Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1KP8
Title	:	Structural Basis for GroEL-assisted Protein Folding from the Crystal Structure of (GroEL-KMgATP)14 at 2.0 A Resolution
Authors	:	Wang, J.
Deposited on	:	2001-12-30
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

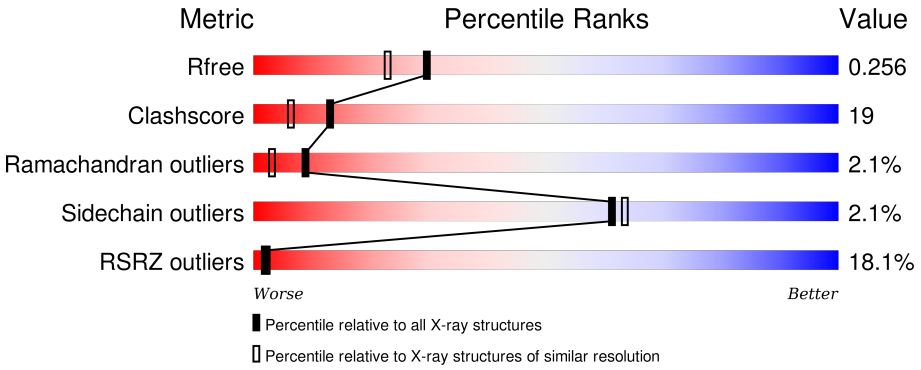
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	547	14% 63% 30%
1	B	547	24% 64% 29%
1	C	547	23% 64% 29%
1	D	547	6% 67% 27%
1	E	547	19% 64% 29%

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Mol	Chain	Length	Quality of chain
1	F	547	22% 66% 27%
1	G	547	9% 65% 28%
1	H	547	12% 65% 29%
1	I	547	16% 65% 28%
1	J	547	17% 65% 28%
1	K	547	26% 64% 29%
1	L	547	17% 64% 29%
1	M	547	26% 64% 29%
1	N	547	13% 67% 26%

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
2	SO4	A	4001	-	-	-	X
2	SO4	A	4007	-	-	-	X
2	SO4	B	4009	-	-	-	X
2	SO4	C	4011	-	-	-	X
2	SO4	E	4005	-	-	-	X
2	SO4	F	4004	-	-	-	X
2	SO4	G	4002	-	-	-	X
2	SO4	H	4017	-	-	-	X
2	SO4	J	4019	-	-	-	X
2	SO4	K	4021	-	-	-	X
2	SO4	L	4003	-	-	-	X
2	SO4	M	4013	-	-	-	X
2	SO4	N	4015	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 57085 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	B	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	C	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	D	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	E	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	F	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	G	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	H	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	I	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	J	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	K	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	L	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	M	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	N	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5

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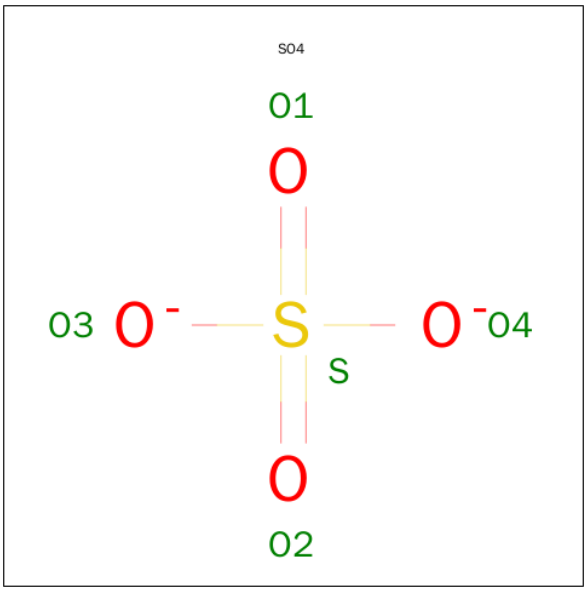
Chain	Residue	Modelled	Actual	Comment	Reference
A	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
A	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
B	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
B	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
B	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
C	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
C	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
C	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
D	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
D	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
D	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
E	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
E	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
E	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
F	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
F	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
F	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
G	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
G	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
G	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
H	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
H	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
H	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
I	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
I	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
I	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
J	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
J	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
J	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
K	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
K	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
K	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
L	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
L	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
L	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
M	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
M	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
M	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
N	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
N	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
N	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0

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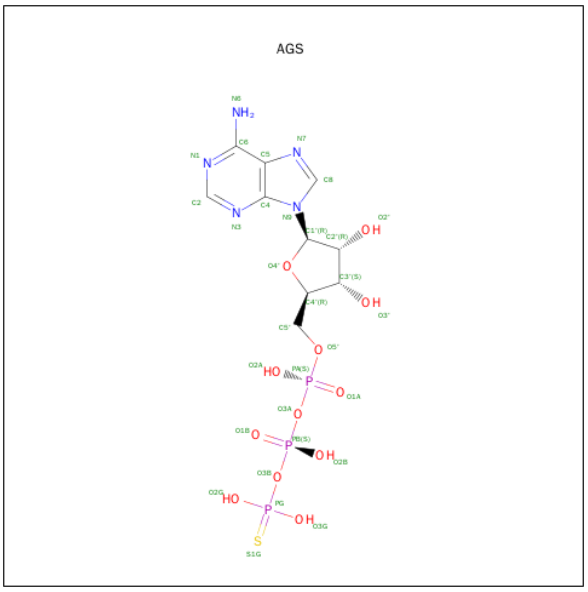
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total K 1 1	0	0
4	J	1	Total K 1 1	0	0
4	D	2	Total K 2 2	0	0
4	K	1	Total K 1 1	0	0
4	E	2	Total K 2 2	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	I	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	N	1	Total K 1 1	0	0
4	L	1	Total K 1 1	0	0
4	F	1	Total K 1 1	0	0
4	M	1	Total K 1 1	0	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	K	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	L	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	M	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is water.

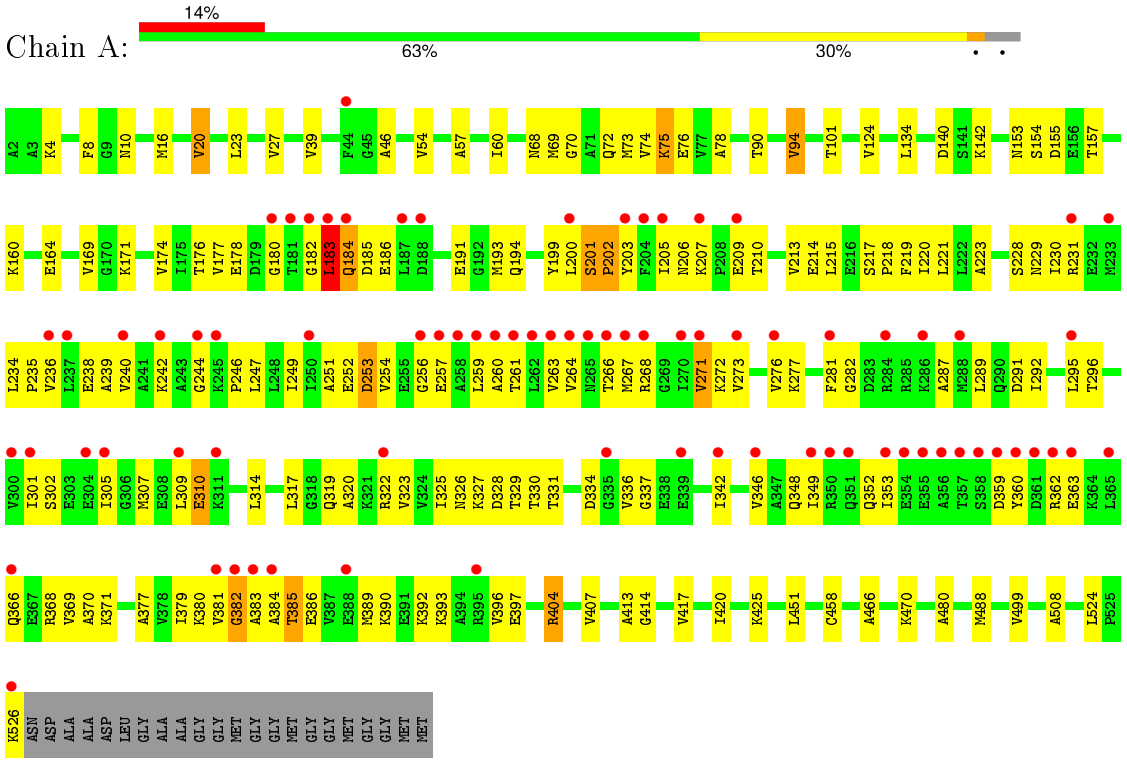
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	156	Total O 156 156	0	0
6	B	214	Total O 214 214	0	0
6	C	149	Total O 149 149	0	0
6	D	261	Total O 261 261	0	0
6	E	217	Total O 217 217	0	0
6	F	200	Total O 200 200	0	0
6	G	269	Total O 269 269	0	0
6	H	204	Total O 204 204	0	0
6	I	145	Total O 145 145	0	0
6	J	139	Total O 139 139	0	0
6	K	133	Total O 133 133	0	0
6	L	163	Total O 163 163	0	0
6	M	138	Total O 138 138	0	0
6	N	153	Total O 153 153	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.

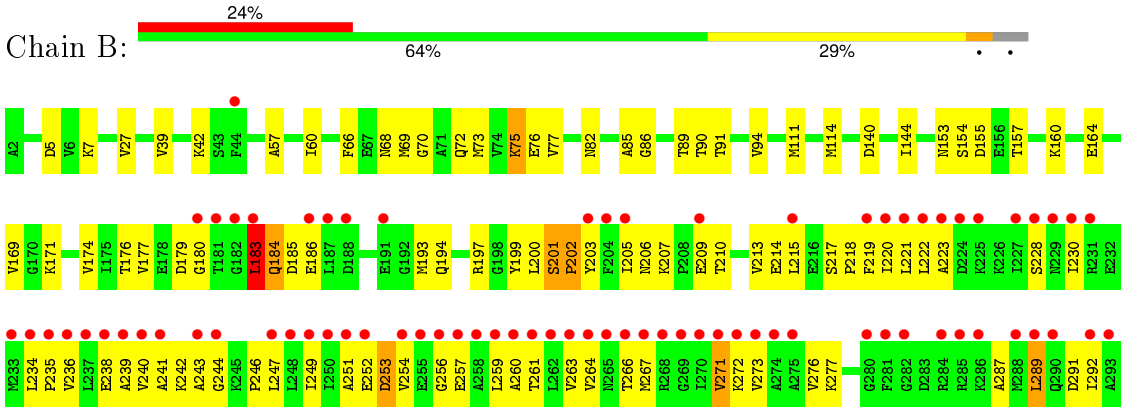
- Molecule 1: groEL protein

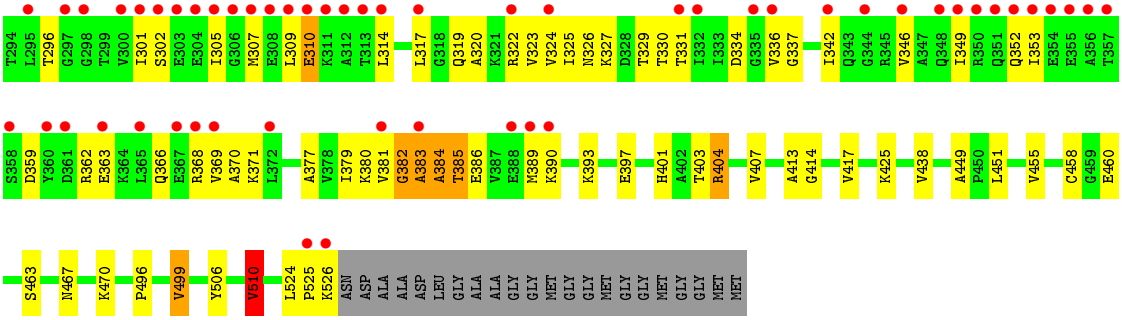
Chain A:



- Molecule 1: groEL protein

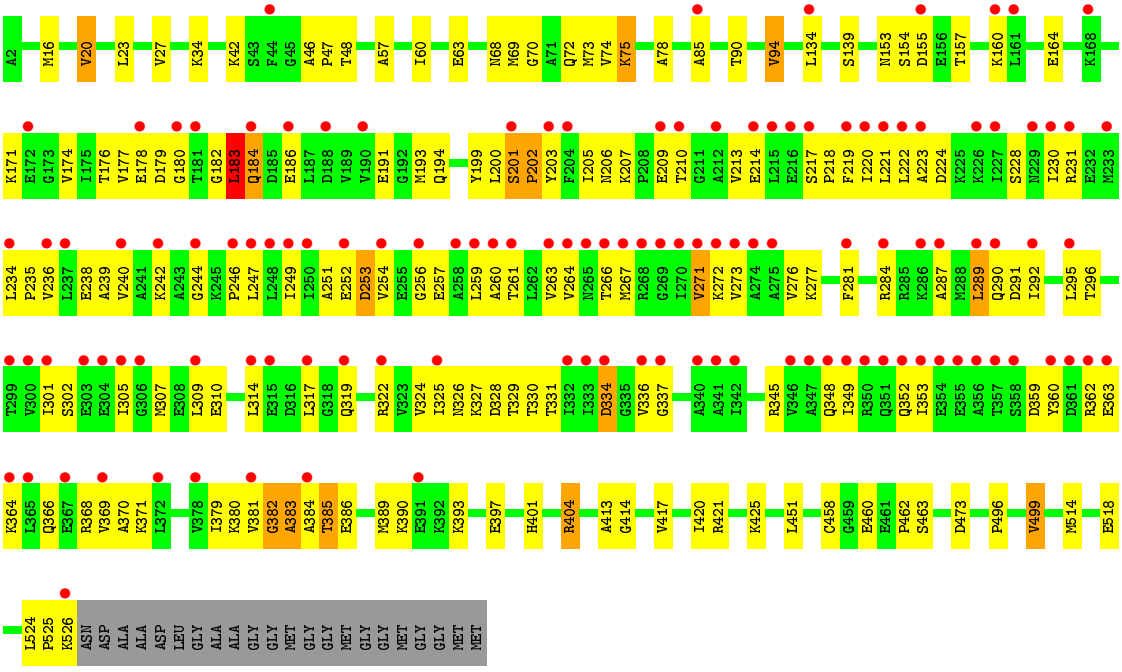
Chain B:





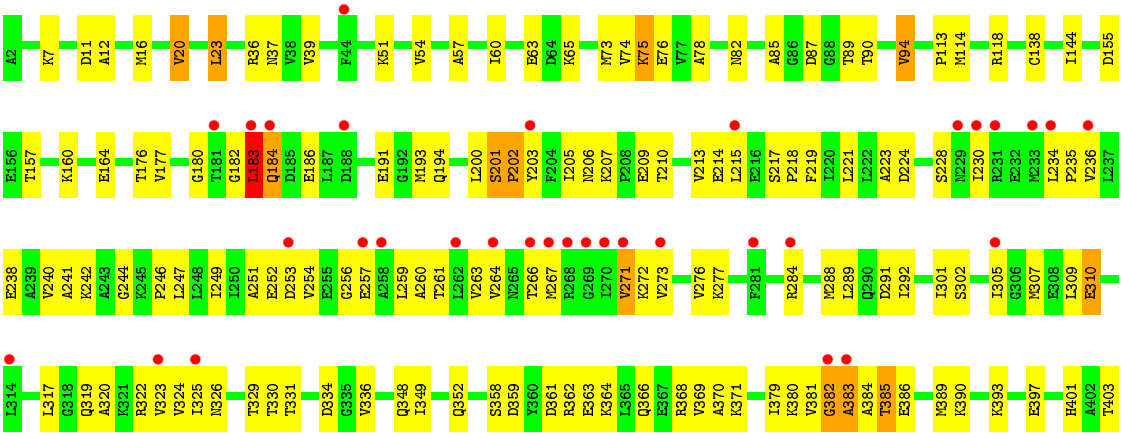
• Molecule 1: groEL protein

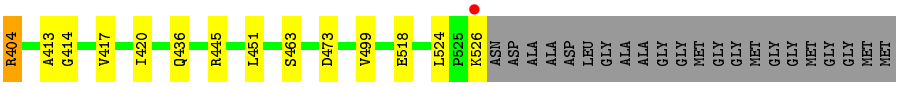
Chain C:



• Molecule 1: groEL protein

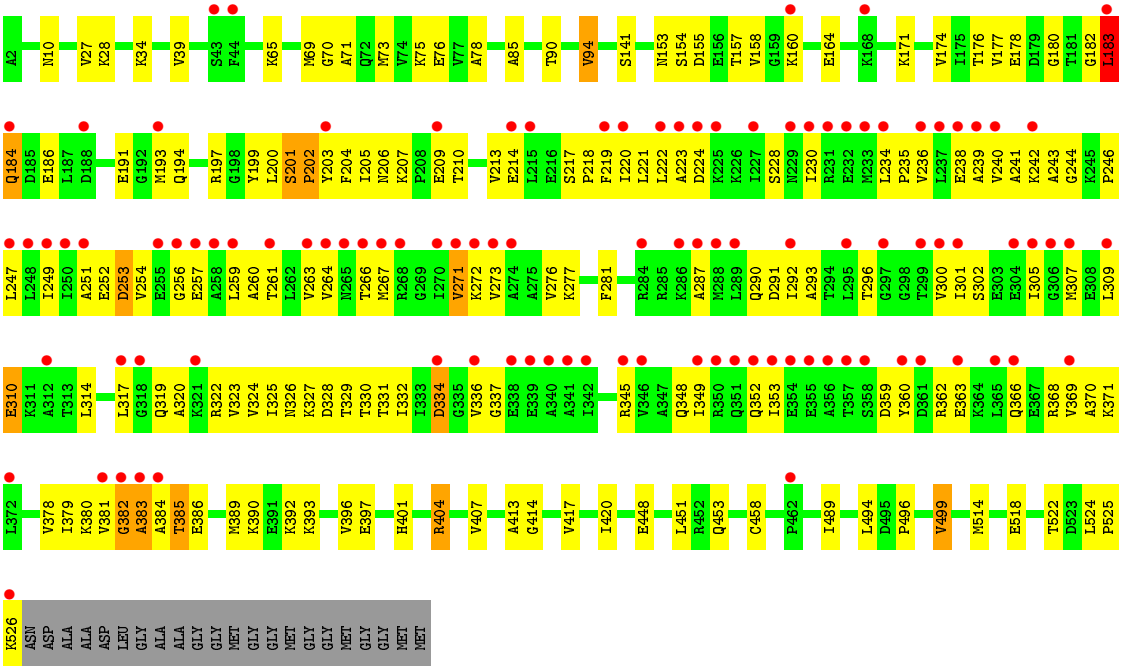
Chain D:





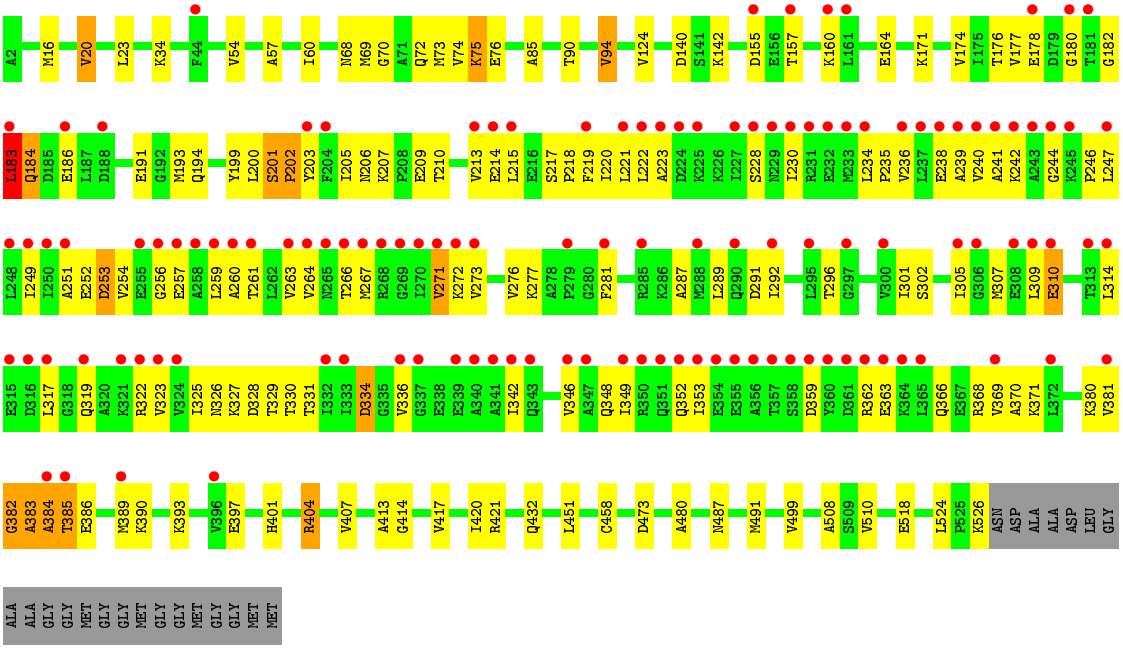
• Molecule 1: groEL protein

Chain E:



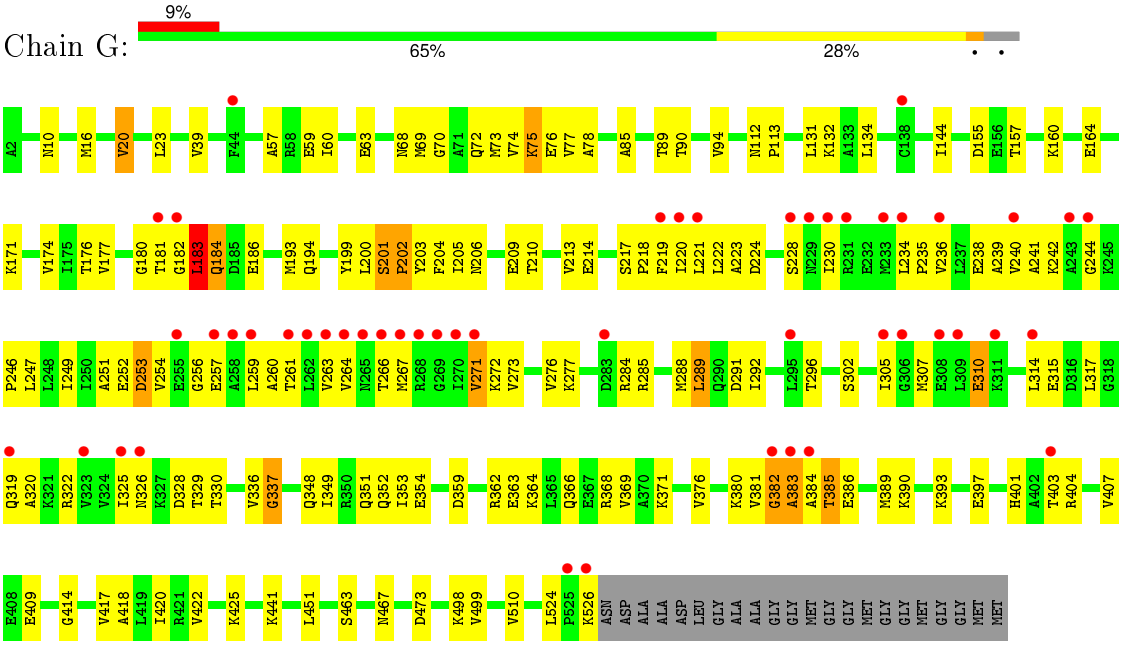
• Molecule 1: groEL protein

Chain F:



