N	1104	PO4	P-O1	3.15	1.66	1.52
4	L	1100	OGK	C05-C06	3.16	1.57	1.52
5	J	1102	PO4	P-O1	3.16	1.66	1.52
5	P	1104	PO4	P-O3	3.17	1.64	1.53
5	H	1103	PO4	P-O1	3.17	1.66	1.52
5	L	1104	PO4	P-O3	3.19	1.64	1.53
5	P	1103	PO4	P-O1	3.19	1.66	1.52
5	F	1103	PO4	P-O4	3.20	1.64	1.53
5	J	1104	PO4	P-O3	3.20	1.64	1.53
5	J	1103	PO4	P-O3	3.21	1.64	1.53
5	B	1103	PO4	P-O1	3.22	1.66	1.52
5	P	1101	PO4	P-O3	3.23	1.65	1.53
5	L	1103	PO4	P-O1	3.26	1.66	1.52
5	L	1104	PO4	P-O1	3.26	1.66	1.52
4	J	1100	OGK	C05-C06	3.27	1.57	1.52
5	L	1104	PO4	P-O4	3.27	1.65	1.53
5	H	1102	PO4	P-O1	3.27	1.66	1.52
5	P	1104	PO4	P-O4	3.28	1.65	1.53
5	D	1104	PO4	P-O3	3.29	1.65	1.53
5	F	1104	PO4	P-O1	3.30	1.66	1.52
5	N	1104	PO4	P-O3	3.30	1.65	1.53
5	B	1104	PO4	P-O4	3.31	1.65	1.53
5	B	1102	PO4	P-O4	3.33	1.65	1.53
5	N	1102	PO4	P-O3	3.34	1.65	1.53
5	F	1103	PO4	P-O1	3.34	1.67	1.52
5	P	1103	PO4	P-O3	3.35	1.65	1.53
5	P	1103	PO4	P-O4	3.35	1.65	1.53
5	J	1101	PO4	P-O4	3.36	1.65	1.53
5	L	1102	PO4	P-O4	3.37	1.65	1.53
5	B	1103	PO4	P-O3	3.37	1.65	1.53
5	J	1102	PO4	P-O4	3.40	1.65	1.53
5	D	1101	PO4	P-O4	3.45	1.65	1.53
5	N	1102	PO4	P-O4	3.46	1.65	1.53
5	N	1103	PO4	P-O3	3.46	1.65	1.53
5	H	1101	PO4	P-O4	3.47	1.65	1.53
5	H	1104	PO4	P-O3	3.48	1.65	1.53
5	P	1102	PO4	P-O4	3.49	1.65	1.53
5	D	1102	PO4	P-O4	3.49	1.65	1.53
5	F	1102	PO4	P-O4	3.50	1.66	1.53
5	B	1102	PO4	P-O3	3.50	1.66	1.53
5	B	1104	PO4	P-O3	3.50	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1103	PO4	P-O3	3.55	1.66	1.53
5	L	1103	PO4	P-O3	3.56	1.66	1.53
5	L	1101	PO4	P-O3	3.56	1.66	1.53
5	L	1102	PO4	P-O3	3.59	1.66	1.53
5	H	1104	PO4	P-O4	3.59	1.66	1.53
5	N	1101	PO4	P-O4	3.61	1.66	1.53
5	D	1104	PO4	P-O4	3.64	1.66	1.53
5	F	1102	PO4	P-O3	3.68	1.66	1.53
5	P	1102	PO4	P-O3	3.69	1.66	1.53
5	N	1101	PO4	P-O3	3.72	1.66	1.53
4	N	1100	OGK	C23-C22	3.73	1.59	1.53
5	P	1101	PO4	P-O4	3.75	1.66	1.53
5	H	1102	PO4	P-O4	3.75	1.66	1.53
5	N	1104	PO4	P-O4	3.76	1.66	1.53
5	J	1101	PO4	P-O3	3.80	1.67	1.53
5	J	1102	PO4	P-O3	3.81	1.67	1.53
5	D	1101	PO4	P-O3	3.81	1.67	1.53
5	D	1102	PO4	P-O3	3.81	1.67	1.53
4	P	1100	OGK	C23-C22	3.81	1.59	1.53
5	H	1101	PO4	P-O3	3.83	1.67	1.53
5	F	1101	PO4	P-O3	3.84	1.67	1.53