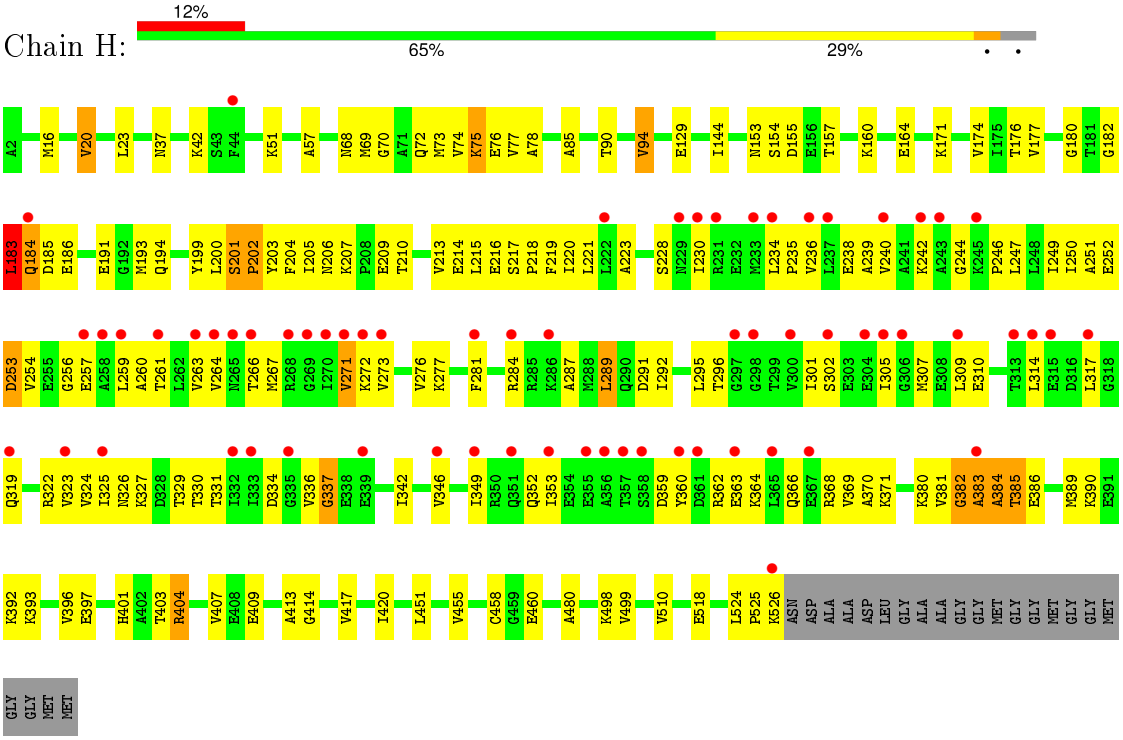
• Molecule 1: groEL protein

Chain G:



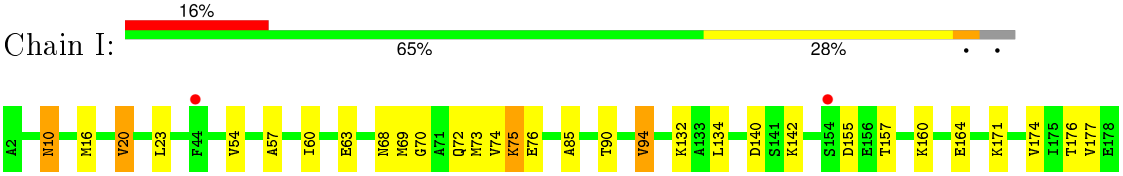
• Molecule 1: groEL protein

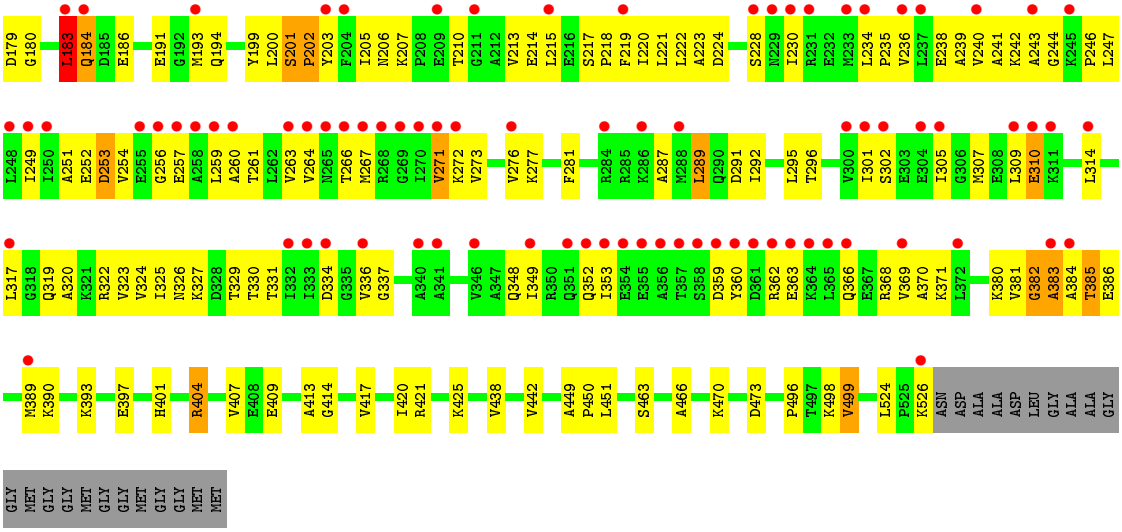
Chain H:



• Molecule 1: groEL protein

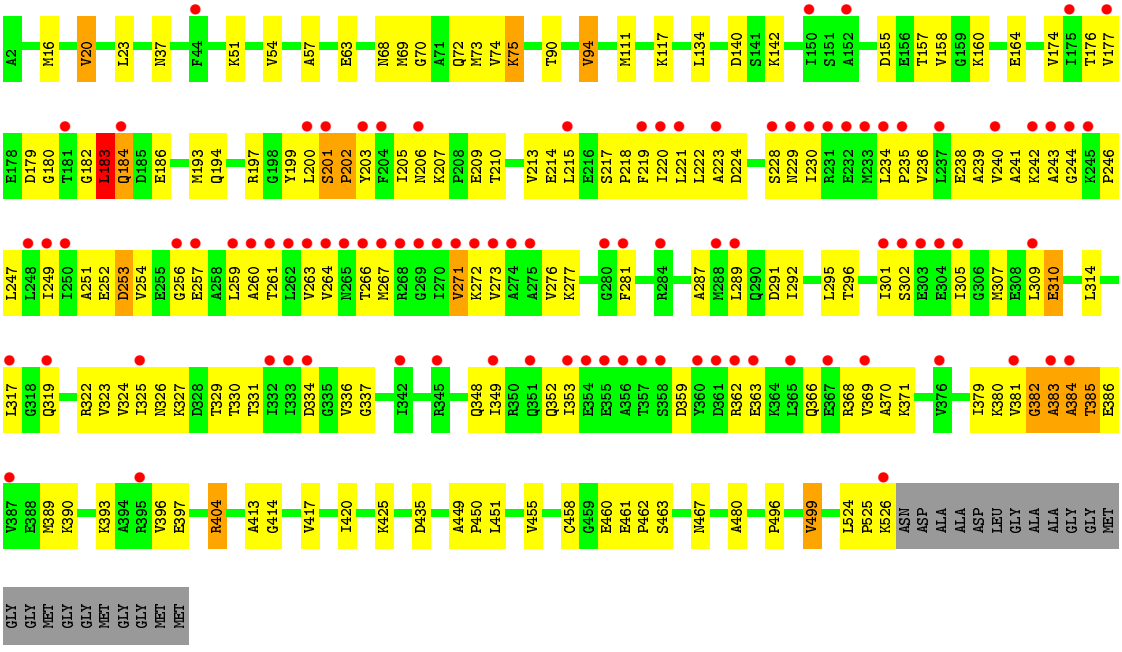
Chain I:





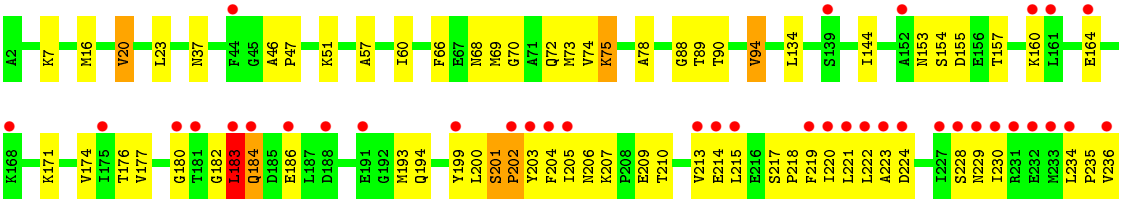
• Molecule 1: groEL protein

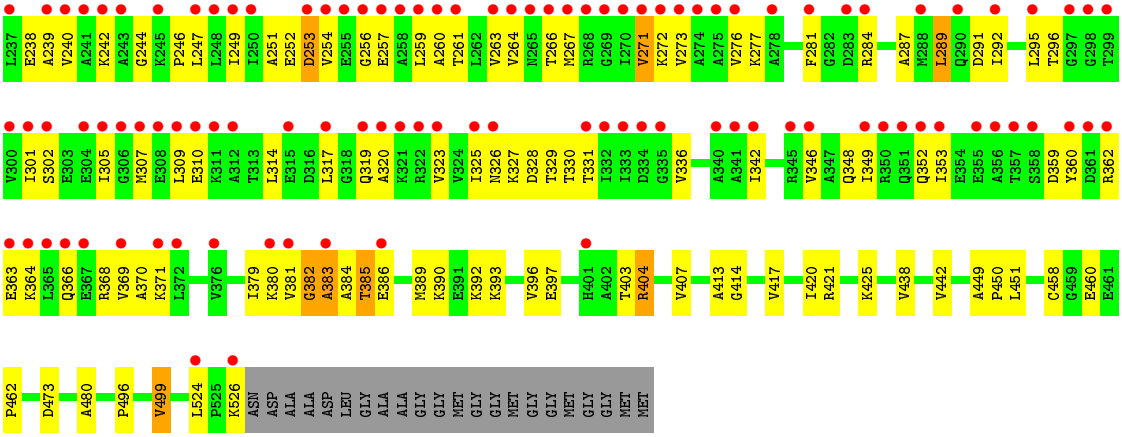
Chain J:



• Molecule 1: groEL protein

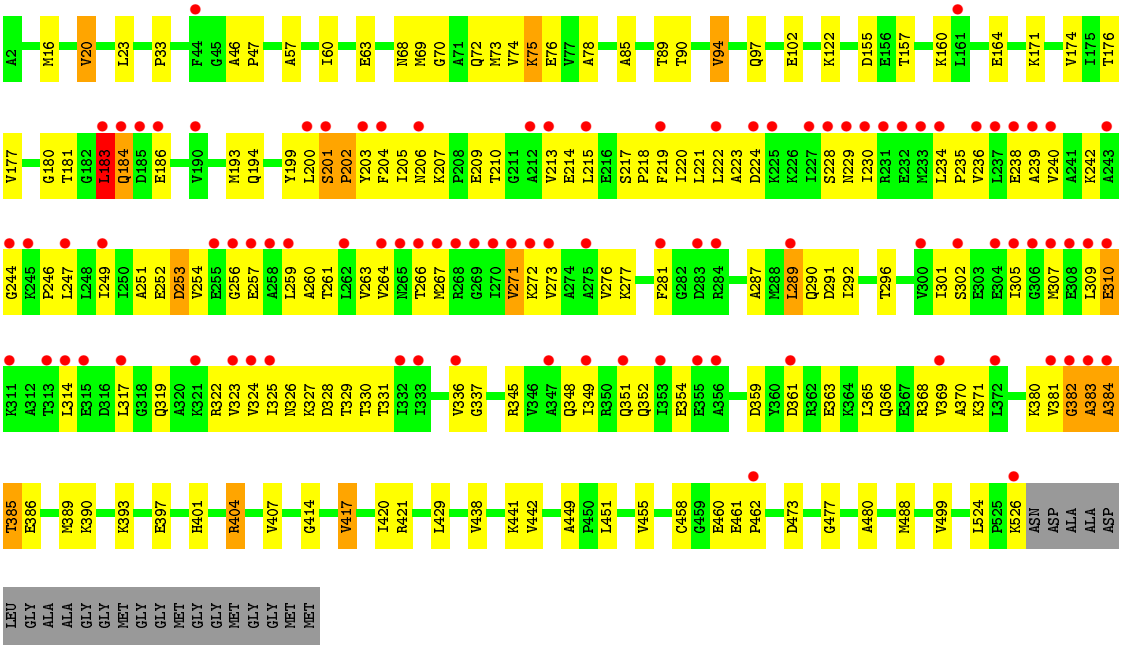
Chain K:





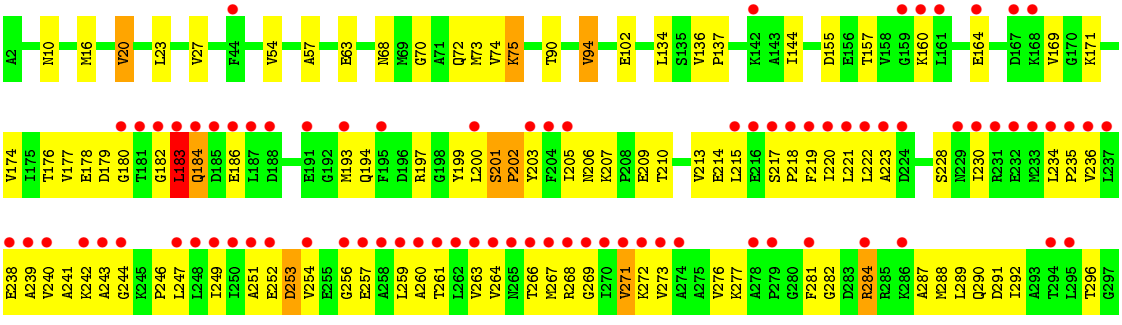
• Molecule 1: groEL protein

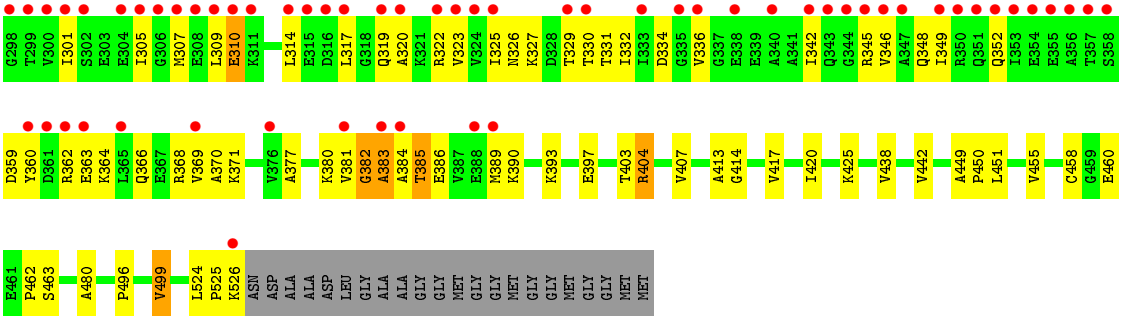
Chain L:



• Molecule 1: groEL protein

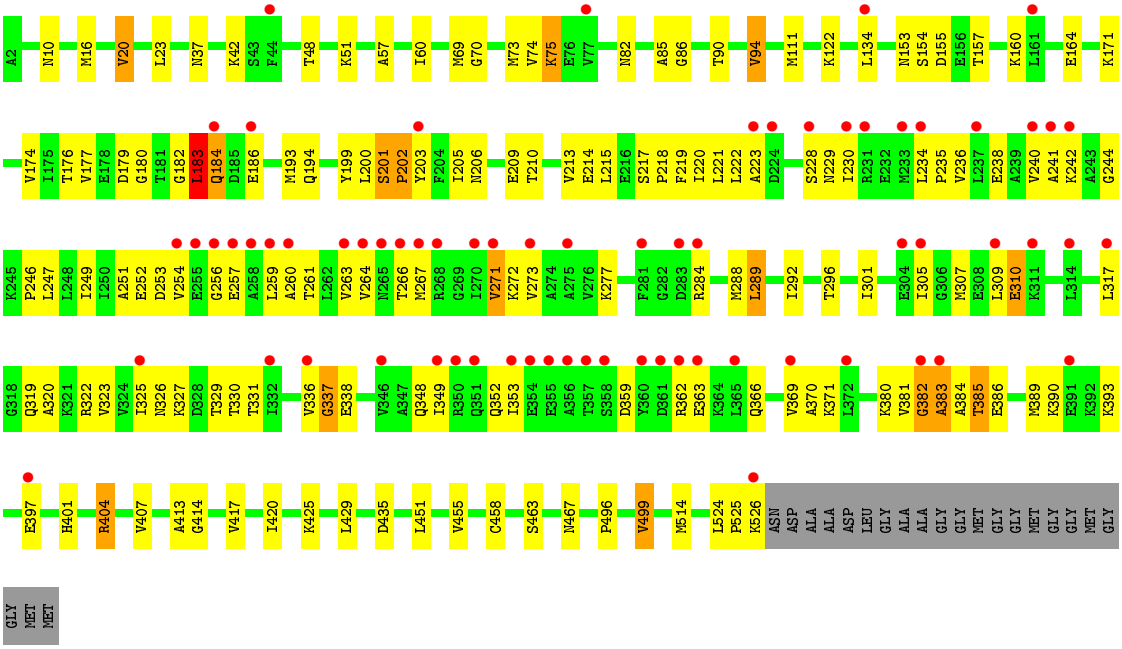
Chain M:





- Molecule 1: groEL protein

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.57Å 260.11Å 150.20Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	39.89 – 2.00 39.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.9 (39.89-2.00) 79.1 (39.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.57 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.258 0.241 , 0.256	Depositor DCC
R_{free} test set	10647 reflections (1.97%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 645898 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	57085	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MG, AGS, K, SO4

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	0.32	0/3883	0.55	0/5243
1	B	0.35	0/3883	0.57	1/5243 (0.0%)
1	C	0.32	0/3883	0.55	0/5243
1	D	0.36	0/3883	0.58	0/5243
1	E	0.34	0/3883	0.57	0/5243
1	F	0.32	0/3883	0.55	0/5243
1	G	0.36	0/3883	0.58	0/5243
1	H	0.33	0/3883	0.56	0/5243
1	I	0.30	0/3883	0.55	0/5243
1	J	0.30	0/3883	0.54	0/5243
1	K	0.30	0/3883	0.54	0/5243
1	L	0.32	0/3883	0.55	0/5243
1	M	0.30	0/3883	0.54	0/5243
1	N	0.31	0/3883	0.55	0/5243
All	All	0.32	0/54362	0.55	1/73402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	510	VAL	CB-CA-C	-5.51	100.94	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3982	161	0
1	B	3855	0	3982	170	0
1	C	3855	0	3982	153	0
1	D	3855	0	3982	146	0
1	E	3855	0	3982	154	0
1	F	3855	0	3982	136	0
1	G	3855	0	3982	153	1
1	H	3855	0	3982	149	0
1	I	3855	0	3982	150	0
1	J	3855	0	3982	149	0
1	K	3855	0	3982	154	0
1	L	3855	0	3982	149	0
1	M	3855	0	3982	151	0
1	N	3855	0	3982	145	1
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	5	0	0	0	0
2	M	10	0	0	0	0
2	N	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	31	0	12	3	0
5	B	31	0	12	4	0
5	C	31	0	12	3	0
5	D	31	0	12	4	0
5	E	31	0	12	4	0
5	F	31	0	12	3	0
5	G	31	0	12	4	0
5	H	31	0	12	4	0
5	I	31	0	12	4	0
5	J	31	0	12	3	0
5	K	31	0	12	5	0
5	L	31	0	12	5	0
5	M	31	0	12	5	0
5	N	31	0	12	4	0
6	A	156	0	0	7	0
6	B	214	0	0	8	0
6	C	149	0	0	9	0
6	D	261	0	0	19	0
6	E	217	0	0	12	0
6	F	200	0	0	5	0
6	G	269	0	0	12	0
6	H	204	0	0	8	0
6	I	145	0	0	5	0
6	J	139	0	0	2	0
6	K	133	0	0	0	0
6	L	163	0	0	9	0
6	M	138	0	0	6	0
6	N	153	0	0	7	0
All	All	57085	0	55916	2099	1

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 19.

All (2099) 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)
5:B:1:AGS:PG	5:B:1:AGS:S1G	1.50	1.50
5:A:1:AGS:S1G	5:A:1:AGS:PG	1.50	1.49
5:H:1:AGS:PG	5:H:1:AGS:S1G	1.49	1.49
5:M:1:AGS:S1G	5:M:1:AGS:PG	1.49	1.48
5:K:1:AGS:S1G	5:K:1:AGS:PG	1.49	1.48
5:D:551:AGS:PG	5:D:551:AGS:S1G	1.48	1.48
5:J:1:AGS:S1G	5:J:1:AGS:PG	1.49	1.48
5:F:1:AGS:PG	5:F:1:AGS:S1G	1.49	1.48
5:L:1:AGS:PG	5:L:1:AGS:S1G	1.49	1.47
5:N:1:AGS:PG	5:N:1:AGS:S1G	1.49	1.47
5:E:1:AGS:PG	5:E:1:AGS:S1G	1.48	1.47
5:C:1:AGS:PG	5:C:1:AGS:S1G	1.49	1.47
5:I:1:AGS:PG	5:I:1:AGS:S1G	1.49	1.47
5:G:1:AGS:PG	5:G:1:AGS:S1G	1.48	1.46
1:B:77:VAL:HG21	1:B:510:VAL:HG22	1.23	1.15
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.31	1.10
1:J:183:LEU:H	1:J:383:ALA:HB3	1.12	1.10
1:I:183:LEU:H	1:I:383:ALA:HB3	1.13	1.10
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.33	1.10
1:D:183:LEU:H	1:D:383:ALA:HB3	1.15	1.10
1:D:7:LYS:HB3	6:D:2704:HOH:O	1.47	1.10
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.33	1.09
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.33	1.09
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.30	1.09
1:L:183:LEU:H	1:L:383:ALA:HB3	1.08	1.09
1:B:183:LEU:H	1:B:383:ALA:HB3	1.07	1.08
1:F:183:LEU:H	1:F:383:ALA:HB3	1.19	1.08
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.31	1.07
1:K:183:LEU:H	1:K:383:ALA:HB3	1.19	1.07
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.32	1.07
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.31	1.06
1:N:183:LEU:H	1:N:383:ALA:HB3	1.17	1.06
1:H:183:LEU:H	1:H:383:ALA:HB3	1.13	1.06
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.36	1.06
1:A:183:LEU:H	1:A:383:ALA:HB3	1.20	1.06
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.37	1.06
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.36	1.04
1:G:325:ILE:HB	6:G:2628:HOH:O	1.55	1.04
1:B:77:VAL:HG13	1:B:506:TYR:HB3	1.36	1.04
1:E:183:LEU:H	1:E:383:ALA:HB3	1.19	1.03
1:C:183:LEU:H	1:C:383:ALA:HB3	1.23	1.03
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.33	1.03
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.34	1.02
1:M:183:LEU:H	1:M:383:ALA:HB3	1.27	0.99
1:G:183:LEU:H	1:G:383:ALA:HB3	1.25	0.99
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.46	0.98
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.48	0.96
1:H:383:ALA:HB1	1:I:281:PHE:HZ	1.31	0.95
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.48	0.95
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.48	0.95
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.49	0.95
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.50	0.94
1:J:383:ALA:HB1	1:K:281:PHE:HZ	1.33	0.94
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.49	0.94
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.49	0.94
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.50	0.93
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.47	0.93
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.50	0.93
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.51	0.93
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.49	0.93
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.50	0.93
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.52	0.92
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.51	0.92
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.52	0.91
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.53	0.91
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.53	0.91
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.49	0.91
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.53	0.90
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.52	0.90
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.54	0.90
1:B:383:ALA:HB1	1:C:281:PHE:HZ	1.36	0.90
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.55	0.89
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.51	0.89
1:A:281:PHE:HZ	1:G:383:ALA:HB1	1.36	0.89
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.51	0.89
1:B:383:ALA:HB1	1:C:281:PHE:CZ	2.07	0.89
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HB	6:B:2545:HOH:O	1.70	0.88
1:L:383:ALA:HB1	1:M:281:PHE:HZ	1.36	0.88
1:G:57:ALA:O	1:G:75:LYS:HE2	1.73	0.88
1:C:171:LYS:HE2	6:C:2796:HOH:O	1.74	0.88
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.55	0.88
1:D:359:ASP:O	1:D:363:GLU:HG2	1.75	0.87
1:L:183:LEU:N	1:L:383:ALA:HB3	1.89	0.86
1:B:183:LEU:N	1:B:383:ALA:HB3	1.89	0.86
1:L:383:ALA:HB1	1:M:281:PHE:CZ	2.10	0.86
1:H:281:PHE:HZ	1:N:383:ALA:HB1	1.38	0.86
1:D:383:ALA:HB1	1:E:281:PHE:HZ	1.42	0.85
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.40	0.85
1:G:359:ASP:O	1:G:363:GLU:HG2	1.75	0.85
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.58	0.85
1:A:281:PHE:CZ	1:G:383:ALA:HB1	2.12	0.84
1:D:57:ALA:O	1:D:75:LYS:HE2	1.77	0.84
1:E:293:ALA:HB2	6:E:2717:HOH:O	1.77	0.84
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.60	0.83
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.60	0.83
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.60	0.83
1:H:183:LEU:N	1:H:383:ALA:HB3	1.93	0.82
1:E:222:LEU:HD13	6:E:2717:HOH:O	1.79	0.82
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.60	0.82
1:H:289:LEU:HG	6:H:2938:HOH:O	1.77	0.82
1:J:57:ALA:O	1:J:75:LYS:HE2	1.80	0.82
1:I:183:LEU:N	1:I:383:ALA:HB3	1.93	0.82
1:B:86:GLY:HA3	1:B:401:HIS:CE1	2.15	0.82
1:D:183:LEU:N	1:D:383:ALA:HB3	1.94	0.81
1:I:57:ALA:O	1:I:75:LYS:HE2	1.80	0.81
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.62	0.81
1:B:77:VAL:CG2	1:B:510:VAL:HG22	2.07	0.81
1:J:183:LEU:N	1:J:383:ALA:HB3	1.92	0.81
1:H:383:ALA:HB1	1:I:281:PHE:CZ	2.16	0.80
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.63	0.80
1:N:420:ILE:HD12	1:N:451:LEU:HD13	1.62	0.80
1:J:383:ALA:HB1	1:K:281:PHE:CZ	2.17	0.80
1:M:359:ASP:O	1:M:363:GLU:HG2	1.82	0.80
1:N:57:ALA:O	1:N:75:LYS:HE2	1.80	0.80
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.64	0.80
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.64	0.80
1:F:57:ALA:O	1:F:75:LYS:HE2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.64	0.79
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.64	0.79
1:J:359:ASP:O	1:J:363:GLU:HG2	1.81	0.79
1:C:463:SER:HB2	6:C:2549:HOH:O	1.82	0.79
1:C:359:ASP:O	1:C:363:GLU:HG2	1.83	0.79
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.65	0.79
1:C:57:ALA:O	1:C:75:LYS:HE2	1.83	0.78
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.64	0.78
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.65	0.78
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.66	0.78
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.65	0.78
1:K:183:LEU:N	1:K:383:ALA:HB3	1.98	0.78
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.65	0.78
1:H:57:ALA:O	1:H:75:LYS:HE2	1.83	0.78
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.66	0.78
1:N:183:LEU:N	1:N:383:ALA:HB3	1.97	0.77
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.65	0.77
1:B:359:ASP:O	1:B:363:GLU:HG2	1.85	0.77
1:M:57:ALA:O	1:M:75:LYS:HE2	1.85	0.77
1:K:359:ASP:O	1:K:363:GLU:HG2	1.85	0.77
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.66	0.77
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.66	0.77
1:F:359:ASP:O	1:F:363:GLU:HG2	1.85	0.77
1:I:420:ILE:HD12	1:I:451:LEU:HD13	1.67	0.77
1:M:463:SER:HB2	6:M:3029:HOH:O	1.85	0.77
1:N:359:ASP:O	1:N:363:GLU:HG2	1.84	0.76
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.68	0.76
1:I:359:ASP:O	1:I:363:GLU:HG2	1.86	0.76
1:G:213:VAL:HB	1:G:325:ILE:CG1	2.15	0.76
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.68	0.76
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.68	0.76
1:F:414:GLY:O	1:F:417:VAL:HG13	1.86	0.76
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.65	0.76
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.66	0.75
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.66	0.75
1:L:359:ASP:O	1:L:363:GLU:HG2	1.85	0.75
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.68	0.75
1:F:183:LEU:N	1:F:383:ALA:HB3	1.97	0.75
1:J:381:VAL:HG21	1:J:393:LYS:HA	1.68	0.75
1:E:194:GLN:O	1:E:371:LYS:HE3	1.87	0.75
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.67	0.75
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.67	0.75
1:H:359:ASP:O	1:H:363:GLU:HG2	1.86	0.75
1:E:359:ASP:O	1:E:363:GLU:HG2	1.87	0.74
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.69	0.74
1:D:183:LEU:H	1:D:383:ALA:CB	1.99	0.74
1:E:183:LEU:N	1:E:383:ALA:HB3	2.00	0.74
5:J:1:AGS:O3B	5:J:1:AGS:S1G	2.45	0.74
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.70	0.74
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.70	0.74
1:C:514:MET:HE3	6:C:2670:HOH:O	1.88	0.73
1:I:194:GLN:O	1:I:371:LYS:HE3	1.87	0.73
1:A:359:ASP:O	1:A:363:GLU:HG2	1.88	0.73
5:G:1:AGS:S1G	5:G:1:AGS:O3B	2.45	0.73
1:C:183:LEU:N	1:C:383:ALA:HB3	2.02	0.73
1:A:183:LEU:N	1:A:383:ALA:HB3	1.99	0.73
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.69	0.73
1:G:473:ASP:HB2	6:G:2130:HOH:O	1.89	0.73
1:L:414:GLY:O	1:L:417:VAL:HG13	1.88	0.73
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.71	0.73
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.71	0.73
5:H:1:AGS:S1G	5:H:1:AGS:O3B	2.46	0.72
1:J:194:GLN:O	1:J:371:LYS:HE3	1.88	0.72
5:N:1:AGS:O3G	5:N:1:AGS:S1G	2.46	0.72
1:A:57:ALA:O	1:A:75:LYS:HE2	1.89	0.72
5:G:1:AGS:S1G	5:G:1:AGS:O3G	2.46	0.72
1:F:263:VAL:O	1:F:267:MET:HB2	1.89	0.72
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.72	0.72
1:L:420:ILE:HD12	1:L:451:LEU:HD13	1.72	0.72
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.72	0.72
5:D:551:AGS:O3B	5:D:551:AGS:S1G	2.46	0.72
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.71	0.72
1:B:194:GLN:O	1:B:371:LYS:HE3	1.89	0.72
1:K:57:ALA:O	1:K:75:LYS:HE2	1.89	0.72
1:I:383:ALA:HB1	1:J:281:PHE:HZ	1.55	0.72
1:C:514:MET:HB3	6:C:2670:HOH:O	1.89	0.72
5:K:1:AGS:S1G	5:K:1:AGS:O3G	2.46	0.72
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.70	0.72
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.72	0.72
1:F:432:GLN:HG2	6:F:2120:HOH:O	1.88	0.72
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1:AGS:O3B	5:I:1:AGS:S1G	2.47	0.71
1:A:414:GLY:O	1:A:417:VAL:HG13	1.90	0.71
5:C:1:AGS:O3B	5:C:1:AGS:S1G	2.48	0.71
1:H:404:ARG:NH1	6:H:2827:HOH:O	2.24	0.71
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.72	0.71
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.71	0.71
1:L:57:ALA:O	1:L:75:LYS:HE2	1.89	0.71
1:M:183:LEU:N	1:M:383:ALA:HB3	2.05	0.71
1:G:177:VAL:HG21	1:G:397:GLU:CG	2.21	0.71
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.73	0.71
5:F:1:AGS:S1G	5:F:1:AGS:O3B	2.48	0.71
1:B:305:ILE:HD12	1:B:307:MET:HE2	1.72	0.71
1:G:263:VAL:O	1:G:267:MET:HB2	1.91	0.71
5:E:1:AGS:O3B	5:E:1:AGS:S1G	2.48	0.70
1:B:183:LEU:H	1:B:383:ALA:CB	1.95	0.70
1:D:263:VAL:O	1:D:267:MET:HB2	1.91	0.70
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.72	0.70
1:K:414:GLY:O	1:K:417:VAL:HG13	1.91	0.70
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.72	0.70
1:I:183:LEU:H	1:I:383:ALA:CB	1.98	0.70
1:M:194:GLN:O	1:M:371:LYS:HE3	1.91	0.70
1:L:194:GLN:O	1:L:371:LYS:HE3	1.91	0.70
1:F:305:ILE:HD12	1:F:307:MET:HE2	1.72	0.70
1:A:183:LEU:H	1:A:383:ALA:CB	2.03	0.70
5:M:1:AGS:S1G	5:M:1:AGS:O3B	2.50	0.70
5:F:1:AGS:S1G	5:F:1:AGS:O3G	2.46	0.70
5:C:1:AGS:S1G	5:C:1:AGS:O3G	2.45	0.70
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.72	0.70
1:E:525:PRO:HD3	6:E:1182:HOH:O	1.91	0.70
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.92	0.69
1:L:183:LEU:H	1:L:383:ALA:CB	1.95	0.69
1:K:263:VAL:O	1:K:267:MET:HB2	1.92	0.69
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.73	0.69
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.58	0.69
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.23	0.69
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.74	0.69
1:A:263:VAL:O	1:A:267:MET:HB2	1.91	0.69
5:D:551:AGS:S1G	5:D:551:AGS:O3G	2.45	0.69
5:J:1:AGS:O3G	5:J:1:AGS:S1G	2.47	0.69
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.74	0.69
1:J:414:GLY:O	1:J:417:VAL:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:GLN:O	1:H:371:LYS:HE3	1.91	0.69
5:I:1:AGS:O3G	5:I:1:AGS:S1G	2.45	0.69
1:H:183:LEU:H	1:H:383:ALA:CB	1.98	0.69
1:M:414:GLY:O	1:M:417:VAL:HG13	1.92	0.69
1:C:525:PRO:HD3	6:C:1993:HOH:O	1.93	0.69
5:N:1:AGS:O3B	5:N:1:AGS:S1G	2.50	0.69
5:A:1:AGS:O3B	5:A:1:AGS:S1G	2.48	0.69
1:C:194:GLN:O	1:C:371:LYS:HE3	1.91	0.69
1:N:263:VAL:O	1:N:267:MET:HB2	1.93	0.69
1:H:525:PRO:HD3	6:H:2151:HOH:O	1.93	0.69
1:K:305:ILE:HD12	1:K:307:MET:HE2	1.75	0.69
1:D:213:VAL:HB	1:D:325:ILE:CG1	2.23	0.69
5:H:1:AGS:O3G	5:H:1:AGS:S1G	2.48	0.69
5:K:1:AGS:O3B	5:K:1:AGS:S1G	2.50	0.69
5:E:1:AGS:O3G	5:E:1:AGS:S1G	2.46	0.69
1:L:263:VAL:O	1:L:267:MET:HB2	1.93	0.69
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.75	0.69
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.23	0.69
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.74	0.69
1:H:183:LEU:HD23	1:H:384:ALA:HB2	1.76	0.68
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.75	0.68
1:L:449:ALA:HB1	6:L:2642:HOH:O	1.93	0.68
1:J:183:LEU:H	1:J:383:ALA:CB	1.98	0.68
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.75	0.68
1:H:263:VAL:O	1:H:267:MET:HB2	1.92	0.68
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.23	0.68
1:B:263:VAL:O	1:B:267:MET:HB2	1.93	0.68
1:H:305:ILE:HD12	1:H:307:MET:HE2	1.76	0.68
1:C:263:VAL:O	1:C:267:MET:HB2	1.93	0.68
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.75	0.68
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.76	0.68
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.75	0.68
1:B:414:GLY:O	1:B:417:VAL:HG13	1.93	0.68
1:A:228:SER:O	1:A:257:GLU:HB3	1.94	0.68
1:B:213:VAL:HB	1:B:325:ILE:CG1	2.24	0.68
5:L:1:AGS:O3B	5:L:1:AGS:S1G	2.49	0.68
1:D:194:GLN:O	1:D:371:LYS:HE3	1.94	0.67
1:J:263:VAL:O	1:J:267:MET:HB2	1.93	0.67
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.74	0.67
1:M:263:VAL:O	1:M:267:MET:HB2	1.93	0.67
1:K:383:ALA:HB1	1:L:281:PHE:HZ	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:VAL:O	1:I:267:MET:HB2	1.93	0.67
5:B:1:AGS:O3B	5:B:1:AGS:S1G	2.50	0.67
1:G:183:LEU:N	1:G:383:ALA:HB3	2.04	0.67
1:M:177:VAL:HG21	1:M:397:GLU:HG3	1.75	0.67
1:N:219:PHE:HB3	1:N:317:LEU:HD23	1.77	0.67
1:G:285:ARG:HD2	6:G:2626:HOH:O	1.95	0.67
1:H:177:VAL:HG21	1:H:397:GLU:CG	2.25	0.67
1:C:228:SER:O	1:C:257:GLU:HB3	1.95	0.67
5:B:1:AGS:O3G	5:B:1:AGS:S1G	2.48	0.67
1:J:384:ALA:HA	1:K:360:TYR:OH	1.95	0.67
1:E:263:VAL:O	1:E:267:MET:HB2	1.94	0.67
1:N:305:ILE:HD12	1:N:307:MET:HE2	1.76	0.66
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.76	0.66
1:D:160:LYS:O	1:D:164:GLU:HG3	1.95	0.66
1:G:183:LEU:HD23	1:G:384:ALA:HB2	1.77	0.66
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.75	0.66
1:D:383:ALA:HB1	1:E:281:PHE:CZ	2.29	0.66
5:M:1:AGS:O3G	5:M:1:AGS:S1G	2.47	0.66
1:H:174:VAL:HG22	1:H:194:GLN:HE21	1.61	0.66
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.60	0.66
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.78	0.66
1:D:414:GLY:O	1:D:417:VAL:HG13	1.96	0.66
1:N:183:LEU:HD23	1:N:384:ALA:HB2	1.78	0.66
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.75	0.66
1:L:177:VAL:HG21	1:L:397:GLU:CG	2.25	0.66
1:F:177:VAL:HG21	1:F:397:GLU:CG	2.26	0.66
1:E:414:GLY:O	1:E:417:VAL:HG13	1.95	0.66
1:B:183:LEU:HD23	1:B:384:ALA:HB2	1.77	0.66
1:A:194:GLN:O	1:A:371:LYS:HE3	1.94	0.66
5:A:1:AGS:S1G	5:A:1:AGS:O3G	2.47	0.66
1:C:414:GLY:O	1:C:417:VAL:HG13	1.96	0.66
1:L:183:LEU:HD23	1:L:384:ALA:HB2	1.78	0.66
1:I:160:LYS:O	1:I:164:GLU:HG3	1.96	0.66
1:I:183:LEU:HD23	1:I:384:ALA:HB2	1.78	0.66
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.76	0.66
1:E:392:LYS:HE3	6:E:2648:HOH:O	1.96	0.66
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.77	0.66
1:F:228:SER:O	1:F:257:GLU:HB3	1.95	0.66
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.78	0.65
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.78	0.65
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:414:GLY:O	1:I:417:VAL:HG13	1.96	0.65
1:H:228:SER:O	1:H:257:GLU:HB3	1.97	0.65
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	0.65
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.78	0.65
1:H:404:ARG:CG	1:H:404:ARG:HH11	2.08	0.65
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.77	0.65
1:F:178:GLU:OE2	1:F:322:ARG:HD3	1.96	0.65
1:D:326:ASN:HD22	1:D:329:THR:HB	1.61	0.65
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.27	0.65
1:L:228:SER:O	1:L:257:GLU:HB3	1.97	0.65
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.26	0.65
1:G:242:LYS:C	1:G:244:GLY:H	1.98	0.65
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.79	0.65
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.78	0.65
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.78	0.65
1:B:228:SER:O	1:B:257:GLU:HB3	1.97	0.65
1:D:78:ALA:HB3	6:D:2581:HOH:O	1.95	0.65
1:H:281:PHE:CZ	1:N:383:ALA:HB1	2.28	0.65
1:C:221:LEU:HD23	1:C:249:ILE:HD12	1.79	0.65
1:B:91:THR:O	1:B:94:VAL:HG22	1.96	0.65
1:K:228:SER:O	1:K:257:GLU:HB3	1.97	0.65
1:H:42:LYS:HB2	6:H:2847:HOH:O	1.96	0.65
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.79	0.65
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.77	0.65
1:B:60:ILE:O	1:B:75:LYS:HE3	1.98	0.64
1:E:206:ASN:HD21	1:E:214:GLU:H	1.45	0.64
1:C:305:ILE:HD12	1:C:307:MET:HE2	1.78	0.64
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.79	0.64
1:H:69:MET:O	1:H:73:MET:HG3	1.96	0.64
1:G:228:SER:O	1:G:257:GLU:HB3	1.97	0.64
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.79	0.64
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.79	0.64
1:H:414:GLY:O	1:H:417:VAL:HG13	1.98	0.64
1:F:194:GLN:O	1:F:371:LYS:HE3	1.97	0.64
1:I:383:ALA:HB1	1:J:281:PHE:CZ	2.32	0.64
1:F:183:LEU:HD23	1:F:384:ALA:HB2	1.80	0.64
1:A:349:ILE:HA	1:A:352:GLN:CG	2.27	0.64
1:I:177:VAL:HG21	1:I:397:GLU:CG	2.28	0.64
1:I:206:ASN:HD21	1:I:214:GLU:H	1.43	0.64
1:B:160:LYS:O	1:B:164:GLU:HG3	1.97	0.64
1:M:221:LEU:HD23	1:M:249:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LEU:O	1:D:184:GLN:HB2	1.98	0.64
1:K:183:LEU:HD23	1:K:384:ALA:HB2	1.80	0.64
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.63	0.64
1:D:177:VAL:HG21	1:D:397:GLU:CG	2.27	0.64
1:E:177:VAL:HG21	1:E:397:GLU:CG	2.27	0.64
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.80	0.64
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.80	0.64
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.80	0.64
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.28	0.64
1:K:404:ARG:HH11	1:K:404:ARG:HG2	1.63	0.64
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.64
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.28	0.64
1:A:268:ARG:O	1:B:257:GLU:HG3	1.97	0.64
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.28	0.64
1:K:183:LEU:H	1:K:383:ALA:CB	2.03	0.63
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.28	0.63
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.80	0.63
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.79	0.63
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.80	0.63
1:K:194:GLN:O	1:K:371:LYS:HE3	1.98	0.63
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.80	0.63
1:M:326:ASN:HD22	1:M:329:THR:HB	1.64	0.63
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.79	0.63
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.80	0.63
1:A:183:LEU:HD23	1:A:384:ALA:HB2	1.81	0.63
1:C:213:VAL:HB	1:C:325:ILE:CG1	2.28	0.63
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.80	0.63
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.81	0.63
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.80	0.63
1:C:90:THR:O	1:C:94:VAL:HG13	1.98	0.63
1:D:193:MET:CE	1:D:292:ILE:HG12	2.28	0.63
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.81	0.63
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	0.63
1:F:183:LEU:H	1:F:383:ALA:CB	2.03	0.63
1:N:177:VAL:HG21	1:N:397:GLU:CG	2.29	0.63
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.80	0.63
1:E:305:ILE:HD12	1:E:307:MET:HE2	1.80	0.63
1:H:362:ARG:O	1:H:366:GLN:HG3	1.99	0.63
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.81	0.63
1:D:193:MET:HE2	1:D:292:ILE:HG12	1.80	0.63
1:J:54:VAL:HG23	6:J:2067:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.79	0.63
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.29	0.63
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.81	0.62
1:G:194:GLN:O	1:G:371:LYS:HE3	1.99	0.62
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.64	0.62
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.81	0.62
1:G:305:ILE:HD12	1:G:307:MET:HE2	1.81	0.62
1:N:228:SER:O	1:N:257:GLU:HB3	1.99	0.62
1:M:228:SER:O	1:M:257:GLU:HB3	1.99	0.62
5:L:1:AGS:S1G	5:L:1:AGS:O3G	2.49	0.62
1:C:139:SER:HB3	6:C:2796:HOH:O	2.00	0.62
1:K:200:LEU:O	1:K:201:SER:HB3	1.99	0.62
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.81	0.62
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.80	0.62
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.80	0.62
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.81	0.62
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.63	0.62
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.27	0.62
1:F:160:LYS:O	1:F:164:GLU:HG3	2.00	0.62
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.82	0.62
1:E:228:SER:O	1:E:257:GLU:HB3	1.99	0.62
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.81	0.62
1:A:360:TYR:OH	1:G:384:ALA:HA	2.00	0.62
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.81	0.62
1:D:82:ASN:HA	6:D:2757:HOH:O	1.98	0.62
1:C:404:ARG:HH11	1:C:404:ARG:HG2	1.63	0.62
1:N:183:LEU:H	1:N:383:ALA:CB	2.02	0.62
1:C:200:LEU:O	1:C:201:SER:HB3	1.99	0.62
1:B:68:ASN:O	1:B:72:GLN:HG2	1.98	0.62
1:F:413:ALA:HB3	1:F:417:VAL:HG22	1.82	0.62
1:D:200:LEU:O	1:D:201:SER:HB3	2.00	0.62
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.00	0.62
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.81	0.62
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.80	0.62
1:N:272:LYS:HD2	1:N:272:LYS:N	2.15	0.62
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.80	0.62
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.80	0.62
1:H:206:ASN:HD21	1:H:214:GLU:H	1.46	0.62
1:H:384:ALA:HA	1:I:360:TYR:OH	2.00	0.62
1:L:218:PRO:CB	1:L:246:PRO:HG2	2.27	0.62
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:LEU:HD23	1:J:249:ILE:HD12	1.82	0.61
1:B:77:VAL:CG1	1:B:506:TYR:HB3	2.22	0.61
1:H:349:ILE:HA	1:H:352:GLN:CG	2.28	0.61
1:L:78:ALA:HB3	6:L:2535:HOH:O	1.99	0.61
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.65	0.61
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.81	0.61
1:N:414:GLY:O	1:N:417:VAL:HG13	2.00	0.61
1:F:16:MET:O	1:F:20:VAL:HG13	2.00	0.61
1:M:525:PRO:HD3	6:M:2817:HOH:O	1.99	0.61
1:J:177:VAL:HG21	1:J:397:GLU:CG	2.30	0.61
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.83	0.61
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.82	0.61
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.82	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.81	0.61
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.82	0.61
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.01	0.61
1:B:200:LEU:O	1:B:201:SER:HB3	2.00	0.61
1:D:404:ARG:NH1	6:D:2552:HOH:O	2.33	0.61
1:G:78:ALA:HB3	6:G:1724:HOH:O	1.98	0.61
1:E:78:ALA:HB3	6:E:2338:HOH:O	2.00	0.61
1:D:183:LEU:HD23	1:D:384:ALA:HB2	1.83	0.61
1:N:200:LEU:O	1:N:201:SER:HB3	2.00	0.61
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.82	0.61
1:M:268:ARG:O	1:N:257:GLU:HG3	1.99	0.61
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.00	0.61
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.83	0.61
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.83	0.61
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.83	0.61
1:J:160:LYS:O	1:J:164:GLU:HG3	2.01	0.61
1:G:183:LEU:O	1:G:184:GLN:HB2	2.00	0.61
1:A:69:MET:O	1:A:73:MET:HG3	2.00	0.61
1:C:183:LEU:HD12	1:C:184:GLN:HG3	1.83	0.61
1:M:177:VAL:HG21	1:M:397:GLU:CG	2.30	0.61
1:C:272:LYS:HD2	1:C:272:LYS:N	2.16	0.61
1:M:319:GLN:O	1:M:336:VAL:HG23	2.01	0.61
1:I:228:SER:O	1:I:257:GLU:HB3	2.01	0.60
1:J:183:LEU:HD12	1:J:184:GLN:HG3	1.83	0.60
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.83	0.60
1:F:206:ASN:HD21	1:F:214:GLU:H	1.49	0.60
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.83	0.60