5	F	1104	PO4	P-O3	3.85	1.67	1.53
5	B	1101	PO4	P-O3	3.87	1.67	1.53
5	H	1102	PO4	P-O3	3.95	1.67	1.53
5	P	1104	PO4	P-O1	3.97	1.69	1.52
4	H	1100	OGK	C23-C22	4.02	1.60	1.53
4	L	1100	OGK	C23-C22	4.02	1.60	1.53
4	D	1100	OGK	C06-N08	5.40	1.45	1.34
4	H	1100	OGK	C06-N08	5.51	1.46	1.34
4	J	1100	OGK	C06-N08	5.79	1.46	1.34
4	B	1100	OGK	C06-N08	6.22	1.47	1.34
4	F	1100	OGK	C06-N08	6.56	1.48	1.34
4	L	1100	OGK	C06-N08	6.59	1.48	1.34
4	P	1100	OGK	C06-N08	6.62	1.48	1.34
4	N	1100	OGK	C06-N08	6.83	1.49	1.34

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1100	OGK	C13-C14-C09	-7.72	56.76	60.38
4	L	1100	OGK	C13-C14-C09	-6.77	57.21	60.38
4	P	1100	OGK	C13-C14-C09	-6.74	57.22	60.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1100	OGK	C13-C14-C09	-6.61	57.28	60.38
4	P	1100	OGK	C13-C09-N08	-6.49	108.01	117.71
4	J	1100	OGK	C13-C14-C09	-6.35	57.41	60.38
4	N	1100	OGK	C13-C14-C09	-6.00	57.57	60.38
4	F	1100	OGK	C13-C14-C09	-5.80	57.66	60.38
4	L	1100	OGK	C18-C17-C05	-5.71	98.30	116.96
4	B	1100	OGK	C13-C14-C09	-5.68	57.72	60.38
4	P	1100	OGK	C18-C17-C05	-5.51	98.93	116.96
4	F	1100	OGK	C18-C17-C05	-5.24	99.83	116.96
4	P	1100	OGK	C04-C03-C02	-4.93	104.11	112.80
4	P	1100	OGK	O07-C06-C05	-4.93	115.90	121.56
4	B	1100	OGK	C04-C03-C02	-4.86	104.24	112.80
4	D	1100	OGK	C04-C03-C02	-4.32	105.18	112.80
4	L	1100	OGK	C04-C03-C02	-4.21	105.37	112.80
4	N	1100	OGK	C04-C03-C02	-3.99	105.76	112.80
4	B	1100	OGK	C18-C17-C05	-3.89	104.25	116.96
4	L	1100	OGK	C13-C09-N08	-3.80	112.03	117.71
4	D	1100	OGK	C18-C17-C05	-3.76	104.68	116.96
4	J	1100	OGK	C18-C17-C05	-3.75	104.70	116.96
4	J	1100	OGK	C04-C03-C02	-3.52	106.59	112.80
4	N	1100	OGK	C18-C17-C05	-3.50	105.50	116.96
4	H	1100	OGK	C18-C17-C05	-3.47	105.61	116.96
4	B	1100	OGK	O07-C06-C05	-3.33	117.74	121.56
4	D	1100	OGK	C13-C09-N08	-3.29	112.80	117.71
4	F	1100	OGK	C04-C03-C02	-3.15	107.24	112.80
4	H	1100	OGK	O07-C06-N08	-3.12	115.80	123.04
4	L	1100	OGK	O07-C06-N08	-3.12	115.81	123.04
4	F	1100	OGK	C18-C19-C20	-2.94	102.44	105.45
4	H	1100	OGK	O07-C06-C05	-2.70	118.46	121.56
4	F	1100	OGK	O07-C06-C05	-2.58	118.60	121.56
4	B	1100	OGK	C17-C22-C20	-2.58	100.07	104.07