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.01	0.60
1:D:39:VAL:HG12	1:E:69:MET:HE2	1.83	0.60
1:C:177:VAL:HG21	1:C:397:GLU:CG	2.31	0.60
1:B:90:THR:O	1:B:94:VAL:HG13	2.02	0.60
1:I:218:PRO:CB	1:I:246:PRO:HG2	2.28	0.60
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.81	0.60
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.82	0.60
1:M:362:ARG:O	1:M:366:GLN:HG3	2.02	0.60
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.83	0.60
1:B:177:VAL:HG21	1:B:397:GLU:CG	2.32	0.60
1:B:221:LEU:HD23	1:B:249:ILE:HD12	1.82	0.60
1:M:200:LEU:O	1:M:201:SER:HB3	1.99	0.60
1:A:46:ALA:CB	1:B:76:GLU:HG3	2.31	0.60
1:B:425:LYS:HB2	6:B:2916:HOH:O	2.01	0.60
1:G:414:GLY:O	1:G:417:VAL:HG13	2.01	0.60
1:G:420:ILE:HD12	1:G:451:LEU:HD13	1.82	0.60
1:J:23:LEU:CD2	1:J:74:VAL:HG13	2.31	0.60
1:D:272:LYS:HD2	1:D:272:LYS:N	2.17	0.60
1:D:228:SER:O	1:D:257:GLU:HB3	2.01	0.60
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.83	0.60
1:B:57:ALA:O	1:B:75:LYS:HE2	2.01	0.60
1:N:194:GLN:O	1:N:371:LYS:HE3	2.00	0.60
1:A:177:VAL:HG21	1:A:397:GLU:CG	2.31	0.60
1:J:228:SER:O	1:J:257:GLU:HB3	2.02	0.60
1:F:383:ALA:O	1:F:384:ALA:HB3	2.01	0.59
1:J:349:ILE:HA	1:J:352:GLN:CG	2.31	0.59
1:J:272:LYS:N	1:J:272:LYS:HD2	2.17	0.59
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.84	0.59
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.67	0.59
1:C:183:LEU:HD23	1:C:384:ALA:HB2	1.85	0.59
1:E:349:ILE:HA	1:E:352:GLN:CG	2.32	0.59
1:E:183:LEU:HD23	1:E:384:ALA:HB2	1.85	0.59
1:J:218:PRO:CB	1:J:246:PRO:HG2	2.28	0.59
1:A:23:LEU:HD22	1:A:74:VAL:HG13	1.85	0.59
1:E:489:ILE:HD13	1:E:494:LEU:HD21	1.85	0.59
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.82	0.59
1:D:242:LYS:C	1:D:244:GLY:H	2.03	0.59
1:F:90:THR:O	1:F:94:VAL:HG13	2.02	0.59
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.03	0.59
1:K:177:VAL:HG21	1:K:397:GLU:CG	2.32	0.59
1:M:349:ILE:HA	1:M:352:GLN:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.85	0.59
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.02	0.59
1:M:206:ASN:HD21	1:M:214:GLU:H	1.51	0.59
1:B:449:ALA:HB1	6:B:2545:HOH:O	2.02	0.59
1:B:114:MET:HB3	6:B:2278:HOH:O	2.02	0.59
1:M:160:LYS:O	1:M:164:GLU:HG3	2.03	0.59
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.83	0.59
1:I:272:LYS:N	1:I:272:LYS:HD2	2.18	0.59
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.84	0.59
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.84	0.59
1:C:362:ARG:O	1:C:366:GLN:HG3	2.03	0.59
1:L:90:THR:O	1:L:94:VAL:HG13	2.03	0.59
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.85	0.59
1:E:272:LYS:HD2	1:E:272:LYS:N	2.17	0.59
1:C:349:ILE:HA	1:C:352:GLN:CG	2.31	0.58
1:F:349:ILE:HA	1:F:352:GLN:CG	2.33	0.58
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.83	0.58
1:A:362:ARG:O	1:A:366:GLN:HG3	2.03	0.58
1:F:386:GLU:O	1:F:390:LYS:HG2	2.03	0.58
1:A:272:LYS:HD2	1:A:272:LYS:N	2.18	0.58
1:J:174:VAL:HG22	1:J:194:GLN:HE21	1.68	0.58
1:C:155:ASP:OD1	1:C:157:THR:HB	2.03	0.58
1:G:272:LYS:N	1:G:272:LYS:HD2	2.17	0.58
1:K:272:LYS:HD2	1:K:272:LYS:N	2.18	0.58
1:D:362:ARG:O	1:D:366:GLN:HG3	2.03	0.58
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.84	0.58
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.69	0.58
1:F:362:ARG:O	1:F:366:GLN:HG3	2.04	0.58
1:D:11:ASP:HB2	6:D:2704:HOH:O	2.02	0.58
1:I:200:LEU:O	1:I:201:SER:HB3	2.03	0.58
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.85	0.58
1:G:183:LEU:H	1:G:383:ALA:CB	2.08	0.58
1:H:218:PRO:CB	1:H:246:PRO:HG2	2.30	0.58
1:A:404:ARG:NH1	6:A:2654:HOH:O	2.36	0.58
1:I:183:LEU:HD12	1:I:184:GLN:HG3	1.85	0.58
1:H:183:LEU:O	1:H:184:GLN:HB2	2.03	0.58
1:K:218:PRO:CB	1:K:246:PRO:HG2	2.30	0.58
1:N:160:LYS:O	1:N:164:GLU:HG3	2.03	0.58
1:M:183:LEU:HD23	1:M:384:ALA:HB2	1.85	0.58
1:N:349:ILE:HA	1:N:352:GLN:CG	2.33	0.58
1:K:349:ILE:HA	1:K:352:GLN:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:417:VAL:HG11	1:L:488:MET:HG3	1.84	0.58
1:C:206:ASN:HD21	1:C:214:GLU:H	1.50	0.58
1:H:272:LYS:N	1:H:272:LYS:HD2	2.19	0.58
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.68	0.58
1:E:183:LEU:O	1:E:184:GLN:HB2	2.04	0.57
1:F:200:LEU:O	1:F:201:SER:HB3	2.02	0.57
1:H:174:VAL:HG22	1:H:194:GLN:NE2	2.18	0.57
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.86	0.57
1:L:383:ALA:O	1:L:384:ALA:HB3	2.04	0.57
1:L:349:ILE:HA	1:L:352:GLN:CG	2.34	0.57
1:D:463:SER:HB2	6:D:2645:HOH:O	2.03	0.57
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.85	0.57
1:A:382:GLY:O	1:A:389:MET:HG2	2.04	0.57
1:L:272:LYS:HD2	1:L:272:LYS:N	2.19	0.57
1:B:272:LYS:HD2	1:B:272:LYS:N	2.19	0.57
1:G:213:VAL:HB	1:G:325:ILE:HG13	1.86	0.57
1:E:183:LEU:H	1:E:383:ALA:CB	2.05	0.57
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.27	0.57
1:G:382:GLY:O	1:G:389:MET:HG2	2.04	0.57
1:A:420:ILE:HD12	1:A:451:LEU:HD13	1.87	0.57
1:J:206:ASN:HD21	1:J:214:GLU:H	1.51	0.57
1:D:11:ASP:CB	6:D:2704:HOH:O	2.52	0.57
1:N:183:LEU:HD12	1:N:184:GLN:HG3	1.87	0.57
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.85	0.57
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.87	0.57
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.87	0.57
1:F:85:ALA:O	1:F:401:HIS:HE1	1.88	0.57
1:D:90:THR:O	1:D:94:VAL:HG13	2.05	0.57
1:K:183:LEU:HD12	1:K:184:GLN:HG3	1.87	0.57
1:H:360:TYR:OH	1:N:384:ALA:HA	2.04	0.57
1:N:183:LEU:CD1	1:N:184:GLN:HG3	2.34	0.57
1:I:349:ILE:HA	1:I:352:GLN:CG	2.33	0.57
1:A:326:ASN:HD22	1:A:329:THR:HB	1.70	0.57
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.86	0.57
1:L:386:GLU:O	1:L:390:LYS:HG2	2.04	0.57
1:N:362:ARG:O	1:N:366:GLN:HG3	2.05	0.57
1:I:183:LEU:O	1:I:184:GLN:HB2	2.05	0.57
1:A:235:PRO:CG	1:A:310:GLU:HA	2.29	0.57
1:A:218:PRO:CB	1:A:246:PRO:HG2	2.32	0.57
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.57
1:N:206:ASN:HD21	1:N:214:GLU:H	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.85	0.57
1:K:206:ASN:HD21	1:K:214:GLU:H	1.51	0.57
1:B:382:GLY:O	1:B:389:MET:HG2	2.05	0.57
1:E:200:LEU:O	1:E:201:SER:HB3	2.03	0.57
1:I:326:ASN:HD22	1:I:329:THR:HB	1.70	0.57
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.85	0.57
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.85	0.57
1:L:242:LYS:C	1:L:244:GLY:H	2.06	0.57
1:A:16:MET:O	1:A:20:VAL:HG13	2.04	0.57
1:A:281:PHE:HZ	1:G:383:ALA:CB	2.15	0.57
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.29	0.57
1:D:160:LYS:NZ	1:D:160:LYS:HB2	2.20	0.57
1:K:326:ASN:HD22	1:K:329:THR:HB	1.70	0.57
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.86	0.57
1:L:193:MET:CE	1:L:292:ILE:HG12	2.35	0.57
1:F:404:ARG:HH11	1:F:404:ARG:HG2	1.70	0.57
1:A:200:LEU:O	1:A:201:SER:HB3	2.04	0.56
1:A:155:ASP:OD1	1:A:157:THR:HB	2.04	0.56
1:N:183:LEU:O	1:N:184:GLN:HB2	2.05	0.56
1:A:46:ALA:HB2	1:B:76:GLU:HG3	1.87	0.56
6:B:1684:HOH:O	1:C:518:GLU:HG2	2.04	0.56
1:J:383:ALA:O	1:J:384:ALA:HB3	2.05	0.56
1:L:183:LEU:O	1:L:184:GLN:HB2	2.06	0.56
1:L:384:ALA:HA	1:M:360:TYR:OH	2.05	0.56
1:A:183:LEU:O	1:A:184:GLN:HB2	2.06	0.56
1:J:247:LEU:HB3	1:J:273:VAL:HG22	1.85	0.56
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.04	0.56
1:D:138:CYS:HB2	6:D:2989:HOH:O	2.05	0.56
1:E:155:ASP:OD1	1:E:157:THR:HB	2.03	0.56
1:D:386:GLU:O	1:D:390:LYS:HG2	2.05	0.56
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.88	0.56
1:L:160:LYS:O	1:L:164:GLU:HG3	2.05	0.56
1:N:242:LYS:C	1:N:244:GLY:H	2.07	0.56
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.88	0.56
1:B:183:LEU:HD12	1:B:184:GLN:HG3	1.86	0.56
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.88	0.56
1:E:71:ALA:O	1:E:75:LYS:HB2	2.05	0.56
1:M:272:LYS:N	1:M:272:LYS:HD2	2.19	0.56
1:L:155:ASP:OD1	1:L:157:THR:HB	2.05	0.56
1:H:68:ASN:O	1:H:72:GLN:HG2	2.04	0.56
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:HA3	1:G:181:THR:O	2.05	0.56
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:M:382:GLY:O	1:M:389:MET:HG2	2.06	0.56
1:B:155:ASP:OD1	1:B:157:THR:HB	2.05	0.56
1:J:242:LYS:C	1:J:244:GLY:H	2.09	0.56
1:E:300:VAL:HG22	6:E:2717:HOH:O	2.04	0.56
1:B:349:ILE:HA	1:B:352:GLN:CG	2.34	0.56
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.35	0.56
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.04	0.56
1:H:242:LYS:C	1:H:244:GLY:H	2.09	0.56
1:F:54:VAL:HG23	6:F:2017:HOH:O	2.06	0.56
1:E:301:ILE:HG21	1:E:309:LEU:HD23	1.88	0.56
1:E:242:LYS:C	1:E:244:GLY:H	2.08	0.56
1:E:193:MET:CE	1:E:292:ILE:HG12	2.37	0.56
1:G:252:GLU:O	1:G:253:ASP:HB2	2.06	0.56
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.35	0.56
1:I:362:ARG:O	1:I:366:GLN:HG3	2.06	0.56
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.88	0.56
1:C:183:LEU:H	1:C:383:ALA:CB	2.08	0.55
1:F:326:ASN:HD22	1:F:329:THR:HB	1.71	0.55
1:L:181:THR:O	1:M:282:GLY:HA3	2.06	0.55
1:D:114:MET:HG2	6:D:2375:HOH:O	2.06	0.55
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.88	0.55
1:M:462:PRO:HD2	6:M:2751:HOH:O	2.05	0.55
1:F:183:LEU:O	1:F:184:GLN:HB2	2.07	0.55
1:G:199:TYR:N	6:G:2628:HOH:O	2.39	0.55
1:H:205:ILE:HA	1:H:213:VAL:HG22	1.86	0.55
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.88	0.55
1:M:242:LYS:C	1:M:244:GLY:H	2.10	0.55
1:G:176:THR:HG21	1:G:322:ARG:HH12	1.72	0.55
1:K:383:ALA:HB1	1:L:281:PHE:CZ	2.39	0.55
1:M:235:PRO:CG	1:M:310:GLU:HA	2.32	0.55
1:J:326:ASN:HD22	1:J:329:THR:HB	1.71	0.55
1:H:23:LEU:CD2	1:H:74:VAL:HG13	2.37	0.55
1:H:386:GLU:O	1:H:390:LYS:HG2	2.07	0.55
1:K:242:LYS:C	1:K:244:GLY:H	2.08	0.55
1:J:183:LEU:CD1	1:J:184:GLN:HG3	2.36	0.55
1:J:235:PRO:CG	1:J:310:GLU:HA	2.32	0.55
1:J:180:GLY:HA3	1:J:381:VAL:O	2.07	0.55
1:I:266:THR:CG2	1:I:273:VAL:H	2.19	0.55
1:C:193:MET:CE	1:C:292:ILE:HG12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:ALA:O	1:I:384:ALA:HB3	2.07	0.55
1:N:266:THR:CG2	1:N:273:VAL:H	2.19	0.55
1:J:362:ARG:O	1:J:366:GLN:HG3	2.06	0.55
1:I:155:ASP:OD1	1:I:157:THR:HB	2.06	0.55
1:K:155:ASP:OD1	1:K:157:THR:HB	2.06	0.55
1:A:183:LEU:HD12	1:A:184:GLN:HG3	1.89	0.55
1:D:218:PRO:CB	1:D:246:PRO:HG2	2.33	0.55
1:D:60:ILE:O	1:D:75:LYS:HE3	2.07	0.55
1:L:200:LEU:O	1:L:201:SER:HB3	2.07	0.55
1:G:200:LEU:O	1:G:201:SER:HB3	2.07	0.55
1:A:174:VAL:HG22	1:A:194:GLN:HE21	1.70	0.55
1:L:73:MET:O	1:L:76:GLU:HB2	2.07	0.55
1:K:272:LYS:NZ	1:L:229:ASN:HD21	2.04	0.55
1:I:193:MET:CE	1:I:292:ILE:HG12	2.36	0.55
1:A:206:ASN:HD21	1:A:214:GLU:H	1.54	0.55
1:G:310:GLU:OE1	1:G:310:GLU:N	2.40	0.55
1:E:453:GLN:NE2	2:E:4005:SO4:O1	2.40	0.55
1:K:386:GLU:O	1:K:390:LYS:HG2	2.07	0.55
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.55
1:B:183:LEU:O	1:B:184:GLN:HB2	2.06	0.55
1:M:180:GLY:HA3	1:M:381:VAL:O	2.07	0.55
1:E:326:ASN:HD22	1:E:329:THR:HB	1.72	0.55
1:E:160:LYS:O	1:E:164:GLU:HG3	2.07	0.55
1:G:183:LEU:CD1	1:G:184:GLN:HG3	2.37	0.55
1:N:60:ILE:O	1:N:75:LYS:HE3	2.07	0.55
1:C:178:GLU:OE2	1:C:322:ARG:HD3	2.07	0.55
1:D:54:VAL:HG23	6:D:1693:HOH:O	2.07	0.55
1:C:218:PRO:CB	1:C:246:PRO:HG2	2.35	0.55
1:A:331:THR:HG22	6:A:2839:HOH:O	2.06	0.55
1:K:362:ARG:O	1:K:366:GLN:HG3	2.07	0.55
1:B:362:ARG:O	1:B:366:GLN:HG3	2.07	0.55
1:G:386:GLU:O	1:G:390:LYS:HG2	2.07	0.55
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.89	0.55
1:B:384:ALA:O	1:B:385:THR:HG23	2.08	0.54
1:F:183:LEU:HD12	1:F:184:GLN:HG3	1.89	0.54
1:J:200:LEU:O	1:J:201:SER:HB3	2.05	0.54
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.06	0.54
1:G:418:ALA:N	6:G:2394:HOH:O	2.38	0.54
1:D:114:MET:HB3	6:D:2178:HOH:O	2.05	0.54
1:A:160:LYS:O	1:A:164:GLU:HG3	2.08	0.54
1:A:386:GLU:O	1:A:390:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.31	0.54
1:N:382:GLY:O	1:N:389:MET:HG2	2.07	0.54
1:J:176:THR:HG21	1:J:322:ARG:HH12	1.71	0.54
1:B:386:GLU:O	1:B:390:LYS:HG2	2.07	0.54
1:C:260:ALA:O	1:C:264:VAL:HG23	2.07	0.54
1:C:183:LEU:CD1	1:C:184:GLN:HG3	2.38	0.54
1:B:218:PRO:CB	1:B:246:PRO:HG2	2.29	0.54
1:I:305:ILE:HB	1:I:307:MET:HE2	1.89	0.54
1:H:160:LYS:O	1:H:164:GLU:HG3	2.06	0.54
1:K:383:ALA:O	1:K:384:ALA:HB3	2.08	0.54
1:B:235:PRO:CG	1:B:310:GLU:HA	2.30	0.54
1:G:362:ARG:O	1:G:366:GLN:HG3	2.07	0.54
1:J:183:LEU:O	1:J:184:GLN:HB2	2.08	0.54
1:N:218:PRO:CB	1:N:246:PRO:HG2	2.34	0.54
1:H:200:LEU:O	1:H:201:SER:HB3	2.07	0.54
1:G:236:VAL:O	1:G:240:VAL:HG23	2.07	0.54
1:E:489:ILE:HD13	1:E:494:LEU:CD2	2.38	0.54
1:H:16:MET:O	1:H:20:VAL:HG13	2.07	0.54
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.90	0.54
1:H:193:MET:CE	1:H:292:ILE:HG12	2.38	0.54
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.07	0.54
1:H:305:ILE:O	1:H:305:ILE:HG22	2.08	0.54
1:J:259:LEU:O	1:J:263:VAL:HG23	2.08	0.54
1:I:16:MET:O	1:I:20:VAL:HG13	2.08	0.54
1:M:183:LEU:HD12	1:M:184:GLN:HG3	1.90	0.54
1:C:382:GLY:O	1:C:389:MET:HG2	2.08	0.54
1:E:382:GLY:O	1:E:389:MET:HG2	2.08	0.54
1:J:305:ILE:O	1:J:305:ILE:HG22	2.08	0.54
1:F:160:LYS:NZ	1:F:160:LYS:HB2	2.23	0.54
1:B:206:ASN:HD21	1:B:214:GLU:H	1.56	0.54
1:F:242:LYS:C	1:F:244:GLY:H	2.10	0.54
1:D:85:ALA:HB1	6:D:2188:HOH:O	2.07	0.54
1:H:176:THR:HG22	1:H:177:VAL:N	2.22	0.54
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.88	0.54
1:I:183:LEU:CD1	1:I:184:GLN:HG3	2.38	0.54
1:M:183:LEU:O	1:M:184:GLN:HB2	2.08	0.54
1:J:236:VAL:O	1:J:240:VAL:HG23	2.08	0.54
1:G:266:THR:CG2	1:G:273:VAL:H	2.21	0.54
1:B:383:ALA:O	1:B:384:ALA:HB3	2.08	0.53
1:B:85:ALA:O	1:B:401:HIS:HE1	1.90	0.53
1:H:382:GLY:O	1:H:389:MET:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:ILE:HG22	1:F:305:ILE:O	2.07	0.53
1:H:160:LYS:HB2	1:H:160:LYS:NZ	2.23	0.53
1:L:16:MET:O	1:L:20:VAL:HG13	2.08	0.53
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.90	0.53
1:B:242:LYS:C	1:B:244:GLY:H	2.11	0.53
1:I:90:THR:O	1:I:94:VAL:HG13	2.08	0.53
1:A:281:PHE:CZ	1:G:383:ALA:CB	2.89	0.53
1:G:218:PRO:CB	1:G:246:PRO:HG2	2.32	0.53
1:F:176:THR:HG22	1:F:177:VAL:N	2.23	0.53
1:H:73:MET:O	1:H:76:GLU:HB2	2.09	0.53
1:J:193:MET:CE	1:J:292:ILE:HG12	2.38	0.53
1:J:90:THR:O	1:J:94:VAL:HG13	2.09	0.53
1:D:16:MET:O	1:D:20:VAL:HG13	2.08	0.53
1:K:183:LEU:CD1	1:K:184:GLN:HG3	2.38	0.53
1:H:183:LEU:HD12	1:H:184:GLN:HG3	1.91	0.53
1:C:383:ALA:O	1:C:384:ALA:HB3	2.08	0.53
1:M:183:LEU:CD1	1:M:184:GLN:HG3	2.38	0.53
1:I:174:VAL:HG22	1:I:194:GLN:HE21	1.73	0.53
1:M:176:THR:HG22	1:M:177:VAL:N	2.24	0.53
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.88	0.53
1:A:305:ILE:HG22	1:A:305:ILE:O	2.08	0.53
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.88	0.53
1:H:319:GLN:O	1:H:336:VAL:HG23	2.08	0.53
1:K:319:GLN:O	1:K:336:VAL:HG23	2.08	0.53
1:A:229:ASN:ND2	1:G:244:GLY:CA	2.71	0.53
1:G:349:ILE:HA	1:G:352:GLN:CG	2.37	0.53
1:H:129:GLU:HG2	6:H:1634:HOH:O	2.09	0.53
1:A:301:ILE:HG21	1:A:309:LEU:HD23	1.90	0.53
1:I:242:LYS:C	1:I:244:GLY:H	2.11	0.53
1:G:206:ASN:HD21	1:G:214:GLU:H	1.56	0.53
1:J:310:GLU:N	1:J:310:GLU:OE1	2.41	0.53
1:G:155:ASP:OD1	1:G:157:THR:HB	2.08	0.53
1:M:219:PHE:O	1:M:247:LEU:HD12	2.09	0.53
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.90	0.53
1:B:219:PHE:O	1:B:247:LEU:HD12	2.08	0.53
1:A:202:PRO:O	1:A:203:TYR:HB2	2.08	0.53
1:M:301:ILE:HG21	1:M:309:LEU:HD23	1.90	0.53
1:I:90:THR:OG1	5:I:1:AGS:S1G	2.65	0.53
1:B:183:LEU:CD1	1:B:184:GLN:HG3	2.38	0.53
1:M:183:LEU:H	1:M:383:ALA:CB	2.10	0.53
1:C:235:PRO:CG	1:C:310:GLU:HA	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:O	1:A:253:ASP:HB2	2.09	0.53
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.74	0.53
1:N:326:ASN:HD22	1:N:329:THR:HB	1.74	0.53
1:E:362:ARG:O	1:E:366:GLN:HG3	2.09	0.53
1:M:155:ASP:OD1	1:M:157:THR:HB	2.08	0.53
1:N:23:LEU:CD2	1:N:74:VAL:HG13	2.38	0.53
1:L:319:GLN:O	1:L:336:VAL:HG23	2.09	0.53
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.90	0.53
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.89	0.53
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.91	0.53
1:B:239:ALA:O	1:B:314:LEU:HD11	2.09	0.53
1:E:386:GLU:O	1:E:390:LYS:HG2	2.09	0.53
1:B:319:GLN:O	1:B:336:VAL:HG23	2.08	0.53
1:C:236:VAL:O	1:C:240:VAL:HG23	2.09	0.53
1:D:383:ALA:O	1:D:384:ALA:HB3	2.09	0.53
1:L:183:LEU:CD1	1:L:184:GLN:HG3	2.39	0.53
1:G:325:ILE:HG22	1:G:330:THR:HA	1.91	0.53
1:G:183:LEU:HD12	1:G:184:GLN:HG3	1.90	0.53
1:C:176:THR:HG22	1:C:177:VAL:N	2.23	0.53
1:K:16:MET:O	1:K:20:VAL:HG13	2.09	0.53
1:J:155:ASP:OD1	1:J:157:THR:HB	2.09	0.53
1:K:239:ALA:O	1:K:314:LEU:HD11	2.08	0.53
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.74	0.53
1:F:183:LEU:CD1	1:F:184:GLN:HG3	2.39	0.53
1:B:310:GLU:OE1	1:B:310:GLU:N	2.42	0.53
1:H:266:THR:CG2	1:H:273:VAL:H	2.22	0.53
1:G:193:MET:CE	1:G:292:ILE:HG12	2.39	0.53
1:C:386:GLU:O	1:C:390:LYS:HG2	2.09	0.53
1:F:155:ASP:OD1	1:F:157:THR:HB	2.08	0.53
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.39	0.53
1:G:16:MET:O	1:G:20:VAL:HG13	2.09	0.53
1:E:383:ALA:O	1:E:384:ALA:HB3	2.09	0.52
1:M:383:ALA:O	1:M:384:ALA:HB3	2.09	0.52
1:I:382:GLY:O	1:I:389:MET:HG2	2.08	0.52
1:E:180:GLY:HA3	1:E:381:VAL:O	2.09	0.52
1:K:174:VAL:HG22	1:K:194:GLN:HE21	1.72	0.52
1:K:176:THR:HG22	1:K:177:VAL:N	2.24	0.52
1:B:176:THR:HG22	1:B:177:VAL:N	2.24	0.52
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.92	0.52
1:K:193:MET:CE	1:K:292:ILE:HG12	2.40	0.52
1:G:160:LYS:O	1:G:164:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.10	0.52
1:F:272:LYS:N	1:F:272:LYS:HD2	2.24	0.52
1:H:383:ALA:O	1:H:384:ALA:HB3	2.09	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.39	0.52
1:N:219:PHE:O	1:N:247:LEU:HD12	2.08	0.52
1:K:524:LEU:O	1:K:526:LYS:N	2.41	0.52
1:G:235:PRO:CG	1:G:310:GLU:HA	2.32	0.52
1:C:305:ILE:HG22	1:C:305:ILE:O	2.09	0.52
1:A:242:LYS:C	1:A:244:GLY:H	2.12	0.52
1:K:90:THR:O	1:K:94:VAL:HG13	2.09	0.52
1:I:310:GLU:OE1	1:I:310:GLU:N	2.42	0.52
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.92	0.52
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.90	0.52
1:G:160:LYS:HB2	1:G:160:LYS:NZ	2.25	0.52
1:C:242:LYS:C	1:C:244:GLY:H	2.11	0.52
1:B:90:THR:OG1	5:B:1:AGS:S1G	2.67	0.52
1:H:183:LEU:CD1	1:H:184:GLN:HG3	2.40	0.52
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.10	0.52
1:L:193:MET:HE2	1:L:292:ILE:HG12	1.90	0.52
1:C:239:ALA:O	1:C:314:LEU:HD11	2.10	0.52
1:F:202:PRO:O	1:F:203:TYR:HB2	2.10	0.52
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.92	0.52
1:B:160:LYS:NZ	1:B:160:LYS:HB2	2.24	0.52
1:B:470:LYS:HD3	6:B:2745:HOH:O	2.10	0.52
1:H:90:THR:OG1	5:H:1:AGS:S1G	2.63	0.52
1:J:252:GLU:O	1:J:253:ASP:HB2	2.10	0.52
1:N:193:MET:CE	1:N:292:ILE:HG12	2.39	0.52
1:J:496:PRO:HB2	1:J:499:VAL:CG1	2.40	0.52
1:M:90:THR:O	1:M:94:VAL:HG13	2.10	0.52
1:E:310:GLU:OE1	1:E:310:GLU:N	2.43	0.52
1:K:180:GLY:HA3	1:K:381:VAL:O	2.10	0.52
1:K:382:GLY:O	1:K:389:MET:HG2	2.10	0.52
1:F:271:VAL:HG12	1:F:273:VAL:HG23	1.92	0.52
1:M:134:LEU:HD21	1:M:425:LYS:NZ	2.25	0.52
1:I:235:PRO:CG	1:I:310:GLU:HA	2.33	0.52
1:E:69:MET:O	1:E:73:MET:HG3	2.09	0.52
1:J:386:GLU:O	1:J:390:LYS:HG2	2.10	0.52
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.92	0.52
1:C:180:GLY:HA3	1:C:381:VAL:O	2.10	0.52
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.92	0.52
1:E:193:MET:HE2	1:E:292:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLU:O	1:E:253:ASP:HB2	2.10	0.52
1:C:160:LYS:O	1:C:164:GLU:HG3	2.10	0.52
1:E:319:GLN:O	1:E:336:VAL:HG23	2.10	0.52
1:M:284:ARG:NH1	1:M:364:LYS:NZ	2.58	0.51
1:K:235:PRO:CG	1:K:310:GLU:HA	2.35	0.51
1:M:305:ILE:O	1:M:305:ILE:HG22	2.09	0.51
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.51
1:I:305:ILE:HG22	1:I:305:ILE:O	2.10	0.51
1:G:305:ILE:O	1:G:305:ILE:HG22	2.10	0.51
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.10	0.51
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.51
1:C:160:LYS:NZ	1:C:160:LYS:HB2	2.24	0.51
1:I:68:ASN:O	1:I:72:GLN:HG2	2.10	0.51
1:E:524:LEU:O	1:E:526:LYS:N	2.43	0.51
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.92	0.51
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.92	0.51
1:F:68:ASN:O	1:F:72:GLN:HG2	2.10	0.51
1:F:382:GLY:O	1:F:389:MET:HG2	2.10	0.51
1:A:310:GLU:N	1:A:310:GLU:OE1	2.44	0.51
1:E:174:VAL:HG22	1:E:194:GLN:HE21	1.74	0.51
1:C:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:K:305:ILE:O	1:K:305:ILE:HG22	2.10	0.51
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.93	0.51
1:C:134:LEU:HD21	1:C:425:LYS:NZ	2.25	0.51
1:I:239:ALA:O	1:I:314:LEU:HD11	2.10	0.51
1:B:193:MET:CE	1:B:292:ILE:HG12	2.40	0.51
1:D:384:ALA:HA	1:E:360:TYR:OH	2.11	0.51
1:E:183:LEU:CD1	1:E:184:GLN:HG3	2.40	0.51
1:C:384:ALA:O	1:C:385:THR:HG23	2.11	0.51
1:I:219:PHE:O	1:I:247:LEU:HD12	2.09	0.51
1:J:16:MET:O	1:J:20:VAL:HG13	2.11	0.51
1:A:54:VAL:HG23	6:A:2015:HOH:O	2.10	0.51
1:F:223:ALA:O	1:F:251:ALA:HA	2.10	0.51
1:E:305:ILE:O	1:E:305:ILE:HG22	2.10	0.51
1:A:160:LYS:HB2	1:A:160:LYS:NZ	2.26	0.51
1:L:305:ILE:O	1:L:305:ILE:HG22	2.10	0.51
1:B:305:ILE:O	1:B:305:ILE:HG22	2.11	0.51
1:L:266:THR:CG2	1:L:273:VAL:H	2.24	0.51
1:I:176:THR:HG22	1:I:177:VAL:N	2.25	0.51
1:M:287:ALA:HB1	1:M:368:ARG:NH1	2.25	0.51
1:F:239:ALA:O	1:F:314:LEU:HD11	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:MET:CE	1:A:292:ILE:HG12	2.41	0.51
1:M:252:GLU:O	1:M:253:ASP:HB2	2.10	0.51
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.92	0.51
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.93	0.51
1:M:16:MET:O	1:M:20:VAL:HG13	2.11	0.51
1:I:386:GLU:O	1:I:390:LYS:HG2	2.11	0.51
1:E:183:LEU:HD12	1:E:184:GLN:HG3	1.93	0.51
1:A:200:LEU:HG	1:A:276:VAL:HA	1.93	0.51
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.92	0.51
1:E:271:VAL:HG12	1:E:273:VAL:HG23	1.93	0.51
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.51	0.51
1:N:383:ALA:O	1:N:384:ALA:HB3	2.10	0.51
1:N:266:THR:HG22	1:N:271:VAL:O	2.11	0.51
1:A:176:THR:HG22	1:A:177:VAL:N	2.25	0.51
1:G:319:GLN:O	1:G:336:VAL:HG23	2.11	0.51
1:L:260:ALA:O	1:L:264:VAL:HG23	2.11	0.51
1:F:193:MET:CE	1:F:292:ILE:HG12	2.41	0.51
1:D:155:ASP:OD1	1:D:157:THR:HB	2.11	0.51
1:K:183:LEU:O	1:K:184:GLN:HB2	2.11	0.51
1:F:310:GLU:OE1	1:F:310:GLU:N	2.44	0.51
1:D:305:ILE:O	1:D:305:ILE:HG22	2.10	0.51
1:J:202:PRO:O	1:J:203:TYR:HB2	2.11	0.51
1:K:252:GLU:O	1:K:253:ASP:HB2	2.11	0.51
1:M:310:GLU:OE1	1:M:310:GLU:N	2.44	0.50
1:A:231:ARG:NH2	1:G:241:ALA:HB1	2.26	0.50
1:G:242:LYS:C	1:G:244:GLY:N	2.64	0.50
1:B:271:VAL:HG12	1:B:273:VAL:HG23	1.93	0.50
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.93	0.50
1:H:78:ALA:HB3	6:H:2660:HOH:O	2.11	0.50
1:G:90:THR:O	1:G:94:VAL:HG13	2.11	0.50
1:N:496:PRO:HD2	6:N:2145:HOH:O	2.10	0.50
1:E:383:ALA:HB1	1:F:281:PHE:HZ	1.75	0.50
1:N:305:ILE:O	1:N:305:ILE:HG22	2.11	0.50
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.93	0.50
1:I:54:VAL:HG23	6:I:2135:HOH:O	2.11	0.50
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.93	0.50
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.92	0.50
1:C:85:ALA:O	1:C:401:HIS:HE1	1.94	0.50
1:I:234:LEU:O	1:I:238:GLU:HG3	2.12	0.50
1:L:310:GLU:OE1	1:L:310:GLU:N	2.44	0.50
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:ILE:HG21	1:H:309:LEU:HD23	1.92	0.50
1:G:441:LYS:HE2	6:G:1481:HOH:O	2.11	0.50
1:M:496:PRO:HB2	1:M:499:VAL:CG1	2.41	0.50
1:J:271:VAL:HG12	1:J:273:VAL:HG23	1.92	0.50
1:E:413:ALA:CB	1:E:417:VAL:HG22	2.41	0.50
1:F:266:THR:CG2	1:F:273:VAL:H	2.25	0.50
1:N:319:GLN:O	1:N:336:VAL:HG23	2.12	0.50
1:K:193:MET:HE2	1:K:292:ILE:HG12	1.93	0.50
1:G:326:ASN:HD22	1:G:329:THR:HB	1.75	0.50
1:N:202:PRO:O	1:N:203:TYR:HB2	2.11	0.50
1:K:223:ALA:O	1:K:251:ALA:HA	2.12	0.50
1:D:183:LEU:CD1	1:D:184:GLN:HG3	2.40	0.50
1:L:183:LEU:HD12	1:L:184:GLN:HG3	1.93	0.50
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.94	0.50
1:K:236:VAL:O	1:K:240:VAL:HG23	2.11	0.50
1:K:266:THR:CG2	1:K:273:VAL:H	2.24	0.50
1:C:325:ILE:HG22	1:C:330:THR:HA	1.92	0.50
1:N:514:MET:SD	6:N:2800:HOH:O	2.60	0.50
1:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.50
1:L:174:VAL:HG22	1:L:194:GLN:HE21	1.75	0.50
1:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.50
1:I:206:ASN:OD1	1:I:207:LYS:HG3	2.11	0.50
1:D:260:ALA:O	1:D:264:VAL:HG23	2.11	0.50
1:L:23:LEU:HD22	1:L:74:VAL:HG13	1.93	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.12	0.50
1:D:381:VAL:O	1:D:382:GLY:O	2.30	0.50
1:H:252:GLU:O	1:H:253:ASP:HB2	2.12	0.50
1:F:301:ILE:HG21	1:F:309:LEU:HD23	1.93	0.50
1:M:209:GLU:OE1	1:M:209:GLU:N	2.44	0.50
1:K:310:GLU:OE1	1:K:310:GLU:N	2.44	0.50
1:N:310:GLU:OE1	1:N:310:GLU:N	2.45	0.50
1:L:180:GLY:HA3	1:L:381:VAL:O	2.11	0.50
1:K:271:VAL:HG12	1:K:273:VAL:HG23	1.93	0.50
1:M:266:THR:CG2	1:M:273:VAL:H	2.25	0.50
1:D:271:VAL:HG12	1:D:273:VAL:HG23	1.92	0.50
1:I:202:PRO:O	1:I:203:TYR:HB2	2.11	0.50
1:I:223:ALA:O	1:I:251:ALA:HA	2.12	0.50
1:G:383:ALA:O	1:G:384:ALA:HB3	2.12	0.50
1:J:266:THR:CG2	1:J:273:VAL:H	2.25	0.50
1:F:236:VAL:O	1:F:240:VAL:HG23	2.12	0.50
1:M:272:LYS:NZ	1:N:228:SER:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.94	0.49
1:M:413:ALA:HB3	1:M:417:VAL:HG22	1.94	0.49
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.75	0.49
1:A:287:ALA:HB1	1:A:368:ARG:NH1	2.26	0.49
1:G:23:LEU:CD2	1:G:74:VAL:HG13	2.42	0.49
1:L:301:ILE:HG21	1:L:309:LEU:HD23	1.94	0.49
1:E:239:ALA:O	1:E:314:LEU:HD11	2.12	0.49
1:B:183:LEU:HD13	1:B:184:GLN:N	2.26	0.49
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.94	0.49
1:C:219:PHE:O	1:C:247:LEU:HD12	2.11	0.49
1:D:371:LYS:HG2	6:D:1228:HOH:O	2.11	0.49
1:I:160:LYS:HB2	1:I:160:LYS:NZ	2.27	0.49
1:M:236:VAL:O	1:M:240:VAL:HG23	2.12	0.49
1:A:319:GLN:O	1:A:336:VAL:HG23	2.12	0.49
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.94	0.49
1:N:348:GLN:O	1:N:352:GLN:HG2	2.13	0.49
1:L:252:GLU:O	1:L:253:ASP:HB2	2.11	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.92	0.49
1:D:78:ALA:HB1	1:D:89:THR:HB	1.94	0.49
1:F:174:VAL:HG22	1:F:194:GLN:HE21	1.77	0.49
1:H:325:ILE:HG22	1:H:330:THR:HA	1.95	0.49
1:E:236:VAL:O	1:E:240:VAL:HG23	2.12	0.49
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.93	0.49
1:G:202:PRO:O	1:G:203:TYR:HB2	2.12	0.49
1:H:176:THR:HG21	1:H:322:ARG:HH12	1.76	0.49
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.94	0.49
1:E:266:THR:CG2	1:E:273:VAL:H	2.25	0.49
1:F:23:LEU:HD22	1:F:74:VAL:HG13	1.94	0.49
1:E:90:THR:OG1	5:E:1:AGS:S1G	2.66	0.49
1:H:310:GLU:N	1:H:310:GLU:OE1	2.45	0.49
1:A:229:ASN:ND2	1:G:244:GLY:HA3	2.28	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.11	0.49
1:H:413:ALA:HB3	1:H:417:VAL:HG22	1.93	0.49
1:C:68:ASN:O	1:C:72:GLN:HG2	2.12	0.49
1:L:287:ALA:HB1	1:L:368:ARG:NH1	2.27	0.49
1:M:386:GLU:O	1:M:390:LYS:HG2	2.12	0.49
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.94	0.49
1:L:202:PRO:O	1:L:203:TYR:HB2	2.12	0.49
1:E:171:LYS:HB2	1:E:407:VAL:HG11	1.93	0.49
1:D:202:PRO:O	1:D:203:TYR:HB2	2.12	0.49
1:A:266:THR:CG2	1:A:273:VAL:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PRO:O	1:B:203:TYR:HB2	2.12	0.49
1:L:223:ALA:O	1:L:251:ALA:HA	2.12	0.49
1:K:69:MET:O	1:K:73:MET:HG3	2.12	0.49
1:B:326:ASN:HD22	1:B:329:THR:HB	1.76	0.49
1:L:524:LEU:O	1:L:526:LYS:N	2.45	0.49
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.95	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.13	0.49
1:N:218:PRO:HD2	1:N:320:ALA:O	2.13	0.49
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.42	0.49
1:J:382:GLY:O	1:J:389:MET:HG2	2.13	0.49
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.27	0.49
1:B:223:ALA:O	1:B:251:ALA:HA	2.13	0.49
1:B:525:PRO:HD3	6:B:1427:HOH:O	2.13	0.49
1:C:319:GLN:O	1:C:336:VAL:HG23	2.13	0.49
1:I:252:GLU:O	1:I:253:ASP:HB2	2.12	0.49
6:C:2466:HOH:O	1:D:518:GLU:HG2	2.12	0.49
1:B:5:ASP:HB2	1:B:524:LEU:HD12	1.95	0.49
1:N:234:LEU:O	1:N:238:GLU:HG3	2.13	0.49
1:A:60:ILE:O	1:A:75:LYS:HE3	2.13	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.95	0.49
1:A:271:VAL:HG12	1:A:273:VAL:HG23	1.94	0.49
1:E:287:ALA:HB1	1:E:368:ARG:NH1	2.27	0.49
1:J:63:GLU:OE2	1:K:526:LYS:HE2	2.12	0.49
1:C:63:GLU:OE2	1:D:526:LYS:HE2	2.13	0.49
1:H:202:PRO:O	1:H:203:TYR:HB2	2.11	0.49
1:F:235:PRO:CG	1:F:310:GLU:HA	2.31	0.48
1:D:310:GLU:OE1	1:D:310:GLU:N	2.46	0.48
1:E:206:ASN:OD1	1:E:207:LYS:HG3	2.13	0.48
1:I:266:THR:HG22	1:I:271:VAL:O	2.13	0.48
1:I:319:GLN:O	1:I:336:VAL:HG23	2.13	0.48
1:M:223:ALA:O	1:M:251:ALA:HA	2.13	0.48
1:K:202:PRO:O	1:K:203:TYR:HB2	2.12	0.48
1:H:384:ALA:O	1:H:385:THR:HG23	2.13	0.48
1:G:259:LEU:O	1:G:263:VAL:HG23	2.13	0.48
1:D:259:LEU:O	1:D:263:VAL:HG23	2.13	0.48
1:D:325:ILE:HG22	1:D:330:THR:HA	1.94	0.48
1:L:326:ASN:HD22	1:L:329:THR:HB	1.77	0.48
1:N:413:ALA:HB3	1:N:417:VAL:HG22	1.94	0.48
1:L:69:MET:O	1:L:73:MET:HG3	2.13	0.48
1:B:179:ASP:HB3	1:B:389:MET:CE	2.44	0.48
1:L:23:LEU:CD2	1:L:74:VAL:HG13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.95	0.48
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.78	0.48
1:E:202:PRO:O	1:E:203:TYR:HB2	2.13	0.48
1:M:202:PRO:O	1:M:203:TYR:HB2	2.13	0.48
1:G:69:MET:O	1:G:73:MET:HG3	2.13	0.48
1:C:183:LEU:O	1:C:184:GLN:HB2	2.14	0.48
1:H:234:LEU:O	1:H:238:GLU:HG3	2.13	0.48
1:F:73:MET:O	1:F:76:GLU:HB2	2.13	0.48
1:J:496:PRO:O	1:J:499:VAL:HG13	2.12	0.48
1:F:319:GLN:O	1:F:336:VAL:HG23	2.12	0.48
1:E:404:ARG:NH1	6:E:2208:HOH:O	2.45	0.48
1:B:77:VAL:HG11	1:B:510:VAL:CG2	2.43	0.48
1:L:384:ALA:O	1:L:385:THR:HG23	2.14	0.48
1:M:281:PHE:H	1:M:284:ARG:HD2	1.76	0.48
1:A:234:LEU:O	1:A:238:GLU:HG3	2.13	0.48
1:C:310:GLU:N	1:C:310:GLU:OE1	2.46	0.48
1:B:252:GLU:O	1:B:253:ASP:HB2	2.13	0.48
1:L:176:THR:HG22	1:L:177:VAL:N	2.28	0.48
1:J:206:ASN:OD1	1:J:207:LYS:HG3	2.13	0.48
1:J:496:PRO:HB2	1:J:499:VAL:HG12	1.94	0.48
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.78	0.48
6:E:1217:HOH:O	1:F:518:GLU:HG2	2.12	0.48
1:A:239:ALA:O	1:A:314:LEU:HD11	2.13	0.48
1:I:73:MET:O	1:I:76:GLU:HB2	2.13	0.48
1:G:425:LYS:NZ	6:G:2070:HOH:O	2.45	0.48
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.95	0.48
1:B:153:ASN:O	1:B:154:SER:HB2	2.14	0.48
1:K:160:LYS:O	1:K:164:GLU:HG3	2.12	0.48
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.96	0.48
1:C:524:LEU:O	1:C:526:LYS:N	2.45	0.48
1:M:193:MET:CE	1:M:292:ILE:HG12	2.43	0.48
1:E:235:PRO:CG	1:E:310:GLU:HA	2.32	0.48
1:M:200:LEU:HG	1:M:276:VAL:HA	1.95	0.48
1:M:266:THR:HG22	1:M:271:VAL:O	2.14	0.48
1:B:236:VAL:O	1:B:240:VAL:HG23	2.12	0.48
1:A:266:THR:HG22	1:A:271:VAL:O	2.13	0.48
1:N:499:VAL:HG11	6:N:2145:HOH:O	2.13	0.48
1:H:223:ALA:O	1:H:251:ALA:HA	2.12	0.48
1:D:384:ALA:O	1:D:385:THR:HG23	2.14	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.48
1:L:174:VAL:HG22	1:L:194:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:413:ALA:HB3	1:J:417:VAL:HG22	1.95	0.48
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.95	0.48
1:D:63:GLU:OE2	1:E:526:LYS:HE2	2.13	0.48
1:A:260:ALA:O	1:A:264:VAL:HG23	2.13	0.48
1:I:524:LEU:O	1:I:526:LYS:N	2.46	0.48
1:N:222:LEU:HB3	1:N:289:LEU:CD2	2.43	0.48
1:E:153:ASN:O	1:E:154:SER:HB2	2.13	0.48
1:B:200:LEU:HG	1:B:276:VAL:HA	1.96	0.48
1:L:219:PHE:O	1:L:247:LEU:HD12	2.13	0.48
1:A:46:ALA:HB2	1:B:76:GLU:HG2	1.93	0.48
1:A:176:THR:HG21	1:A:322:ARG:HH12	1.79	0.48
1:G:266:THR:HG22	1:G:271:VAL:O	2.14	0.48
1:A:206:ASN:OD1	1:A:207:LYS:HG3	2.13	0.48
1:G:362:ARG:HD2	6:G:1728:HOH:O	2.13	0.48
1:L:291:ASP:OD2	1:L:368:ARG:HD2	2.14	0.48
1:L:441:LYS:HE2	6:L:2814:HOH:O	2.13	0.48
1:N:16:MET:O	1:N:20:VAL:HG13	2.13	0.48
1:K:384:ALA:O	1:K:385:THR:HG23	2.14	0.48
1:M:174:VAL:HG22	1:M:194:GLN:HE21	1.77	0.48
1:N:325:ILE:HG22	1:N:330:THR:HA	1.96	0.48
1:E:353:ILE:HD13	1:E:366:GLN:HG2	1.96	0.48
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.44	0.48
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.95	0.48
1:J:319:GLN:O	1:J:336:VAL:HG23	2.14	0.48
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.95	0.48
1:L:209:GLU:OE1	1:L:209:GLU:N	2.47	0.48
1:F:180:GLY:HA3	1:F:381:VAL:O	2.13	0.48
1:F:252:GLU:O	1:F:253:ASP:HB2	2.14	0.48
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	0.48
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.93	0.48
1:H:219:PHE:O	1:H:247:LEU:HD12	2.13	0.48
1:E:259:LEU:O	1:E:263:VAL:HG23	2.14	0.48
1:K:325:ILE:HG22	1:K:330:THR:HA	1.96	0.48
1:B:185:ASP:OD1	1:B:382:GLY:N	2.47	0.48
1:D:113:PRO:HD2	6:D:2375:HOH:O	2.14	0.48
1:D:524:LEU:O	1:D:526:LYS:N	2.46	0.48
1:N:386:GLU:O	1:N:390:LYS:HG2	2.14	0.48
1:N:223:ALA:O	1:N:251:ALA:HA	2.14	0.48
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.49	0.48
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.96	0.48
1:H:266:THR:HG22	1:H:271:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:413:ALA:HB3	1:I:417:VAL:HG22	1.94	0.48
1:G:73:MET:O	1:G:76:GLU:HB2	2.13	0.48
1:F:222:LEU:HB3	1:F:289:LEU:CD2	2.44	0.48
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.48
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:D:85:ALA:O	1:D:401:HIS:HE1	1.95	0.47
1:A:223:ALA:O	1:A:251:ALA:HA	2.14	0.47
1:G:239:ALA:O	1:G:314:LEU:HD11	2.14	0.47
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.96	0.47
1:B:171:LYS:HB2	1:B:407:VAL:HG11	1.96	0.47
1:G:348:GLN:O	1:G:352:GLN:HG2	2.14	0.47
1:A:413:ALA:HB3	1:A:417:VAL:HG22	1.95	0.47
1:K:259:LEU:O	1:K:263:VAL:HG23	2.14	0.47
1:L:177:VAL:HG21	1:L:397:GLU:HG2	1.94	0.47
1:H:206:ASN:ND2	1:H:214:GLU:H	2.12	0.47
1:J:353:ILE:HD13	1:J:366:GLN:HG2	1.96	0.47
1:A:193:MET:HE2	1:A:292:ILE:HG12	1.96	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.95	0.47
1:B:260:ALA:O	1:B:264:VAL:HG23	2.15	0.47
1:C:259:LEU:O	1:C:263:VAL:HG23	2.14	0.47
1:D:23:LEU:CD2	1:D:74:VAL:HG13	2.44	0.47
1:I:236:VAL:O	1:I:240:VAL:HG23	2.14	0.47
1:I:271:VAL:HG12	1:I:273:VAL:HG23	1.95	0.47
1:J:325:ILE:HG22	1:J:330:THR:HA	1.97	0.47
1:M:366:GLN:O	1:M:369:VAL:HG22	2.15	0.47
1:K:206:ASN:OD1	1:K:207:LYS:HG3	2.13	0.47
1:K:287:ALA:HB1	1:K:368:ARG:NH1	2.28	0.47
1:K:37:ASN:HD21	1:K:51:LYS:HE3	1.80	0.47
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.96	0.47
1:K:234:LEU:O	1:K:238:GLU:HG3	2.13	0.47
1:G:234:LEU:N	1:G:235:PRO:HD2	2.29	0.47
1:K:219:PHE:O	1:K:247:LEU:HD12	2.13	0.47
1:B:266:THR:CG2	1:B:273:VAL:H	2.27	0.47
1:J:287:ALA:HB1	1:J:368:ARG:NH1	2.29	0.47
1:L:206:ASN:OD1	1:L:207:LYS:HG3	2.15	0.47
1:I:287:ALA:HB1	1:I:368:ARG:NH1	2.29	0.47
1:F:524:LEU:O	1:F:526:LYS:N	2.46	0.47
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.50	0.47
1:I:10:ASN:ND2	6:I:2045:HOH:O	2.47	0.47
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.97	0.47
1:H:209:GLU:OE1	1:H:209:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:GLU:OE1	1:G:209:GLU:N	2.44	0.47
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	0.47
1:A:231:ARG:NH1	1:G:242:LYS:HG2	2.28	0.47
1:D:217:SER:N	1:D:218:PRO:CD	2.78	0.47
1:H:271:VAL:HG12	1:H:273:VAL:HG23	1.96	0.47
1:L:78:ALA:HB1	1:L:89:THR:HB	1.97	0.47
1:N:160:LYS:HB2	1:N:160:LYS:NZ	2.29	0.47
1:B:206:ASN:OD1	1:B:207:LYS:HG3	2.13	0.47
1:H:239:ALA:O	1:H:314:LEU:HD11	2.15	0.47
1:M:524:LEU:O	1:M:526:LYS:N	2.46	0.47
1:A:209:GLU:OE1	1:A:209:GLU:N	2.44	0.47
1:B:383:ALA:HB1	1:C:281:PHE:CE2	2.49	0.47
1:L:234:LEU:O	1:L:238:GLU:HG3	2.15	0.47
1:N:236:VAL:O	1:N:240:VAL:HG23	2.14	0.47
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.96	0.47
1:D:89:THR:HG23	6:D:2757:HOH:O	2.13	0.47
1:A:305:ILE:HB	1:A:307:MET:HE2	1.95	0.47
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.95	0.47
1:C:301:ILE:HG21	1:C:309:LEU:HD23	1.95	0.47
1:D:12:ALA:N	6:D:2704:HOH:O	2.47	0.47
1:N:183:LEU:HD13	1:N:184:GLN:N	2.29	0.47
1:A:183:LEU:CD2	1:A:384:ALA:HB2	2.44	0.47
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.47
1:L:234:LEU:N	1:L:235:PRO:HD2	2.30	0.47
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.95	0.47
1:J:266:THR:HG22	1:J:271:VAL:O	2.15	0.47
1:I:206:ASN:ND2	1:I:214:GLU:H	2.12	0.47
1:J:176:THR:HG22	1:J:177:VAL:N	2.29	0.47
1:G:302:SER:H	1:G:307:MET:CE	2.28	0.47
1:H:206:ASN:OD1	1:H:207:LYS:HG3	2.15	0.47
1:M:206:ASN:OD1	1:M:207:LYS:HG3	2.14	0.47
1:I:272:LYS:NZ	1:J:229:ASN:OD1	2.47	0.47
1:J:369:VAL:HG23	1:J:370:ALA:N	2.30	0.47
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.96	0.47
1:L:366:GLN:HA	1:L:369:VAL:HG22	1.95	0.47
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.50	0.47
1:M:260:ALA:O	1:M:264:VAL:HG23	2.15	0.47
1:D:252:GLU:O	1:D:253:ASP:HB2	2.15	0.47
1:K:183:LEU:CD2	1:K:384:ALA:HB2	2.43	0.47
1:H:185:ASP:OD1	1:H:382:GLY:N	2.46	0.47
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:GLY:O	1:D:389:MET:HG2	2.15	0.47
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.96	0.47
1:F:206:ASN:OD1	1:F:207:LYS:HG3	2.14	0.47
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.97	0.47
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.97	0.47
1:A:134:LEU:HD21	1:A:425:LYS:NZ	2.30	0.47
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.50	0.47
1:J:525:PRO:HD3	6:J:2970:HOH:O	2.14	0.47
1:E:90:THR:O	1:E:94:VAL:HG13	2.14	0.47
1:C:183:LEU:HD13	1:C:184:GLN:N	2.30	0.47
1:L:325:ILE:HG22	1:L:330:THR:HA	1.97	0.47
1:M:160:LYS:NZ	1:M:160:LYS:HB2	2.29	0.47
1:K:160:LYS:HB2	1:K:160:LYS:NZ	2.30	0.47
1:E:260:ALA:O	1:E:264:VAL:HG23	2.15	0.47
1:L:236:VAL:O	1:L:240:VAL:HG23	2.15	0.47
1:J:111:MET:HG2	1:J:435:ASP:OD1	2.15	0.47
1:C:252:GLU:O	1:C:253:ASP:HB2	2.14	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:M:90:THR:OG1	5:M:1:AGS:S1G	2.63	0.47
1:J:234:LEU:O	1:J:238:GLU:HG3	2.13	0.47
1:C:23:LEU:CD2	1:C:74:VAL:HG13	2.45	0.47
1:D:302:SER:H	1:D:307:MET:HE1	1.80	0.47
1:L:271:VAL:HG12	1:L:273:VAL:HG23	1.96	0.47
1:A:236:VAL:O	1:A:240:VAL:HG23	2.15	0.47
1:D:206:ASN:HD21	1:D:214:GLU:H	1.63	0.47
1:M:269:GLY:O	1:N:229:ASN:OD1	2.33	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:F:384:ALA:O	1:F:385:THR:HG23	2.14	0.46
1:F:234:LEU:O	1:F:238:GLU:HG3	2.14	0.46
1:D:238:GLU:O	1:D:241:ALA:HB3	2.15	0.46
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.96	0.46
1:A:73:MET:O	1:A:76:GLU:HB2	2.15	0.46
1:L:242:LYS:C	1:L:244:GLY:N	2.69	0.46
1:H:199:TYR:CZ	1:H:327:LYS:HA	2.51	0.46
1:I:140:ASP:OD2	1:I:142:LYS:HB3	2.16	0.46
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.97	0.46
1:G:384:ALA:O	1:G:385:THR:HG23	2.15	0.46
1:C:60:ILE:O	1:C:75:LYS:HE3	2.15	0.46
1:I:325:ILE:HG22	1:I:330:THR:HA	1.98	0.46
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.98	0.46
1:A:169:VAL:HG13	1:A:377:ALA:HB2	1.97	0.46
1:N:155:ASP:OD1	1:N:157:THR:HB	2.14	0.46
1:I:260:ALA:O	1:I:264:VAL:HG23	2.14	0.46
1:M:63:GLU:OE2	1:N:526:LYS:HE2	2.15	0.46
5:G:1:AGS:O2G	5:G:1:AGS:S1G	2.53	0.46
1:C:234:LEU:N	1:C:235:PRO:HD2	2.30	0.46
1:G:78:ALA:HB1	1:G:89:THR:HB	1.96	0.46
1:M:239:ALA:O	1:M:314:LEU:HD11	2.15	0.46
1:M:323:VAL:HG12	1:M:332:ILE:HA	1.98	0.46
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.50	0.46
1:I:463:SER:HB2	6:I:2586:HOH:O	2.14	0.46
1:E:451:LEU:HD23	1:E:451:LEU:C	2.35	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.46
1:F:381:VAL:O	1:F:382:GLY:O	2.33	0.46
1:K:183:LEU:HD13	1:K:184:GLN:N	2.30	0.46
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.46
1:B:325:ILE:HG22	1:B:330:THR:HA	1.96	0.46
1:G:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:F:353:ILE:HD13	1:F:366:GLN:HG2	1.98	0.46
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.46
1:N:122:LYS:HE2	1:N:429:LEU:HD11	1.97	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.98	0.46
1:B:169:VAL:CG1	1:B:377:ALA:HB2	2.45	0.46
1:D:209:GLU:N	1:D:209:GLU:OE1	2.45	0.46
1:M:234:LEU:N	1:M:235:PRO:HD2	2.30	0.46
1:H:234:LEU:N	1:H:235:PRO:HD2	2.30	0.46
1:I:381:VAL:O	1:I:382:GLY:O	2.34	0.46
1:K:60:ILE:O	1:K:75:LYS:HE3	2.16	0.46
1:K:325:ILE:HA	1:K:329:THR:O	2.15	0.46
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.96	0.46
1:L:455:VAL:O	1:L:458:CYS:HB2	2.14	0.46
1:A:90:THR:O	1:A:94:VAL:HG13	2.14	0.46
1:K:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.46
1:F:383:ALA:O	1:F:384:ALA:CB	2.63	0.46
1:A:182:GLY:HA2	1:A:383:ALA:HB3	1.97	0.46
1:F:234:LEU:N	1:F:235:PRO:HD2	2.30	0.46
1:J:234:LEU:N	1:J:235:PRO:HD2	2.31	0.46
1:M:234:LEU:O	1:M:238:GLU:HG3	2.14	0.46
1:D:235:PRO:CG	1:D:310:GLU:HA	2.34	0.46
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:ILE:HG22	6:H:2938:HOH:O	2.15	0.46
1:F:200:LEU:HG	1:F:276:VAL:HA	1.98	0.46
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.96	0.46
1:E:223:ALA:O	1:E:251:ALA:HA	2.16	0.46
1:E:10:ASN:HB2	6:E:1989:HOH:O	2.14	0.46
1:C:209:GLU:OE1	1:C:209:GLU:N	2.45	0.46
1:G:60:ILE:O	1:G:75:LYS:HE3	2.16	0.46
1:J:174:VAL:HG22	1:J:194:GLN:NE2	2.31	0.46
1:D:266:THR:CG2	1:D:273:VAL:H	2.28	0.46
1:A:366:GLN:O	1:A:369:VAL:HG22	2.15	0.46
1:M:10:ASN:HA	6:M:2195:HOH:O	2.15	0.46
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.97	0.46
1:A:199:TYR:CZ	1:A:327:LYS:HA	2.51	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.16	0.46
1:I:217:SER:N	1:I:218:PRO:CD	2.79	0.46
1:H:217:SER:N	1:H:218:PRO:CD	2.79	0.46
1:C:234:LEU:O	1:C:238:GLU:HG3	2.15	0.46
1:E:217:SER:N	1:E:218:PRO:HD3	2.31	0.46
1:F:217:SER:N	1:F:218:PRO:HD3	2.31	0.46
1:N:234:LEU:N	1:N:235:PRO:HD2	2.31	0.46
1:J:219:PHE:O	1:J:247:LEU:HD12	2.15	0.46
1:M:325:ILE:HA	1:M:329:THR:O	2.16	0.46
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.30	0.46
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.96	0.46
1:A:78:ALA:HB3	6:A:2430:HOH:O	2.15	0.46
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.98	0.46
1:M:438:VAL:O	1:M:442:VAL:HG23	2.16	0.46
1:J:223:ALA:O	1:J:251:ALA:HA	2.15	0.46
1:H:183:LEU:CD2	1:H:384:ALA:HB2	2.45	0.46
1:E:234:LEU:N	1:E:235:PRO:HD2	2.31	0.46
1:B:180:GLY:HA3	1:B:381:VAL:O	2.15	0.46
1:H:353:ILE:HD13	1:H:366:GLN:HG2	1.98	0.46
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.97	0.46
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.98	0.46
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.97	0.46
1:C:290:GLN:HB3	1:C:345:ARG:NH2	2.31	0.46
1:I:301:ILE:HG21	1:I:309:LEU:HD23	1.97	0.46
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.98	0.46
1:K:78:ALA:HB1	1:K:89:THR:HB	1.98	0.46
1:L:68:ASN:O	1:L:72:GLN:HG2	2.16	0.46
1:K:234:LEU:N	1:K:235:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HG22	1:A:330:THR:HA	1.98	0.46
1:I:69:MET:O	1:I:73:MET:HG3	2.15	0.46
1:A:524:LEU:O	1:A:526:LYS:N	2.48	0.46
1:K:210:THR:HG22	1:K:210:THR:O	2.16	0.46
1:K:302:SER:H	1:K:307:MET:HE1	1.81	0.45
1:K:177:VAL:HA	1:K:379:ILE:O	2.16	0.45
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.98	0.45
1:A:353:ILE:HD13	1:A:366:GLN:HG2	1.97	0.45
1:B:404:ARG:NH1	6:B:2253:HOH:O	2.48	0.45
1:L:171:LYS:HB2	1:L:407:VAL:HG11	1.98	0.45
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.57	0.45
1:A:101:THR:HG23	6:A:2971:HOH:O	2.16	0.45
1:J:183:LEU:HD13	1:J:184:GLN:N	2.30	0.45
1:B:183:LEU:CD2	1:B:384:ALA:HB2	2.43	0.45
1:H:235:PRO:CG	1:H:310:GLU:HA	2.35	0.45
1:G:234:LEU:O	1:G:238:GLU:HG3	2.17	0.45
1:N:271:VAL:HG12	1:N:273:VAL:HG23	1.97	0.45
1:I:353:ILE:HD13	1:I:366:GLN:HG2	1.98	0.45
1:I:369:VAL:HG23	1:I:370:ALA:N	2.31	0.45
1:K:369:VAL:HG23	1:K:370:ALA:N	2.31	0.45
1:N:215:LEU:HB2	1:N:323:VAL:CG2	2.47	0.45
1:D:319:GLN:O	1:D:336:VAL:HG23	2.17	0.45
1:C:324:VAL:O	1:C:331:THR:HG22	2.16	0.45
1:J:260:ALA:O	1:J:264:VAL:HG23	2.16	0.45
1:A:182:GLY:HA2	1:A:383:ALA:CB	2.46	0.45
1:F:217:SER:N	1:F:218:PRO:CD	2.79	0.45
1:I:60:ILE:O	1:I:75:LYS:HE3	2.16	0.45
1:E:325:ILE:HG22	1:E:330:THR:HA	1.97	0.45
1:N:266:THR:HG21	1:N:273:VAL:H	1.80	0.45
1:E:206:ASN:ND2	1:E:214:GLU:H	2.11	0.45
1:M:325:ILE:HG22	1:M:330:THR:HA	1.97	0.45
1:J:325:ILE:HA	1:J:329:THR:O	2.16	0.45
1:F:160:LYS:HB2	1:F:160:LYS:HZ2	1.81	0.45
1:E:219:PHE:O	1:E:247:LEU:HD12	2.16	0.45
1:F:193:MET:HE2	1:F:292:ILE:HG12	1.99	0.45
1:J:524:LEU:O	1:J:526:LYS:N	2.49	0.45
1:C:78:ALA:HB3	6:C:1582:HOH:O	2.16	0.45
1:D:301:ILE:HG21	1:D:309:LEU:HD23	1.98	0.45
1:A:384:ALA:O	1:A:385:THR:HG23	2.16	0.45
1:I:217:SER:N	1:I:218:PRO:HD3	2.31	0.45
1:K:217:SER:N	1:K:218:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:C:413:ALA:HB3	1:C:417:VAL:HG22	1.99	0.45
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.99	0.45
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.32	0.45
1:M:169:VAL:HG13	1:M:377:ALA:HB2	1.99	0.45
1:I:134:LEU:HD21	1:I:425:LYS:NZ	2.31	0.45
1:N:10:ASN:ND2	6:N:2158:HOH:O	2.49	0.45
1:E:290:GLN:HB3	1:E:345:ARG:NH2	2.31	0.45
1:G:68:ASN:O	1:G:72:GLN:HG2	2.16	0.45
1:I:183:LEU:CD2	1:I:384:ALA:HB2	2.45	0.45
1:E:182:GLY:O	1:E:183:LEU:O	2.35	0.45
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.99	0.45
1:F:219:PHE:O	1:F:247:LEU:HD12	2.16	0.45
1:E:369:VAL:HG23	1:E:370:ALA:N	2.30	0.45
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.99	0.45
1:J:301:ILE:HG21	1:J:309:LEU:HD23	1.97	0.45
1:K:301:ILE:HG21	1:K:309:LEU:HD23	1.97	0.45
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.98	0.45
1:D:90:THR:OG1	5:D:551:AGS:S1G	2.68	0.45
1:I:183:LEU:HD13	1:I:184:GLN:N	2.31	0.45
1:M:217:SER:N	1:M:218:PRO:HD3	2.32	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.79	0.45
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.98	0.45
1:A:185:ASP:OD1	1:A:382:GLY:N	2.48	0.45
1:L:438:VAL:O	1:L:442:VAL:HG23	2.17	0.45
1:H:524:LEU:O	1:H:526:LYS:N	2.49	0.45
1:G:238:GLU:O	1:G:241:ALA:HB3	2.16	0.45
1:E:158:VAL:HG22	6:E:2648:HOH:O	2.16	0.45
1:D:87:ASP:N	6:D:2757:HOH:O	2.49	0.45
1:A:369:VAL:HG23	1:A:370:ALA:N	2.32	0.45
1:C:206:ASN:OD1	1:C:207:LYS:HG3	2.17	0.45
1:L:524:LEU:HA	1:L:524:LEU:HD12	1.87	0.45
1:A:39:VAL:HG12	1:B:69:MET:CE	2.47	0.45
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.17	0.45
1:M:222:LEU:HB3	1:M:289:LEU:CD2	2.47	0.45
1:L:222:LEU:HB3	1:L:289:LEU:CD2	2.46	0.45
1:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.45
1:N:238:GLU:O	1:N:241:ALA:HB3	2.17	0.45
1:F:325:ILE:HG22	1:F:330:THR:HA	1.98	0.45
1:N:174:VAL:HG22	1:N:194:GLN:HE21	1.82	0.45
1:F:366:GLN:O	1:F:369:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:242:LYS:C	1:H:244:GLY:N	2.70	0.45
1:N:90:THR:O	1:N:94:VAL:HG13	2.16	0.45
1:N:252:GLU:O	1:N:253:ASP:HB2	2.16	0.45
1:G:463:SER:O	1:G:467:ASN:HB2	2.17	0.45
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.47	0.45
1:E:210:THR:HG22	1:E:210:THR:O	2.17	0.45
1:K:88:GLY:HA2	5:K:1:AGS:PB	2.57	0.45
1:K:217:SER:N	1:K:218:PRO:HD3	2.31	0.45
1:B:217:SER:N	1:B:218:PRO:HD3	2.32	0.45
1:A:217:SER:N	1:A:218:PRO:CD	2.80	0.45
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.98	0.45
1:K:174:VAL:HG22	1:K:194:GLN:NE2	2.32	0.45
1:F:325:ILE:HA	1:F:329:THR:O	2.17	0.45
1:J:160:LYS:NZ	1:J:160:LYS:HB2	2.32	0.45
1:J:272:LYS:NZ	1:K:229:ASN:OD1	2.50	0.45
1:D:242:LYS:C	1:D:244:GLY:N	2.67	0.45
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.29	0.45
1:N:242:LYS:C	1:N:244:GLY:N	2.69	0.45
1:C:239:ALA:C	1:C:314:LEU:HD21	2.38	0.45
1:L:369:VAL:HG23	1:L:370:ALA:N	2.32	0.45
1:K:260:ALA:O	1:K:264:VAL:HG23	2.16	0.45
1:K:342:ILE:O	1:K:346:VAL:HG23	2.16	0.45
1:J:239:ALA:O	1:J:314:LEU:HD11	2.16	0.45
1:B:210:THR:HG22	1:B:210:THR:O	2.16	0.45
1:L:90:THR:OG1	5:L:1:AGS:S1G	2.65	0.45
1:J:183:LEU:CD2	1:J:384:ALA:HB2	2.44	0.45
1:A:217:SER:N	1:A:218:PRO:HD3	2.32	0.45
1:M:238:GLU:O	1:M:241:ALA:HB3	2.17	0.45
1:B:39:VAL:HG12	1:C:69:MET:CE	2.47	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.98	0.45
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.57	0.45
1:B:342:ILE:O	1:B:346:VAL:HG23	2.17	0.45
1:E:141:SER:HB3	6:E:2603:HOH:O	2.17	0.45
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.45
1:C:210:THR:HG22	1:C:210:THR:O	2.17	0.45
1:C:182:GLY:HA2	1:C:383:ALA:HB3	1.97	0.44
1:C:381:VAL:O	1:C:382:GLY:O	2.36	0.44
1:C:305:ILE:HB	1:C:307:MET:HE2	1.98	0.44
1:L:266:THR:HG22	1:L:271:VAL:O	2.16	0.44
1:D:73:MET:O	1:D:76:GLU:HB2	2.17	0.44
1:H:284:ARG:HH12	1:H:364:LYS:NZ	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:ASN:HD21	1:J:51:LYS:HE3	1.80	0.44
1:K:209:GLU:OE1	1:K:209:GLU:N	2.47	0.44
1:B:384:ALA:HA	1:C:360:TYR:OH	2.17	0.44
1:A:234:LEU:N	1:A:235:PRO:HD2	2.32	0.44
1:I:174:VAL:HG22	1:I:194:GLN:NE2	2.32	0.44
1:F:194:GLN:HG3	1:F:331:THR:HB	1.99	0.44
1:D:247:LEU:CD2	1:D:249:ILE:HD11	2.47	0.44
1:N:353:ILE:HD13	1:N:366:GLN:HG2	1.99	0.44
1:B:455:VAL:O	1:B:458:CYS:HB2	2.17	0.44
1:I:70:GLY:HA2	1:I:73:MET:HE3	2.00	0.44
1:N:301:ILE:HG21	1:N:309:LEU:HD23	1.99	0.44
1:I:191:GLU:O	1:I:334:ASP:HA	2.16	0.44
1:D:358:SER:HB3	1:D:361:ASP:OD1	2.16	0.44
1:B:209:GLU:OE1	1:B:209:GLU:N	2.48	0.44
1:K:182:GLY:HA2	1:K:383:ALA:HB3	1.99	0.44
1:E:381:VAL:O	1:E:382:GLY:O	2.36	0.44
1:E:325:ILE:HA	1:E:329:THR:O	2.18	0.44
1:G:302:SER:O	1:G:307:MET:HE3	2.17	0.44
1:I:366:GLN:O	1:I:369:VAL:HG22	2.16	0.44
1:N:496:PRO:HB2	1:N:499:VAL:CG1	2.47	0.44
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.00	0.44
1:I:222:LEU:HB3	1:I:289:LEU:CD2	2.47	0.44
1:D:183:LEU:HD12	1:D:184:GLN:HG3	1.99	0.44
1:J:463:SER:O	1:J:467:ASN:HB2	2.18	0.44
1:L:302:SER:H	1:L:307:MET:HE1	1.83	0.44
1:I:325:ILE:HA	1:I:329:THR:O	2.17	0.44
1:E:413:ALA:HB3	1:E:417:VAL:HG22	1.99	0.44
1:K:266:THR:HG22	1:K:271:VAL:O	2.17	0.44
1:G:305:ILE:HB	1:G:307:MET:HE2	1.98	0.44
1:C:287:ALA:HB1	1:C:368:ARG:NH1	2.32	0.44
1:H:336:VAL:O	1:H:337:GLY:C	2.56	0.44
1:H:155:ASP:OD1	1:H:157:THR:HB	2.18	0.44
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.99	0.44
1:K:222:LEU:HB3	1:K:289:LEU:CD2	2.48	0.44
1:D:288:MET:HG2	1:D:368:ARG:HD3	1.99	0.44
1:H:236:VAL:O	1:H:240:VAL:HG23	2.16	0.44
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.99	0.44
1:N:325:ILE:HG22	1:N:330:THR:HG23	1.99	0.44
1:B:524:LEU:C	1:B:526:LYS:H	2.20	0.44
1:J:460:GLU:O	1:J:462:PRO:HD3	2.18	0.44