4	D	1100	OGK	O07-C06-N08	-2.56	117.09	123.04
4	P	1100	OGK	O07-C06-N08	-2.53	117.17	123.04
4	B	1100	OGK	C13-C09-N08	-2.51	113.96	117.71
4	B	1100	OGK	C18-C19-C20	-2.41	102.98	105.45
4	J	1100	OGK	O07-C06-N08	-2.37	117.54	123.04
4	F	1100	OGK	C13-C09-N08	-2.34	114.21	117.71
4	J	1100	OGK	C13-C09-N08	-2.26	114.33	117.71
4	D	1100	OGK	C23-C03-C02	-2.24	108.85	112.80
4	L	1100	OGK	C19-C18-C17	2.09	107.78	104.92
4	J	1100	OGK	O07-C06-C05	2.13	124.01	121.56
4	F	1100	OGK	C04-C03-C23	2.14	113.48	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1100	OGK	C04-C03-C23	2.21	113.60	109.70
4	P	1100	OGK	C18-C17-C22	2.21	106.42	103.87
4	F	1100	OGK	C09-C13-C14	2.27	61.98	60.89
4	H	1100	OGK	C23-C03-C02	2.41	117.04	112.80
4	J	1100	OGK	C13-C09-C14	2.44	60.29	59.04
4	P	1100	OGK	C04-C05-C17	2.52	115.28	110.04
4	F	1100	OGK	C13-C09-C14	2.58	60.36	59.04
4	H	1100	OGK	C04-C05-C17	2.59	115.41	110.04
4	D	1100	OGK	O07-C06-C05	2.62	124.57	121.56
4	H	1100	OGK	C05-C06-N08	2.62	119.77	116.30
4	F	1100	OGK	C04-C05-C06	2.66	117.37	111.16
4	F	1100	OGK	C22-C23-C03	2.71	115.61	109.91
4	N	1100	OGK	C05-C04-C03	2.75	115.70	109.91
4	H	1100	OGK	C09-C13-C14	2.75	62.21	60.89
4	L	1100	OGK	C13-C09-C14	2.76	60.45	59.04
4	B	1100	OGK	C13-C09-C14	2.77	60.46	59.04
4	L	1100	OGK	C22-C23-C03	2.80	115.81	109.91
4	H	1100	OGK	C13-C09-C14	2.88	60.51	59.04
4	J	1100	OGK	C09-C13-C14	2.96	62.31	60.89
4	L	1100	OGK	C09-C13-C14	3.03	62.34	60.89
4	D	1100	OGK	C13-C09-C14	3.05	60.60	59.04
4	H	1100	OGK	C22-C23-C03	3.05	116.34	109.91
4	P	1100	OGK	C04-C05-C06	3.11	118.40	111.16
4	N	1100	OGK	C22-C23-C03	3.13	116.51	109.91
4	J	1100	OGK	C04-C05-C06	3.14	118.48	111.16
4	L	1100	OGK	C05-C06-N08	3.31	120.67	116.30
4	N	1100	OGK	C13-C09-C14	3.38	60.77	59.04
4	H	1100	OGK	C05-C04-C03	3.39	117.06	109.91
4	J	1100	OGK	C18-C17-C22	3.43	107.83	103.87
4	L	1100	OGK	C18-C17-C22	3.49	107.89	103.87
4	D	1100	OGK	C09-C13-C14	3.64	62.64	60.89
4	F	1100	OGK	C04-C05-C17	3.77	117.86	110.04
4	P	1100	OGK	C13-C09-C14	3.78	60.97	59.04
4	L	1100	OGK	C04-C05-C06	3.81	120.04	111.16
4	H	1100	OGK	C04-C05-C06	3.86	120.16	111.16
4	P	1100	OGK	C05-C04-C03	3.91	118.14	109.91