5:K:1:AGS:S1G	5:K:1:AGS:O2G	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:384:ALA:O	1:N:385:THR:HG23	2.17	0.44
1:J:217:SER:N	1:J:218:PRO:HD3	2.32	0.44
1:D:218:PRO:HD2	1:D:320:ALA:O	2.18	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.18	0.44
1:B:302:SER:O	1:B:307:MET:HE3	2.18	0.44
1:K:413:ALA:HB3	1:K:417:VAL:HG22	1.98	0.44
1:N:193:MET:HE2	1:N:292:ILE:HG12	1.99	0.44
1:M:73:MET:HB3	6:M:2221:HOH:O	2.18	0.44
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.99	0.44
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.44
1:C:369:VAL:HG23	1:C:370:ALA:N	2.32	0.44
1:M:290:GLN:HB3	1:M:345:ARG:NH2	2.31	0.44
1:K:134:LEU:HD21	1:K:425:LYS:NZ	2.32	0.44
1:J:324:VAL:O	1:J:331:THR:HG22	2.18	0.44
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.99	0.44
1:G:210:THR:O	1:G:210:THR:HG22	2.17	0.44
1:F:183:LEU:CD2	1:F:384:ALA:HB2	2.47	0.44
1:E:384:ALA:O	1:E:385:THR:HG23	2.17	0.44
1:M:182:GLY:HA2	1:M:383:ALA:HB3	2.00	0.44
1:J:217:SER:N	1:J:218:PRO:CD	2.81	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:L:253:ASP:OD1	1:L:277:LYS:HE2	2.18	0.44
1:H:176:THR:HG22	1:H:177:VAL:H	1.82	0.44
1:D:413:ALA:HB3	1:D:417:VAL:HG22	1.98	0.44
1:C:325:ILE:HA	1:C:329:THR:O	2.17	0.44
1:A:69:MET:CE	1:G:39:VAL:HG12	2.47	0.44
1:F:369:VAL:HG23	1:F:370:ALA:N	2.32	0.44
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.99	0.44
1:H:215:LEU:HB2	1:H:323:VAL:HG22	2.00	0.44
1:J:68:ASN:O	1:J:72:GLN:HG2	2.17	0.44
1:F:210:THR:O	1:F:210:THR:HG22	2.17	0.44
1:I:384:ALA:O	1:I:385:THR:HG23	2.18	0.44
1:A:218:PRO:HD2	1:A:320:ALA:O	2.17	0.44
1:D:234:LEU:N	1:D:235:PRO:HD2	2.33	0.44
1:C:217:SER:N	1:C:218:PRO:CD	2.81	0.44
1:I:496:PRO:O	1:I:499:VAL:HG13	2.17	0.44
1:H:392:LYS:O	1:H:396:VAL:HG23	2.18	0.44
1:N:153:ASN:O	1:N:154:SER:HB2	2.18	0.44
1:J:224:ASP:HB3	1:J:302:SER:HB3	2.00	0.44
1:C:16:MET:O	1:C:20:VAL:HG13	2.17	0.44
1:F:389:MET:N	6:F:2746:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:LEU:O	1:E:238:GLU:HG3	2.17	0.44
1:N:217:SER:N	1:N:218:PRO:CD	2.81	0.44
1:C:179:ASP:HB3	1:C:389:MET:CE	2.48	0.44
1:M:369:VAL:HG23	1:M:370:ALA:N	2.32	0.44
1:E:242:LYS:C	1:E:244:GLY:N	2.71	0.44
1:K:242:LYS:C	1:K:244:GLY:N	2.71	0.44
1:G:336:VAL:O	1:G:337:GLY:C	2.55	0.44
1:N:42:LYS:HE3	1:N:48:THR:OG1	2.18	0.44
1:H:217:SER:N	1:H:218:PRO:HD3	2.33	0.43
1:B:217:SER:N	1:B:218:PRO:CD	2.80	0.43
1:B:325:ILE:HA	1:B:329:THR:O	2.18	0.43
1:G:381:VAL:O	1:G:382:GLY:O	2.36	0.43
1:D:200:LEU:HD13	1:D:254:VAL:HB	2.00	0.43
1:B:259:LEU:O	1:B:263:VAL:HG23	2.18	0.43
1:H:302:SER:H	1:H:307:MET:HE1	1.83	0.43
1:B:413:ALA:HB3	1:B:417:VAL:HG22	2.00	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:G:70:GLY:HA2	1:G:73:MET:HE3	2.01	0.43
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.17	0.43
1:F:260:ALA:O	1:F:264:VAL:HG23	2.18	0.43
1:F:199:TYR:CZ	1:F:327:LYS:HA	2.53	0.43
1:M:210:THR:HG22	1:M:210:THR:O	2.18	0.43
1:C:183:LEU:CD2	1:C:384:ALA:HB2	2.47	0.43
1:C:348:GLN:O	1:C:352:GLN:HG2	2.18	0.43
1:E:200:LEU:HG	1:E:276:VAL:HA	2.01	0.43
1:L:417:VAL:CG1	6:L:2905:HOH:O	2.66	0.43
1:L:417:VAL:HB	6:L:2905:HOH:O	2.18	0.43
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.98	0.43
1:J:242:LYS:C	1:J:244:GLY:N	2.71	0.43
1:F:342:ILE:O	1:F:346:VAL:HG23	2.18	0.43
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.99	0.43
1:H:518:GLU:HG2	6:N:1187:HOH:O	2.18	0.43
1:G:260:ALA:O	1:G:264:VAL:HG23	2.18	0.43
1:L:199:TYR:CZ	1:L:327:LYS:HA	2.53	0.43
1:D:236:VAL:O	1:D:240:VAL:HG23	2.19	0.43
1:B:451:LEU:HD23	1:B:451:LEU:C	2.39	0.43
1:L:421:ARG:CZ	1:L:473:ASP:HA	2.48	0.43
1:N:217:SER:N	1:N:218:PRO:HD3	2.33	0.43
1:A:348:GLN:O	1:A:352:GLN:HG2	2.17	0.43
1:K:348:GLN:O	1:K:352:GLN:HG2	2.19	0.43
1:L:325:ILE:HA	1:L:329:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:O	1:E:76:GLU:HB2	2.18	0.43
1:B:242:LYS:O	1:B:243:ALA:HB3	2.19	0.43
1:G:351:GLN:HA	1:G:354:GLU:HG2	1.99	0.43
1:N:525:PRO:HD3	6:N:2033:HOH:O	2.18	0.43
1:H:260:ALA:O	1:H:264:VAL:HG23	2.18	0.43
1:N:210:THR:HG22	1:N:210:THR:O	2.18	0.43
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.19	0.43
1:N:171:LYS:HB2	1:N:407:VAL:HG11	2.01	0.43
1:I:409:GLU:OE2	1:I:498:LYS:HG3	2.19	0.43
1:A:210:THR:HG22	1:A:210:THR:O	2.18	0.43
1:H:384:ALA:C	1:H:385:THR:HG23	2.39	0.43
1:M:217:SER:N	1:M:218:PRO:CD	2.82	0.43
1:B:218:PRO:HD2	1:B:320:ALA:O	2.18	0.43
1:N:180:GLY:HA3	1:N:381:VAL:O	2.18	0.43
1:N:381:VAL:O	1:N:382:GLY:O	2.37	0.43
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.01	0.43
1:B:266:THR:HG22	1:B:271:VAL:O	2.19	0.43
1:G:224:ASP:HB3	1:G:302:SER:HB3	2.00	0.43
1:J:69:MET:O	1:J:73:MET:HG3	2.19	0.43
1:N:366:GLN:O	1:N:369:VAL:HG22	2.18	0.43
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.54	0.43
1:A:191:GLU:O	1:A:334:ASP:HA	2.18	0.43
1:N:284:ARG:O	1:N:288:MET:HG3	2.19	0.43
1:H:183:LEU:HD13	1:H:184:GLN:N	2.33	0.43
1:D:325:ILE:HG22	1:D:330:THR:HG23	1.99	0.43
1:M:259:LEU:O	1:M:263:VAL:HG23	2.19	0.43
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.99	0.43
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.00	0.43
1:F:178:GLU:OE2	1:F:322:ARG:NH1	2.51	0.43
1:K:205:ILE:CA	1:K:213:VAL:HG22	2.49	0.43
1:B:369:VAL:HG23	1:B:370:ALA:N	2.33	0.43
1:C:242:LYS:C	1:C:244:GLY:N	2.72	0.43
1:N:82:ASN:O	1:N:86:GLY:N	2.49	0.43
1:H:409:GLU:OE2	1:H:498:LYS:HG3	2.19	0.43
1:J:449:ALA:HB3	1:J:450:PRO:HD3	2.01	0.43
1:N:37:ASN:HD21	1:N:51:LYS:HE3	1.84	0.43
1:I:210:THR:HG22	1:I:210:THR:O	2.19	0.43
1:J:210:THR:O	1:J:210:THR:HG22	2.18	0.43
1:F:383:ALA:HA	6:F:2746:HOH:O	2.19	0.43
1:A:384:ALA:O	1:A:385:THR:OG1	2.33	0.43
1:B:234:LEU:O	1:B:238:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:PRO:HD2	1:E:320:ALA:O	2.19	0.43
1:A:194:GLN:OE1	1:A:329:THR:HG21	2.18	0.43
1:E:176:THR:HG22	1:E:177:VAL:N	2.33	0.43
1:G:132:LYS:HG3	6:G:1971:HOH:O	2.19	0.43
1:H:369:VAL:HG23	1:H:370:ALA:N	2.34	0.43
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.52	0.43
1:L:85:ALA:O	1:L:401:HIS:HE1	2.01	0.43
1:J:209:GLU:N	1:J:209:GLU:OE1	2.47	0.43
1:D:349:ILE:CG2	1:D:369:VAL:HG13	2.48	0.43
1:I:259:LEU:O	1:I:263:VAL:HG23	2.18	0.43
1:A:69:MET:HE2	1:G:39:VAL:HG12	2.01	0.43
1:C:272:LYS:NZ	1:D:228:SER:HB2	2.34	0.43
1:B:215:LEU:HB2	1:B:323:VAL:CG2	2.48	0.43
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.49	0.43
1:G:223:ALA:O	1:G:251:ALA:HA	2.19	0.43
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.00	0.43
1:H:37:ASN:ND2	1:H:51:LYS:HE3	2.34	0.43
1:B:463:SER:O	1:B:467:ASN:HB2	2.19	0.43
1:E:324:VAL:O	1:E:331:THR:HG22	2.17	0.43
1:L:239:ALA:O	1:L:314:LEU:HD11	2.18	0.43
1:L:217:SER:N	1:L:218:PRO:CD	2.82	0.43
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.43
1:F:348:GLN:O	1:F:352:GLN:HG2	2.18	0.43
1:L:381:VAL:O	1:L:382:GLY:O	2.37	0.43
1:F:420:ILE:CD1	1:F:451:LEU:HD13	2.49	0.43
1:N:222:LEU:HB3	1:N:289:LEU:HD21	2.01	0.43
1:C:70:GLY:HA2	1:C:73:MET:HE3	2.01	0.43
1:E:65:LYS:HE3	1:E:522:THR:OG1	2.19	0.43
1:M:68:ASN:O	1:M:72:GLN:HG2	2.18	0.43
1:F:209:GLU:OE1	1:F:209:GLU:N	2.49	0.43
1:B:384:ALA:C	1:B:385:THR:HG23	2.38	0.43
1:L:217:SER:N	1:L:218:PRO:HD3	2.33	0.43
1:D:234:LEU:O	1:D:238:GLU:HG3	2.18	0.43
1:A:417:VAL:HG11	1:A:488:MET:HG3	2.00	0.43
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.99	0.43
1:K:220:ILE:CD1	1:K:296:THR:HG21	2.49	0.43
1:N:524:LEU:O	1:N:526:LYS:N	2.51	0.43
1:I:496:PRO:HB2	1:I:499:VAL:CG1	2.49	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.43
1:D:65:LYS:HG2	6:D:1200:HOH:O	2.19	0.43
1:B:241:ALA:HB1	1:C:231:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.00	0.42
5:N:1:AGS:O2G	5:N:1:AGS:S1G	2.54	0.42
1:L:383:ALA:O	1:L:384:ALA:CB	2.66	0.42
1:M:284:ARG:HH11	1:M:364:LYS:CE	2.32	0.42
1:K:182:GLY:HA2	1:K:383:ALA:CB	2.49	0.42
1:J:179:ASP:HB3	1:J:389:MET:CE	2.48	0.42
1:L:60:ILE:O	1:L:75:LYS:HE3	2.19	0.42
1:A:329:THR:HG22	6:A:2839:HOH:O	2.18	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.42
1:E:177:VAL:HA	1:E:379:ILE:O	2.19	0.42
1:B:353:ILE:HD13	1:B:366:GLN:HG2	2.01	0.42
1:K:70:GLY:HA2	1:K:73:MET:HE3	2.01	0.42
1:F:191:GLU:O	1:F:334:ASP:HA	2.18	0.42
1:C:421:ARG:CZ	1:C:473:ASP:HA	2.49	0.42
1:K:384:ALA:C	1:K:385:THR:HG23	2.39	0.42
1:G:302:SER:H	1:G:307:MET:HE1	1.83	0.42
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.00	0.42
1:A:366:GLN:HA	1:A:369:VAL:HG22	2.00	0.42
1:K:319:GLN:HB3	1:K:336:VAL:HG21	2.00	0.42
1:M:496:PRO:O	1:M:499:VAL:HG13	2.19	0.42
1:J:222:LEU:HB3	1:J:289:LEU:CD2	2.50	0.42
1:I:466:ALA:O	1:I:470:LYS:HG3	2.19	0.42
1:I:238:GLU:O	1:I:241:ALA:HB3	2.19	0.42
1:J:200:LEU:HG	1:J:276:VAL:HA	2.01	0.42
1:A:253:ASP:OD1	1:A:277:LYS:HE2	2.19	0.42
1:L:324:VAL:O	1:L:331:THR:HG22	2.19	0.42
1:D:284:ARG:O	1:D:288:MET:HG3	2.19	0.42
1:N:272:LYS:CD	1:N:272:LYS:N	2.83	0.42
1:E:220:ILE:CD1	1:E:296:THR:HG21	2.48	0.42
1:N:336:VAL:O	1:N:337:GLY:C	2.58	0.42
1:B:193:MET:HE3	1:B:292:ILE:HG12	2.02	0.42
1:I:496:PRO:HD2	1:I:499:VAL:CG1	2.49	0.42
1:K:438:VAL:O	1:K:442:VAL:HG23	2.18	0.42
1:D:37:ASN:HD21	1:D:51:LYS:HE3	1.84	0.42
1:C:496:PRO:O	1:C:499:VAL:HG13	2.19	0.42
1:K:421:ARG:CZ	1:K:473:ASP:HA	2.49	0.42
1:L:94:VAL:HB	6:L:2642:HOH:O	2.20	0.42
1:F:384:ALA:C	1:F:385:THR:HG23	2.40	0.42
1:E:348:GLN:O	1:E:352:GLN:HG2	2.19	0.42
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.42
1:F:253:ASP:OD1	1:F:277:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:VAL:HG12	1:C:273:VAL:HG23	2.00	0.42
1:N:193:MET:HE1	1:N:292:ILE:HG12	2.01	0.42
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:N:206:ASN:ND2	1:N:214:GLU:H	2.16	0.42
1:M:288:MET:HA	1:M:291:ASP:OD2	2.19	0.42
1:D:206:ASN:OD1	1:D:207:LYS:HG3	2.19	0.42
1:B:169:VAL:HG13	1:B:377:ALA:HB2	2.00	0.42
1:G:524:LEU:O	1:G:526:LYS:N	2.52	0.42
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.02	0.42
1:A:8:PHE:HB3	6:A:1960:HOH:O	2.20	0.42
1:D:36:ARG:HG3	1:E:518:GLU:HG2	2.00	0.42
1:G:85:ALA:O	1:G:401:HIS:HE1	2.02	0.42
1:L:183:LEU:HD13	1:L:184:GLN:N	2.34	0.42
1:M:284:ARG:HH11	1:M:364:LYS:NZ	2.18	0.42
1:F:183:LEU:HD13	1:F:184:GLN:N	2.34	0.42
1:A:183:LEU:HD13	1:A:184:GLN:N	2.34	0.42
1:J:238:GLU:O	1:J:241:ALA:HB3	2.20	0.42
1:F:60:ILE:O	1:F:75:LYS:HE3	2.19	0.42
1:C:23:LEU:HD13	1:C:75:LYS:HD2	2.01	0.42
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.42
1:A:240:VAL:HG11	1:A:247:LEU:HB2	2.00	0.42
1:L:202:PRO:O	1:L:204:PHE:N	2.46	0.42
1:J:215:LEU:HB2	1:J:323:VAL:CG2	2.50	0.42
1:G:134:LEU:HD22	6:G:2213:HOH:O	2.19	0.42
6:I:2009:HOH:O	1:J:117:LYS:HE3	2.18	0.42
1:H:342:ILE:O	1:H:346:VAL:HG23	2.19	0.42
1:D:445:ARG:HD3	6:D:2123:HOH:O	2.19	0.42
1:J:182:GLY:HA2	1:J:383:ALA:HB3	2.02	0.42
1:G:242:LYS:O	1:G:244:GLY:N	2.52	0.42
6:C:2549:HOH:O	1:J:463:SER:HB2	2.19	0.42
1:J:348:GLN:O	1:J:352:GLN:HG2	2.19	0.42
1:N:259:LEU:O	1:N:263:VAL:HG23	2.20	0.42
1:L:259:LEU:O	1:L:263:VAL:HG23	2.19	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.02	0.42
1:D:404:ARG:HH11	1:D:404:ARG:CG	2.27	0.42
1:N:194:GLN:HG3	1:N:331:THR:HB	2.00	0.42
1:E:266:THR:HG22	1:E:271:VAL:O	2.19	0.42
1:G:266:THR:HG21	1:G:273:VAL:H	1.84	0.42
1:M:220:ILE:CD1	1:M:296:THR:HG21	2.48	0.42
1:H:160:LYS:HB2	1:H:160:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:GLN:HB3	1:F:336:VAL:HG21	2.02	0.42
1:G:131:LEU:HD13	1:G:422:VAL:HG21	2.02	0.42
1:K:460:GLU:O	1:K:462:PRO:HD3	2.18	0.42
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.60	0.42
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.91	0.42
1:E:209:GLU:OE1	1:E:209:GLU:N	2.49	0.42
1:D:182:GLY:HA2	1:D:383:ALA:CB	2.50	0.42
1:H:182:GLY:HA2	1:H:383:ALA:HB3	2.02	0.42
1:I:179:ASP:HB3	1:I:389:MET:CE	2.49	0.42
1:J:206:ASN:ND2	1:J:214:GLU:H	2.17	0.42
1:M:242:LYS:O	1:M:243:ALA:HB3	2.20	0.42
1:I:336:VAL:O	1:I:337:GLY:C	2.58	0.42
1:B:144:ILE:HG23	1:B:403:THR:HG21	2.02	0.42
1:C:191:GLU:O	1:C:334:ASP:HA	2.20	0.42
1:N:111:MET:HG2	1:N:435:ASP:OD1	2.19	0.42
1:K:496:PRO:O	1:K:499:VAL:HG13	2.19	0.42
1:B:197:ARG:HD2	1:B:277:LYS:HB2	2.01	0.42
1:H:381:VAL:O	1:H:382:GLY:O	2.38	0.42
1:J:305:ILE:HB	1:J:307:MET:HE2	2.01	0.42
1:H:325:ILE:HA	1:H:329:THR:O	2.19	0.42
1:I:266:THR:HG21	1:I:273:VAL:H	1.84	0.42
1:G:193:MET:HE2	1:G:292:ILE:HG12	2.00	0.42
1:F:206:ASN:ND2	1:F:214:GLU:H	2.16	0.42
1:A:302:SER:O	1:A:307:MET:HE3	2.20	0.42
1:M:179:ASP:HB3	1:M:389:MET:CE	2.50	0.42
1:H:319:GLN:HB3	1:H:336:VAL:HG21	2.01	0.42
1:B:140:ASP:O	1:B:144:ILE:HG13	2.20	0.42
1:M:524:LEU:HA	1:M:524:LEU:HD12	1.87	0.42
1:J:331:THR:HG23	1:J:331:THR:O	2.20	0.42
1:M:144:ILE:HG23	1:M:403:THR:HG21	2.01	0.42
1:H:210:THR:HG22	1:H:210:THR:O	2.20	0.42
1:B:77:VAL:HG11	1:B:506:TYR:O	2.18	0.42
1:M:348:GLN:O	1:M:352:GLN:HG2	2.20	0.42
1:L:382:GLY:O	1:L:389:MET:HG2	2.20	0.42
1:B:324:VAL:O	1:B:331:THR:HG22	2.20	0.42
1:N:305:ILE:HB	1:N:307:MET:HE2	2.01	0.42
1:N:369:VAL:HG23	1:N:370:ALA:N	2.35	0.42
1:L:206:ASN:ND2	1:L:214:GLU:H	2.18	0.42
1:I:366:GLN:HA	1:I:369:VAL:HG22	2.01	0.42
1:A:4:LYS:HG3	1:G:59:GLU:O	2.19	0.42
1:C:384:ALA:C	1:C:385:THR:HG23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:O	1:F:263:VAL:HG23	2.19	0.42
1:H:240:VAL:HG11	1:H:247:LEU:HB2	2.01	0.42
1:G:219:PHE:O	1:G:247:LEU:HD12	2.19	0.42
1:E:76:GLU:HG3	6:E:2322:HOH:O	2.20	0.42
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.91	0.42
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.35	0.42
1:L:33:PRO:CG	1:L:480:ALA:HB3	2.50	0.42
1:D:223:ALA:O	1:D:251:ALA:HA	2.20	0.42
1:N:183:LEU:CD2	1:N:384:ALA:HB2	2.49	0.41
1:B:305:ILE:HB	1:B:307:MET:HE2	2.02	0.41
1:I:177:VAL:HG21	1:I:397:GLU:HG2	1.99	0.41
1:N:325:ILE:HA	1:N:329:THR:O	2.18	0.41
1:G:417:VAL:HG13	6:G:2394:HOH:O	2.20	0.41
1:F:242:LYS:C	1:F:244:GLY:N	2.73	0.41
1:A:336:VAL:O	1:A:337:GLY:C	2.59	0.41
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.34	0.41
1:F:510:VAL:CG2	6:F:2556:HOH:O	2.67	0.41
1:D:191:GLU:O	1:D:334:ASP:HA	2.20	0.41
1:C:222:LEU:HB3	1:C:289:LEU:CD2	2.50	0.41
1:H:220:ILE:HD12	1:H:296:THR:HG21	2.02	0.41
5:L:1:AGS:O2G	5:L:1:AGS:S1G	2.55	0.41
1:C:200:LEU:HG	1:C:276:VAL:HA	2.02	0.41
1:D:177:VAL:HA	1:D:379:ILE:O	2.20	0.41
1:D:160:LYS:HZ2	1:D:160:LYS:HB2	1.84	0.41
1:A:176:THR:HG22	1:A:177:VAL:H	1.84	0.41
1:M:242:LYS:C	1:M:244:GLY:N	2.72	0.41
1:B:366:GLN:HA	1:B:369:VAL:HG22	2.02	0.41
1:G:353:ILE:HD13	1:G:366:GLN:HG2	2.02	0.41
1:M:496:PRO:HB2	1:M:499:VAL:HG12	2.02	0.41
1:L:97:GLN:HG2	6:L:2018:HOH:O	2.19	0.41
1:F:487:ASN:O	1:F:491:MET:HG3	2.20	0.41
1:M:171:LYS:HB2	1:M:407:VAL:HG11	2.02	0.41
1:G:409:GLU:OE2	1:G:498:LYS:HG3	2.20	0.41
1:F:182:GLY:HA2	1:F:383:ALA:HB3	2.01	0.41
1:E:183:LEU:CD2	1:E:384:ALA:HB2	2.50	0.41
1:G:384:ALA:C	1:G:385:THR:HG23	2.40	0.41
1:E:238:GLU:O	1:E:241:ALA:HB3	2.19	0.41
1:D:217:SER:N	1:D:218:PRO:HD3	2.34	0.41
1:B:194:GLN:OE1	1:B:329:THR:HG21	2.20	0.41
1:C:353:ILE:HD13	1:C:366:GLN:HG2	2.01	0.41
1:K:239:ALA:C	1:K:314:LEU:HD21	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:MET:O	1:N:73:MET:HG3	2.19	0.41
1:M:193:MET:HE2	1:M:292:ILE:HG12	2.02	0.41
1:J:336:VAL:O	1:J:337:GLY:C	2.58	0.41
1:N:524:LEU:HA	1:N:524:LEU:HD12	1.91	0.41
1:G:222:LEU:HB3	1:G:289:LEU:CD2	2.50	0.41
1:L:122:LYS:HE2	1:L:429:LEU:HD11	2.02	0.41
1:A:220:ILE:HD12	1:A:296:THR:HG21	2.02	0.41
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.21	0.41
1:B:222:LEU:HB3	1:B:289:LEU:CD2	2.49	0.41
1:A:153:ASN:O	1:A:154:SER:HB2	2.19	0.41
1:C:224:ASP:HB3	1:C:302:SER:HB3	2.02	0.41
1:E:191:GLU:O	1:E:334:ASP:HA	2.20	0.41
1:N:209:GLU:N	1:N:209:GLU:OE1	2.48	0.41
1:L:210:THR:O	1:L:210:THR:HG22	2.20	0.41
1:I:217:SER:HA	1:I:320:ALA:O	2.20	0.41
1:N:176:THR:HG22	1:N:177:VAL:N	2.35	0.41
1:B:240:VAL:HG11	1:B:247:LEU:HB2	2.01	0.41
1:J:177:VAL:HA	1:J:379:ILE:O	2.20	0.41
1:K:366:GLN:HA	1:K:369:VAL:HG22	2.01	0.41
1:H:16:MET:HE3	6:H:2854:HOH:O	2.21	0.41
1:B:242:LYS:C	1:B:244:GLY:N	2.73	0.41
1:G:351:GLN:HA	1:G:354:GLU:CG	2.49	0.41
1:K:171:LYS:HB2	1:K:407:VAL:HG11	2.02	0.41
1:J:295:LEU:HD13	1:J:295:LEU:O	2.20	0.41
1:D:182:GLY:HA2	1:D:383:ALA:HB3	2.03	0.41
1:A:182:GLY:O	1:A:183:LEU:O	2.39	0.41
1:E:182:GLY:HA2	1:E:383:ALA:HB3	2.02	0.41
1:B:325:ILE:HG22	1:B:330:THR:HG23	2.03	0.41
1:D:284:ARG:NH1	1:D:364:LYS:NZ	2.67	0.41
1:E:325:ILE:HG22	1:E:330:THR:HG23	2.02	0.41
1:A:219:PHE:O	1:A:247:LEU:HD12	2.20	0.41
1:C:177:VAL:HA	1:C:379:ILE:O	2.20	0.41
1:E:28:LYS:HD2	1:E:453:GLN:NE2	2.36	0.41
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.87	0.41
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.50	0.41
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.50	0.41
1:C:460:GLU:O	1:C:462:PRO:HD3	2.21	0.41
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.60	0.41
1:E:178:GLU:OE1	1:E:378:VAL:HG11	2.20	0.41
1:H:153:ASN:O	1:H:154:SER:HB2	2.20	0.41
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:LEU:HD21	1:J:425:LYS:NZ	2.35	0.41
1:M:54:VAL:HG23	6:M:2164:HOH:O	2.20	0.41
1:N:463:SER:O	1:N:467:ASN:HB2	2.19	0.41
1:H:295:LEU:C	1:H:295:LEU:HD13	2.41	0.41
1:C:182:GLY:HA2	1:C:383:ALA:CB	2.50	0.41
1:I:324:VAL:O	1:I:331:THR:HG22	2.21	0.41
1:L:477:GLY:CA	6:L:2905:HOH:O	2.68	0.41
1:D:200:LEU:HG	1:D:276:VAL:HA	2.01	0.41
1:K:204:PHE:C	1:K:213:VAL:HG22	2.41	0.41
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.85	0.41
1:K:366:GLN:O	1:K:369:VAL:HG22	2.20	0.41
1:B:336:VAL:O	1:B:337:GLY:C	2.59	0.41
1:B:193:MET:HE1	1:B:292:ILE:HG12	2.02	0.41
1:M:215:LEU:HB2	1:M:323:VAL:HG22	2.03	0.41
1:H:85:ALA:O	1:H:401:HIS:HE1	2.03	0.41
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.56	0.41
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.41
1:K:295:LEU:HD13	1:K:295:LEU:O	2.20	0.41
1:D:210:THR:HG22	1:D:210:THR:O	2.19	0.41
1:M:136:VAL:HA	1:M:137:PRO:HD3	1.87	0.41
1:A:231:ARG:NH1	1:G:242:LYS:HA	2.35	0.41
1:A:266:THR:HG21	1:A:273:VAL:H	1.86	0.41
1:E:305:ILE:HB	1:E:307:MET:HE2	2.02	0.41
1:A:242:LYS:C	1:A:244:GLY:N	2.73	0.41
1:B:69:MET:O	1:B:73:MET:HG3	2.20	0.41
1:N:455:VAL:O	1:N:458:CYS:HB2	2.21	0.41
1:G:183:LEU:CD2	1:G:384:ALA:HB2	2.48	0.41
1:F:238:GLU:O	1:F:241:ALA:HB3	2.20	0.41
1:D:348:GLN:O	1:D:352:GLN:HG2	2.21	0.41
1:K:381:VAL:O	1:K:382:GLY:O	2.39	0.41
1:D:201:SER:O	1:D:202:PRO:O	2.39	0.41
1:B:302:SER:H	1:B:307:MET:HE1	1.85	0.41
1:L:194:GLN:HG3	1:L:331:THR:HB	2.03	0.41
1:G:266:THR:HG22	1:G:273:VAL:H	1.86	0.41
1:I:242:LYS:O	1:I:243:ALA:HB3	2.20	0.41
1:E:336:VAL:O	1:E:337:GLY:C	2.58	0.41
1:G:202:PRO:C	1:G:204:PHE:H	2.23	0.41
1:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:N:260:ALA:O	1:N:264:VAL:HG23	2.21	0.41
1:J:140:ASP:OD2	1:J:142:LYS:HB3	2.21	0.41
1:D:324:VAL:HB	1:D:331:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ALA:O	1:E:401:HIS:HE1	2.03	0.41
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.61	0.41
1:K:153:ASN:O	1:K:154:SER:HB2	2.20	0.41
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.41
1:J:182:GLY:HA2	1:J:383:ALA:CB	2.50	0.41
1:L:183:LEU:CD2	1:L:384:ALA:HB2	2.49	0.41
1:L:384:ALA:C	1:L:385:THR:HG23	2.40	0.41
1:L:235:PRO:CG	1:L:310:GLU:HA	2.34	0.41
1:M:253:ASP:OD1	1:M:277:LYS:HE2	2.20	0.41
1:L:200:LEU:HG	1:L:276:VAL:HA	2.02	0.41
1:J:381:VAL:O	1:J:382:GLY:O	2.39	0.41
1:G:200:LEU:HG	1:G:276:VAL:HA	2.02	0.41
1:L:477:GLY:HA2	6:L:2905:HOH:O	2.20	0.41
1:B:194:GLN:HG3	1:B:331:THR:HB	2.03	0.41
1:B:174:VAL:HG22	1:B:194:GLN:NE2	2.36	0.41
1:B:205:ILE:CA	1:B:213:VAL:HG22	2.50	0.41
1:H:177:VAL:HG21	1:H:397:GLU:HG2	2.00	0.41
1:A:194:GLN:HG3	1:A:331:THR:HB	2.02	0.41
1:B:177:VAL:HA	1:B:379:ILE:O	2.21	0.41
1:N:194:GLN:OE1	1:N:329:THR:HG21	2.21	0.41
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.34	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.50	0.41
1:G:77:VAL:CG2	1:G:510:VAL:HG21	2.51	0.41
1:J:242:LYS:O	1:J:243:ALA:HB3	2.20	0.41
1:E:160:LYS:HB2	1:E:160:LYS:NZ	2.36	0.41
1:K:353:ILE:HD13	1:K:366:GLN:HG2	2.01	0.41
1:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	0.41
1:E:366:GLN:HA	1:E:369:VAL:HG22	2.03	0.41
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.41
1:I:63:GLU:HB2	1:J:524:LEU:CD2	2.50	0.41
1:C:496:PRO:HB2	1:C:499:VAL:CG1	2.50	0.41
1:L:215:LEU:HB2	1:L:323:VAL:HG22	2.03	0.41
1:L:351:GLN:HA	1:L:354:GLU:HG2	2.02	0.41
1:F:421:ARG:CZ	1:F:473:ASP:HA	2.51	0.41
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.60	0.41
1:H:191:GLU:O	1:H:334:ASP:HA	2.19	0.41
1:L:290:GLN:HB3	1:L:345:ARG:NH2	2.35	0.41
1:N:85:ALA:O	1:N:401:HIS:HE1	2.03	0.41
1:N:134:LEU:HD21	1:N:425:LYS:NZ	2.35	0.41
1:H:324:VAL:O	1:H:331:THR:HG22	2.21	0.41
1:I:171:LYS:HB2	1:I:407:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:449:ALA:HB3	1:M:450:PRO:HD3	2.03	0.41
1:L:46:ALA:HA	1:L:47:PRO:HD3	1.93	0.41
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.19	0.41
1:G:284:ARG:O	1:G:288:MET:HG3	2.21	0.41
1:I:421:ARG:CZ	1:I:473:ASP:HA	2.51	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:A:325:ILE:HA	1:A:329:THR:O	2.20	0.41
1:N:193:MET:HG3	1:N:371:LYS:HB3	2.03	0.41
1:F:23:LEU:CD2	1:F:74:VAL:HG13	2.51	0.41
1:E:202:PRO:C	1:E:204:PHE:H	2.23	0.41
1:M:102:GLU:HB2	1:M:442:VAL:HG13	2.03	0.41
1:C:153:ASN:O	1:C:154:SER:HB2	2.21	0.41
1:E:224:ASP:HB3	1:E:302:SER:HB3	2.01	0.41
1:M:384:ALA:C	1:M:385:THR:HG23	2.42	0.40
1:M:205:ILE:CA	1:M:213:VAL:HG22	2.48	0.40
1:L:160:LYS:NZ	1:L:160:LYS:HB2	2.36	0.40
1:H:77:VAL:HG23	1:H:510:VAL:HG21	2.03	0.40
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.51	0.40
1:K:46:ALA:HA	1:K:47:PRO:HD3	1.88	0.40
1:A:466:ALA:O	1:A:470:LYS:HG3	2.21	0.40
1:N:384:ALA:C	1:N:385:THR:HG23	2.41	0.40
1:G:182:GLY:HA2	1:G:383:ALA:HB3	2.04	0.40
1:K:451:LEU:C	1:K:451:LEU:HD23	2.41	0.40
1:M:197:ARG:HD2	1:M:277:LYS:HB2	2.04	0.40
1:H:200:LEU:HG	1:H:276:VAL:HA	2.02	0.40
1:D:224:ASP:HB3	1:D:302:SER:HB3	2.04	0.40
1:F:302:SER:O	1:F:307:MET:HE3	2.21	0.40
1:I:325:ILE:HG22	1:I:330:THR:HG23	2.02	0.40
1:K:224:ASP:HB3	1:K:302:SER:HB3	2.03	0.40
1:K:194:GLN:OE1	1:K:329:THR:HG21	2.21	0.40
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.31	0.40
1:E:242:LYS:O	1:E:243:ALA:HB3	2.21	0.40
1:J:366:GLN:O	1:J:369:VAL:HG22	2.20	0.40
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.03	0.40
1:K:215:LEU:HB2	1:K:323:VAL:CG2	2.51	0.40
1:I:496:PRO:HD2	1:I:499:VAL:HG11	2.03	0.40
1:K:7:LYS:HE2	1:K:66:PHE:CE2	2.56	0.40
1:C:284:ARG:HH12	1:C:364:LYS:NZ	2.19	0.40
1:M:183:LEU:HD13	1:M:184:GLN:N	2.35	0.40
1:C:174:VAL:HG22	1:C:194:GLN:HE21	1.87	0.40
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:LYS:C	1:I:244:GLY:N	2.73	0.40
1:C:336:VAL:O	1:C:337:GLY:C	2.60	0.40
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.51	0.40
1:K:284:ARG:HH12	1:K:364:LYS:NZ	2.20	0.40
1:M:342:ILE:O	1:M:346:VAL:HG23	2.22	0.40
1:A:342:ILE:O	1:A:346:VAL:HG23	2.21	0.40
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.56	0.40
1:H:455:VAL:HG13	1:H:460:GLU:HB2	2.02	0.40
1:I:295:LEU:HD13	1:I:295:LEU:C	2.42	0.40
1:C:295:LEU:O	1:C:295:LEU:HD13	2.21	0.40
1:I:384:ALA:C	1:I:385:THR:HG23	2.41	0.40
1:N:182:GLY:O	1:N:183:LEU:O	2.40	0.40
1:E:384:ALA:C	1:E:385:THR:HG23	2.42	0.40
1:D:369:VAL:HG23	1:D:370:ALA:N	2.36	0.40
1:C:201:SER:O	1:C:202:PRO:O	2.40	0.40
1:B:253:ASP:OD1	1:B:277:LYS:HE2	2.21	0.40
1:K:200:LEU:HG	1:K:276:VAL:HA	2.03	0.40
1:N:179:ASP:HB3	1:N:389:MET:CE	2.51	0.40
1:I:194:GLN:HG3	1:I:331:THR:HB	2.02	0.40
1:C:266:THR:HG21	1:C:273:VAL:H	1.86	0.40
1:K:240:VAL:HG11	1:K:247:LEU:HB2	2.02	0.40
1:C:160:LYS:HB2	1:C:160:LYS:HZ2	1.87	0.40
1:H:202:PRO:C	1:H:204:PHE:H	2.24	0.40
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.92	0.40
1:I:524:LEU:HA	1:I:524:LEU:HD12	1.93	0.40
1:N:10:ASN:HA	6:N:2143:HOH:O	2.21	0.40
1:L:361:ASP:O	1:L:365:LEU:HG	2.20	0.40
1:D:118:ARG:HD2	1:D:436:GLN:NE2	2.36	0.40
1:K:392:LYS:O	1:K:396:VAL:HG23	2.22	0.40
1:B:111:MET:SD	1:B:438:VAL:HG21	2.62	0.40
1:C:46:ALA:HA	1:C:47:PRO:HD3	1.94	0.40
1:I:438:VAL:O	1:I:442:VAL:HG23	2.21	0.40
1:F:215:LEU:HB2	1:F:323:VAL:HG22	2.03	0.40
1:C:34:LYS:HG3	1:C:458:CYS:SG	2.62	0.40
1:A:295:LEU:HD13	1:A:295:LEU:C	2.42	0.40
5:M:1:AGS:O2G	5:M:1:AGS:S1G	2.54	0.40
1:H:182:GLY:HA2	1:H:383:ALA:CB	2.51	0.40
1:K:217:SER:HA	1:K:320:ALA:O	2.21	0.40
1:H:216:GLU:C	1:H:218:PRO:HD3	2.41	0.40
1:J:253:ASP:OD1	1:J:277:LYS:HE2	2.22	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:GLN:HG3	1:M:331:THR:HB	2.03	0.40
1:H:266:THR:HG21	1:H:273:VAL:H	1.85	0.40
1:K:302:SER:O	1:K:307:MET:HE3	2.22	0.40
1:D:404:ARG:HG2	1:D:404:ARG:NH1	2.33	0.40
1:K:194:GLN:HG3	1:K:331:THR:HB	2.03	0.40
1:H:326:ASN:HD22	1:H:329:THR:HB	1.86	0.40
1:C:206:ASN:ND2	1:C:214:GLU:H	2.18	0.40
1:C:331:THR:O	1:C:331:THR:HG23	2.22	0.40
1:I:85:ALA:O	1:I:401:HIS:HE1	2.04	0.40
1:I:132:LYS:HE2	6:I:1912:HOH:O	2.21	0.40
1:G:174:VAL:HG12	1:G:376:VAL:HG13	2.04	0.40
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.95	0.40

All (1) 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)
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.17	0.03

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	523/547 (96%)	487 (93%)	27 (5%)	9 (2%)	11 4
1	B	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	8 3
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	9 3
1	D	523/547 (96%)	492 (94%)	22 (4%)	9 (2%)	11 4
1	E	523/547 (96%)	485 (93%)	27 (5%)	11 (2%)	9 3
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	8 3
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	9 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	8 3
1	I	523/547 (96%)	486 (93%)	27 (5%)	10 (2%)	10 4
1	J	523/547 (96%)	486 (93%)	25 (5%)	12 (2%)	8 3
1	K	523/547 (96%)	484 (92%)	29 (6%)	10 (2%)	10 4
1	L	523/547 (96%)	488 (93%)	23 (4%)	12 (2%)	8 3
1	M	523/547 (96%)	487 (93%)	25 (5%)	11 (2%)	9 3
1	N	523/547 (96%)	487 (93%)	26 (5%)	10 (2%)	10 4
All	All	7322/7658 (96%)	6820 (93%)	350 (5%)	152 (2%)	9 3

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	E	183	LEU
1	A	183	LEU
1	A	256	GLY
1	A	271	VAL
1	B	256	GLY
1	B	385	THR
1	C	183	LEU
1	C	256	GLY
1	D	183	LEU
1	D	256	GLY
1	D	382	GLY
1	E	256	GLY
1	F	183	LEU
1	F	256	GLY
1	F	271	VAL
1	F	382	GLY
1	G	183	LEU
1	G	256	GLY
1	G	382	GLY
1	H	183	LEU
1	H	256	GLY
1	H	382	GLY
1	I	183	LEU
1	I	256	GLY
1	I	382	GLY
1	J	183	LEU
1	J	256	GLY