4	B	1100	OGK	C05-C04-C03	3.93	118.19	109.91
4	F	1100	OGK	C05-C04-C03	4.22	118.80	109.91
4	J	1100	OGK	C04-C05-C17	4.24	118.83	110.04
4	L	1100	OGK	C04-C05-C17	4.46	119.29	110.04
4	D	1100	OGK	C05-C04-C03	4.54	119.47	109.91
4	D	1100	OGK	C04-C05-C06	4.69	122.09	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1100	OGK	C18-C17-C22	4.73	109.33	103.87
4	J	1100	OGK	C05-C04-C03	4.77	119.96	109.91
4	D	1100	OGK	C04-C05-C17	5.12	120.67	110.04
4	N	1100	OGK	C18-C17-C22	6.12	110.93	103.87
4	L	1100	OGK	C05-C04-C03	6.23	123.03	109.91
4	B	1100	OGK	C04-C05-C17	6.72	123.99	110.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1100	OGK	C05
4	L	1100	OGK	C05
4	D	1100	OGK	C05
4	H	1100	OGK	C03

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1100	OGK	6	0
5	B	1101	PO4	1	0
5	B	1103	PO4	2	0
4	D	1100	OGK	2	0
5	D	1101	PO4	1	0
5	D	1103	PO4	2	0
4	F	1100	OGK	8	0
5	F	1101	PO4	1	0
5	F	1103	PO4	1	0
4	H	1100	OGK	8	0
5	H	1101	PO4	2	0
5	H	1103	PO4	4	0
5	H	1104	PO4	1	0
4	J	1100	OGK	7	0
5	J	1103	PO4	2	0
4	L	1100	OGK	11	0
5	L	1103	PO4	1	0
4	N	1100	OGK	7	0
5	N	1101	PO4	1	0
5	N	1103	PO4	2	0
4	P	1100	OGK	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1101	PO4	1	0
5	P	1103	PO4	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	145/160 (90%)	0.51	9 (6%) 24 15	27, 72, 133, 163	0
1	C	145/160 (90%)	0.93	28 (19%) 2 1	26, 75, 134, 163	0
1	E	145/160 (90%)	0.28	5 (3%) 49 36	28, 70, 133, 161	0
1	G	145/160 (90%)	0.09	7 (4%) 34 23	27, 66, 134, 161	0
1	I	145/160 (90%)	0.57	19 (13%) 5 2	29, 73, 134, 163	0
1	K	145/160 (90%)	0.65	20 (13%) 4 2	28, 75, 134, 165	0
1	M	145/160 (90%)	0.87	23 (15%) 3 1	32, 75, 133, 162	0
1	O	145/160 (90%)	1.28	44 (30%) 1 0	32, 76, 134, 164	0
2	B	566/592 (95%)	-0.08	11 (1%) 70 59	21, 45, 107, 175	0
2	D	566/592 (95%)	-0.07	16 (2%) 56 44	21, 46, 110, 176	0
2	F	566/592 (95%)	-0.15	23 (4%) 41 29	20, 49, 111, 177	0
2	H	562/592 (94%)	-0.54	5 (0%) 85 79	19, 38, 91, 171	0
2	J	566/592 (95%)	-0.23	17 (3%) 54 41	22, 49, 110, 177	0
2	L	566/592 (95%)	-0.26	20 (3%) 48 35	21, 50, 111, 176	0
2	N	566/592 (95%)	0.26	43 (7%) 17 9	24, 53, 112, 178	0
2	P	566/592 (95%)	0.09	37 (6%) 22 13	23, 54, 114, 176	0
3	Q	13/22 (59%)	0.71	0 100 100	79, 102, 125, 126	0
3	R	13/22 (59%)	2.22	7 (53%) 0 0	86, 109, 128, 129	0
3	S	13/22 (59%)	1.29	3 (23%) 1 1	89, 108, 129, 131	0
3	U	13/22 (59%)	1.19	2 (15%) 3 1	87, 111, 128, 130	0
3	V	13/22 (59%)	1.45	5 (38%) 0 0	88, 111, 128, 128	0
3	W	13/22 (59%)	1.47	5 (38%) 0 0	88, 111, 128, 129	0
3	X	13/22 (59%)	1.42	4 (30%) 1 0	89, 110, 128, 129	0
All	All	5775/6170 (93%)	0.06	353 (6%) 25 15	19, 53, 119, 178	0

All (353) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	592	ILE	17.2
2	F	592	ILE	13.3
2	D	12	SER	13.1
2	N	591	PRO	11.1
2	P	12	SER	10.4
1	A	68	SER	9.4
2	N	12	SER	9.3
2	N	361	GLU	8.6
2	N	358	MET	8.1
1	O	80	ASP	8.0
2	P	592	ILE	7.6
2	J	548	ARG	7.6
1	M	68	SER	7.4
2	F	591	PRO	7.3
2	L	592	ILE	7.3
1	K	68	SER	7.0
2	J	592	ILE	7.0
2	J	361	GLU	6.9
2	D	548	ARG	6.9
2	F	12	SER	6.6
2	P	362	GLU	6.5
2	F	356	GLN	6.4
2	P	548	ARG	6.3
2	L	360	ASP	6.2
1	M	37	CYS	6.2
2	L	361	GLU	6.1
2	N	360	ASP	6.1
2	D	361	GLU	5.9
2	N	590	GLU	5.7
1	O	68	SER	5.6
2	N	355	GLU	5.6
1	M	116	LEU	5.5
2	L	356	GLN	5.4
2	D	592	ILE	5.3
2	B	592	ILE	5.3
1	M	80	ASP	5.2
2	F	590	GLU	5.2
2	P	361	GLU	5.2
2	N	359	GLU	5.1
2	N	354	ASP	5.0
2	J	360	ASP	4.9
2	J	591	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	354	ASP	4.8
2	D	360	ASP	4.8
1	E	68	SER	4.7
2	L	359	GLU	4.7
2	L	548	ARG	4.6
1	M	35	ASP	4.5
2	F	355	GLU	4.5
2	N	362	GLU	4.5
1	A	41	GLY	4.5
1	K	13	GLY	4.4
2	N	356	GLN	4.4
2	J	12	SER	4.4
2	B	527	MET	4.3
2	N	527	MET	4.3
2	F	548	ARG	4.3
1	M	115	ASP	4.3
2	J	358	MET	4.3
2	P	527	MET	4.3
1	I	38	VAL	4.2
1	C	20	GLU	4.2
2	P	360	ASP	4.2
1	O	93	ILE	4.1
2	F	359	GLU	4.1
2	P	257	ILE	4.1
2	P	564	HIS	4.1
1	C	118	CYS	4.0
3	V	205	ARG	4.0
2	P	591	PRO	4.0
1	M	18	VAL	4.0
2	P	393	GLU	4.0
2	J	527	MET	4.0
2	L	12	SER	4.0
1	O	63	VAL	4.0
2	P	337	LEU	4.0
2	L	527	MET	4.0
2	P	418	ARG	3.9
1	C	13	GLY	3.9
2	P	340	TYR	3.9
3	R	210	HIS	3.9
1	A	43	PRO	3.9
1	O	53	ALA	3.8
1	O	83	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	37	CYS	3.8
1	C	115	ASP	3.8
1	O	89	ASP	3.8
2	N	373	LEU	3.8
1	G	68	SER	3.8
1	I	37	CYS	3.8
2	P	356	GLN	3.7
2	J	362	GLU	3.7
2	H	527	MET	3.7
1	K	38	VAL	3.7
2	F	527	MET	3.7
2	F	361	GLU	3.7
2	N	13	CYS	3.7
2	N	313	LEU	3.7
1	O	84	LYS	3.7
1	M	67	ALA	3.7
2	H	358	MET	3.6
1	I	29	ILE	3.6
2	H	362	GLU	3.6
3	W	217	LYS	3.6
2	N	266	LEU	3.6
2	P	589	LYS	3.6
3	S	210	HIS	3.5
1	O	31	HIS	3.5
2	B	356	GLN	3.5
1	K	67	ALA	3.5
2	F	358	MET	3.5
1	C	122	ALA	3.5
2	P	401	TYR	3.5
2	N	363	GLY	3.5
1	C	114	LEU	3.4
2	B	548	ARG	3.4
1	I	43	PRO	3.4
1	G	80	ASP	3.4
1	M	84	LYS	3.4
1	M	38	VAL	3.4
3	R	205	ARG	3.4
1	K	43	PRO	3.4
2	N	428	VAL	3.3
3	W	211	ARG	3.3
1	G	35	ASP	3.3
1	I	39	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	547	SER	3.3
1	O	117	THR	3.3
2	L	354	ASP	3.3
2	J	590	GLU	3.3
2	F	363	GLY	3.3
2	N	357	GLY	3.3
3	R	213	LEU	3.2
2	D	356	GLN	3.2
1	E	38	VAL	3.1
1	K	88	ALA	3.1
1	O	114	LEU	3.1
1	O	90	PHE	3.1
1	C	67	ALA	3.1
2	L	591	PRO	3.1
3	R	214	GLU	3.1
2	D	530	GLN	3.1
1	A	107	TYR	3.1
1	O	67	ALA	3.1
1	O	52	LEU	3.1
1	I	36	ASP	3.1
2	J	359	GLU	3.1
2	J	363	GLY	3.1
1	O	116	LEU	3.0
1	E	37	CYS	3.0
1	O	91	MET	3.0
2	D	362	GLU	3.0
2	H	528	THR	3.0
1	O	58	TYR	3.0
3	W	216	ARG	3.0
2	D	358	MET	3.0
1	I	24	LEU	3.0
1	G	81	ASP	3.0
2	J	356	GLN	3.0
2	P	258	GLY	3.0
2	F	362	GLU	3.0
1	O	5	LYS	2.9
1	I	20	GLU	2.9
1	O	65	ALA	2.9
1	C	119	GLN	2.9
2	F	258	GLY	2.9
3	W	205	ARG	2.9
2	P	354	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	17	GLU	2.9
1	O	60	LYS	2.9
1	G	37	CYS	2.9
1	O	21	ALA	2.9
1	M	81	ASP	2.8
2	D	418	ARG	2.8
2	L	418	ARG	2.8
1	I	27	GLN	2.8
1	I	47	VAL	2.8
2	P	375	GLN	2.8
1	O	18	VAL	2.8
1	K	115	ASP	2.8
2	P	461	TYR	2.8
1	O	119	GLN	2.8
1	I	84	LYS	2.8
2	N	401	TYR	2.8
1	C	7	VAL	2.8
2	N	267	VAL	2.8
2	L	258	GLY	2.8
2	P	266	LEU	2.8
2	P	370	LEU	2.8
2	D	527	MET	2.8
3	R	209	LEU	2.7
2	N	536	ALA	2.7
1	C	17	GLU	2.7
2	N	588	LEU	2.7
1	M	27	GLN	2.7
1	O	27	GLN	2.7
2	D	528	THR	2.7
2	N	418	ARG	2.7
1	I	6	ILE	2.7
2	P	267	VAL	2.7
2	N	258	GLY	2.7
1	C	63	VAL	2.7
2	N	548	ARG	2.7
1	C	66	ALA	2.6
1	C	82	ASP	2.6
2	L	524	ARG	2.6
1	O	86	TRP	2.6
1	I	125	ILE	2.6
1	O	92	LYS	2.6
1	O	17	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	55	VAL	2.6
1	A	21	ALA	2.6
1	O	19	GLU	2.6
3	X	210	HIS	2.6
1	C	5	LYS	2.6
1	O	81	ASP	2.6
2	B	528	THR	2.6
1	O	138	ASN	2.6
2	L	362	GLU	2.6
2	D	564	HIS	2.6
1	C	68	SER	2.6
1	K	24	LEU	2.6
1	K	81	ASP	2.6
1	A	59	CYS	2.6
2	N	420	THR	2.6
3	V	211	ARG	2.6
1	M	83	LEU	2.5
2	N	370	LEU	2.5
1	C	40	ASN	2.5
2	P	255	GLU	2.5
3	V	210	HIS	2.5
1	M	6	ILE	2.5
1	M	23	ALA	2.5
1	O	54	LYS	2.5
2	J	422	LEU	2.5
1	C	24	LEU	2.5
1	M	82	ASP	2.5
1	G	38	VAL	2.5
1	O	113	LEU	2.5
2	N	270	ARG	2.5
1	I	22	VAL	2.5
1	O	62	HIS	2.4
2	D	429	ARG	2.4
2	H	12	SER	2.4
1	A	46	ASN	2.4
1	I	80	ASP	2.4
2	L	590	GLU	2.4
1	K	6	ILE	2.4
1	K	80	ASP	2.4
1	M	17	GLU	2.4
1	O	112	ASN	2.4
2	F	360	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	23	GLN	2.4
2	N	257	ILE	2.4
3	X	205	ARG	2.4
2	B	355	GLU	2.4
1	K	114	LEU	2.4
1	C	90	PHE	2.4
1	C	80	ASP	2.4
2	N	259	MET	2.3
3	S	205	ARG	2.3
1	E	39	ASP	2.3
2	P	355	GLU	2.3
2	N	287	ILE	2.3
2	N	416	GLU	2.3
2	B	358	MET	2.3
2	N	371	ILE	2.3
2	D	417	GLU	2.3
2	P	283	ASN	2.3
1	O	56	ILE	2.3
2	P	371	ILE	2.3
2	J	13	CYS	2.3
2	B	14	VAL	2.3
2	F	526	SER	2.3
2	P	27	TYR	2.3
3	R	208	SER	2.3
1	O	20	GLU	2.3
1	I	31	HIS	2.3
1	C	86	TRP	2.3
3	W	214	GLU	2.3
2	J	354	ASP	2.3
1	K	59	CYS	2.3
3	X	208	SER	2.3
2	P	433	ILE	2.3
2	P	420	THR	2.3
1	K	61	ARG	2.3
1	O	59	CYS	2.3
1	C	38	VAL	2.3
2	L	355	GLU	2.2
2	J	364	LEU	2.2
1	O	88	ALA	2.2
2	D	422	LEU	2.2
1	O	51	ILE	2.2
2	P	363	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	565	PRO	2.2
2	F	13	CYS	2.2
1	M	8	LEU	2.2
1	O	57	GLU	2.2
1	E	82	ASP	2.2
1	I	23	ALA	2.2
2	L	357	GLY	2.2
2	N	340	TYR	2.2
1	M	63	VAL	2.2
2	P	25	MET	2.2
1	K	18	VAL	2.2
1	C	23	ALA	2.2
1	O	115	ASP	2.2
3	U	217	LYS	2.2
1	K	20	GLU	2.1
2	N	339	GLN	2.1
3	U	210	HIS	2.1
1	I	40	ASN	2.1
3	X	207	ALA	2.1
1	M	123	ASP	2.1
2	P	359	GLU	2.1
2	N	314	ILE	2.1
2	N	15	ALA	2.1
1	C	37	CYS	2.1
1	A	25	GLU	2.1
1	M	20	GLU	2.1
2	L	475	GLU	2.1
1	K	84	LYS	2.1
2	B	589	LYS	2.1
2	F	564	HIS	2.1
2	B	547	SER	2.1
3	S	214	GLU	2.1
1	C	81	ASP	2.1
1	I	13	GLY	2.1
1	G	60	LYS	2.1
1	K	60	LYS	2.1
2	B	361	GLU	2.1
1	C	83	LEU	2.1
2	P	373	LEU	2.1
1	O	37	CYS	2.1
1	O	64	GLU	2.1
2	N	589	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	15	SER	2.1
2	N	14	VAL	2.1
3	V	208	SER	2.1
2	N	402	LEU	2.1
1	M	92	LYS	2.0
2	P	335	GLU	2.0
1	M	119	GLN	2.0
2	F	422	LEU	2.0
1	C	8	LEU	2.0
3	R	217	LYS	2.0
3	V	207	ALA	2.0
2	F	357	GLY	2.0
1	C	107	TYR	2.0
2	N	334	LEU	2.0
1	C	21	ALA	2.0
2	L	260	PRO	2.0
2	F	418	ARG	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
5	PO4	P	1104	5/5	0.83	0.22	6.12	30,51,77,101	0
5	PO4	N	1104	5/5	0.94	0.24	5.39	32,59,102,105	0
5	PO4	H	1102	5/5	0.79	0.24	4.40	58,70,91,138	0
5	PO4	H	1104	5/5	0.92	0.19	2.60	23,27,62,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PO4	J	1103	5/5	0.99	0.18	2.42	34,39,48,64	0
5	PO4	N	1103	5/5	0.97	0.22	1.96	40,60,78,102	0
5	PO4	L	1104	5/5	0.96	0.17	1.68	54,54,85,104	0
5	PO4	N	1102	5/5	0.91	0.23	1.26	78,89,102,114	0
5	PO4	L	1103	5/5	0.97	0.21	1.15	31,41,62,72	0
5	PO4	N	1101	5/5	0.95	0.20	0.83	47,54,57,87	0
4	OGK	H	1100	23/23	0.97	0.17	0.81	23,41,56,62	0
5	PO4	L	1101	5/5	0.97	0.18	0.30	34,39,58,68	0
5	PO4	P	1102	5/5	0.93	0.19	0.08	70,91,121,132	0
4	OGK	J	1100	23/23	0.96	0.18	0.02	24,36,51,65	0
5	PO4	P	1101	5/5	0.98	0.18	-0.10	47,50,65,73	0
5	PO4	D	1103	5/5	0.98	0.19	-0.17	28,30,38,79	0
4	OGK	L	1100	23/23	0.97	0.17	-0.21	31,43,62,67	0
4	OGK	P	1100	23/23	0.97	0.16	-0.22	40,52,64,68	0
4	OGK	F	1100	23/23	0.96	0.18	-0.24	23,41,50,70	0
5	PO4	F	1103	5/5	0.97	0.18	-0.26	32,36,48,80	0
4	OGK	N	1100	23/23	0.93	0.17	-0.36	33,54,73,77	0
5	PO4	D	1102	5/5	0.94	0.15	-0.70	48,60,103,128	0
5	PO4	F	1101	5/5	0.98	0.15	-0.77	25,37,47,70	0
5	PO4	B	1103	5/5	0.98	0.16	-0.79	23,25,30,45	0
5	PO4	J	1101	5/5	0.98	0.14	-0.81	42,53,62,65	0
5	PO4	D	1101	5/5	0.98	0.16	-0.90	29,32,43,57	0
4	OGK	D	1100	23/23	0.97	0.14	-0.91	24,32,41,45	0
5	PO4	F	1104	5/5	0.95	0.16	-1.05	28,33,60,69	0
5	PO4	P	1103	5/5	0.96	0.15	-1.06	55,56,64,76	0
5	PO4	J	1102	5/5	0.96	0.12	-1.30	54,71,85,106	0
5	PO4	B	1101	5/5	0.98	0.13	-1.84	31,37,44,44	0
4	OGK	B	1100	23/23	0.98	0.14	-1.88	14,26,38,48	0
5	PO4	D	1104	5/5	0.93	0.15	-	32,38,82,83	0
5	PO4	J	1104	5/5	0.97	0.14	-	44,46,72,76	0
5	PO4	H	1101	5/5	0.94	0.15	-	65,65,83,99	0
5	PO4	H	1103	5/5	0.95	0.19	-	45,60,71,83	0
5	PO4	B	1102	5/5	0.98	0.14	-	51,71,81,85	0
5	PO4	B	1104	5/5	0.96	0.13	-	23,44,66,67	0
5	PO4	L	1102	5/5	0.93	0.18	-	56,67,112,139	0
5	PO4	F	1102	5/5	0.83	0.24	-	67,80,101,127	0

6.5 Other polymers

There are no such residues in this entry.