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Mol	Chain	Res	Type
1	K	183	LEU
1	K	256	GLY
1	L	183	LEU
1	L	256	GLY
1	L	382	GLY
1	M	183	LEU
1	M	256	GLY
1	M	271	VAL
1	N	183	LEU
1	N	256	GLY
1	N	382	GLY
1	A	202	PRO
1	A	385	THR
1	B	202	PRO
1	B	271	VAL
1	C	202	PRO
1	C	271	VAL
1	C	382	GLY
1	C	385	THR
1	D	202	PRO
1	D	271	VAL
1	D	385	THR
1	E	202	PRO
1	E	271	VAL
1	E	382	GLY
1	E	385	THR
1	F	202	PRO
1	F	384	ALA
1	F	385	THR
1	G	202	PRO
1	G	271	VAL
1	G	385	THR
1	H	202	PRO
1	H	271	VAL
1	H	385	THR
1	I	202	PRO
1	I	271	VAL
1	I	385	THR
1	J	202	PRO
1	J	271	VAL
1	J	382	GLY
1	J	385	THR

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Mol	Chain	Res	Type
1	K	202	PRO
1	K	271	VAL
1	K	385	THR
1	L	202	PRO
1	L	271	VAL
1	L	384	ALA
1	L	385	THR
1	M	202	PRO
1	M	385	THR
1	N	202	PRO
1	N	271	VAL
1	N	385	THR
1	A	253	ASP
1	B	382	GLY
1	B	384	ALA
1	C	184	GLN
1	C	201	SER
1	C	383	ALA
1	D	201	SER
1	D	383	ALA
1	E	253	ASP
1	F	334	ASP
1	F	383	ALA
1	G	253	ASP
1	G	337	GLY
1	I	253	ASP
1	I	383	ALA
1	J	253	ASP
1	J	383	ALA
1	J	384	ALA
1	K	184	GLN
1	K	201	SER
1	K	253	ASP
1	K	382	GLY
1	L	253	ASP
1	L	383	ALA
1	M	201	SER
1	M	253	ASP
1	M	382	GLY
1	B	184	GLN
1	B	201	SER
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	383	ALA
1	C	253	ASP
1	C	334	ASP
1	E	184	GLN
1	E	334	ASP
1	E	383	ALA
1	F	184	GLN
1	F	201	SER
1	F	253	ASP
1	G	184	GLN
1	H	337	GLY
1	H	383	ALA
1	I	184	GLN
1	J	184	GLN
1	J	334	ASP
1	K	383	ALA
1	L	184	GLN
1	M	334	ASP
1	M	383	ALA
1	N	184	GLN
1	N	201	SER
1	N	383	ALA
1	A	184	GLN
1	A	201	SER
1	B	334	ASP
1	D	184	GLN
1	E	201	SER
1	G	201	SER
1	G	383	ALA
1	H	184	GLN
1	H	253	ASP
1	H	384	ALA
1	I	201	SER
1	J	201	SER
1	M	184	GLN
1	A	382	GLY
1	N	337	GLY
1	H	201	SER
1	L	201	SER
1	L	337	GLY

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	404/413 (98%)	394 (98%)	10 (2%)	55	55
1	B	404/413 (98%)	397 (98%)	7 (2%)	68	71
1	C	404/413 (98%)	396 (98%)	8 (2%)	63	65
1	D	404/413 (98%)	394 (98%)	10 (2%)	55	55
1	E	404/413 (98%)	397 (98%)	7 (2%)	68	71
1	F	404/413 (98%)	396 (98%)	8 (2%)	63	65
1	G	404/413 (98%)	395 (98%)	9 (2%)	60	62
1	H	404/413 (98%)	397 (98%)	7 (2%)	68	71
1	I	404/413 (98%)	395 (98%)	9 (2%)	60	62
1	J	404/413 (98%)	397 (98%)	7 (2%)	68	71
1	K	404/413 (98%)	396 (98%)	8 (2%)	63	65
1	L	404/413 (98%)	394 (98%)	10 (2%)	55	55
1	M	404/413 (98%)	396 (98%)	8 (2%)	63	65
1	N	404/413 (98%)	396 (98%)	8 (2%)	63	65
All	All	5656/5782 (98%)	5540 (98%)	116 (2%)	61	63

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	20	VAL
1	A	75	LYS
1	A	94	VAL
1	A	183	LEU
1	A	289	LEU
1	A	310	GLU
1	A	328	ASP
1	A	404	ARG
1	A	499	VAL
1	B	75	LYS

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	289	LEU
1	B	310	GLU
1	B	404	ARG
1	B	499	VAL
1	B	510	VAL
1	C	20	VAL
1	C	75	LYS
1	C	94	VAL
1	C	183	LEU
1	C	289	LEU
1	C	328	ASP
1	C	404	ARG
1	C	499	VAL
1	D	20	VAL
1	D	23	LEU
1	D	75	LYS
1	D	94	VAL
1	D	183	LEU
1	D	289	LEU
1	D	310	GLU
1	D	404	ARG
1	D	473	ASP
1	D	499	VAL
1	E	94	VAL
1	E	183	LEU
1	E	310	GLU
1	E	328	ASP
1	E	404	ARG
1	E	499	VAL
1	E	514	MET
1	F	20	VAL
1	F	75	LYS
1	F	94	VAL
1	F	183	LEU
1	F	310	GLU
1	F	328	ASP
1	F	404	ARG
1	F	499	VAL
1	G	10	ASN
1	G	20	VAL
1	G	75	LYS

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Mol	Chain	Res	Type
1	G	183	LEU
1	G	289	LEU
1	G	310	GLU
1	G	328	ASP
1	G	404	ARG
1	G	499	VAL
1	H	20	VAL
1	H	75	LYS
1	H	94	VAL
1	H	183	LEU
1	H	289	LEU
1	H	404	ARG
1	H	499	VAL
1	I	10	ASN
1	I	20	VAL
1	I	75	LYS
1	I	94	VAL
1	I	183	LEU
1	I	289	LEU
1	I	310	GLU
1	I	404	ARG
1	I	499	VAL
1	J	20	VAL
1	J	75	LYS
1	J	94	VAL
1	J	183	LEU
1	J	310	GLU
1	J	404	ARG
1	J	499	VAL
1	K	20	VAL
1	K	75	LYS
1	K	94	VAL
1	K	183	LEU
1	K	289	LEU
1	K	328	ASP
1	K	404	ARG
1	K	499	VAL
1	L	20	VAL
1	L	75	LYS
1	L	94	VAL
1	L	183	LEU
1	L	289	LEU

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Mol	Chain	Res	Type
1	L	310	GLU
1	L	328	ASP
1	L	404	ARG
1	L	417	VAL
1	L	499	VAL
1	M	20	VAL
1	M	75	LYS
1	M	94	VAL
1	M	183	LEU
1	M	284	ARG
1	M	310	GLU
1	M	404	ARG
1	M	499	VAL
1	N	20	VAL
1	N	75	LYS
1	N	94	VAL
1	N	183	LEU
1	N	289	LEU
1	N	310	GLU
1	N	404	ARG
1	N	499	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	146	GLN
1	A	229	ASN
1	A	265	ASN
1	A	319	GLN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	B	146	GLN
1	B	265	ASN
1	B	319	GLN
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	366	GLN
1	B	401	HIS
1	B	475	ASN

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Mol	Chain	Res	Type
1	C	37	ASN
1	C	146	GLN
1	C	265	ASN
1	C	319	GLN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	366	GLN
1	C	401	HIS
1	D	37	ASN
1	D	146	GLN
1	D	229	ASN
1	D	265	ASN
1	D	319	GLN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	366	GLN
1	D	401	HIS
1	D	453	GLN
1	D	475	ASN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	319	GLN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	401	HIS
1	E	453	GLN
1	E	475	ASN
1	F	146	GLN
1	F	265	ASN
1	F	319	GLN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	401	HIS
1	G	37	ASN
1	G	146	GLN
1	G	265	ASN
1	G	319	GLN

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Mol	Chain	Res	Type
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	401	HIS
1	G	453	GLN
1	G	475	ASN
1	H	37	ASN
1	H	146	GLN
1	H	265	ASN
1	H	319	GLN
1	H	326	ASN
1	H	348	GLN
1	H	351	GLN
1	H	401	HIS
1	I	37	ASN
1	I	146	GLN
1	I	265	ASN
1	I	319	GLN
1	I	326	ASN
1	I	348	GLN
1	I	351	GLN
1	I	401	HIS
1	J	37	ASN
1	J	146	GLN
1	J	265	ASN
1	J	319	GLN
1	J	326	ASN
1	J	348	GLN
1	J	351	GLN
1	J	453	GLN
1	K	37	ASN
1	K	146	GLN
1	K	265	ASN
1	K	319	GLN
1	K	326	ASN
1	K	348	GLN
1	K	351	GLN
1	K	401	HIS
1	L	37	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN

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Mol	Chain	Res	Type
1	L	319	GLN
1	L	326	ASN
1	L	348	GLN
1	L	351	GLN
1	L	401	HIS
1	L	453	GLN
1	M	37	ASN
1	M	146	GLN
1	M	229	ASN
1	M	265	ASN
1	M	319	GLN
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	M	401	HIS
1	M	453	GLN
1	N	37	ASN
1	N	146	GLN
1	N	265	ASN
1	N	319	GLN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	401	HIS
1	N	453	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 30 are monoatomic - leaving 36 for Mogul analysis.

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	$\#\|Z\| > 2$
5	AGS	A	1	3,4	24,33,33	4.34	1 (4%)	28,52,52	1.20	4 (14%)
2	SO4	A	4001	-	4,4,4	2.24	1 (25%)	6,6,6	0.87	0
2	SO4	A	4007	-	4,4,4	2.20	1 (25%)	6,6,6	0.90	0
2	SO4	A	4008	-	4,4,4	2.24	1 (25%)	6,6,6	0.85	0
5	AGS	B	1	3,4	24,33,33	4.39	1 (4%)	28,52,52	1.27	2 (7%)
2	SO4	B	4009	-	4,4,4	2.23	1 (25%)	6,6,6	0.89	0
2	SO4	B	4010	-	4,4,4	2.28	1 (25%)	6,6,6	0.87	0
5	AGS	C	1	3,4	24,33,33	4.45	2 (8%)	28,52,52	1.21	2 (7%)
2	SO4	C	4011	-	4,4,4	2.25	1 (25%)	6,6,6	0.89	0
2	SO4	C	4012	-	4,4,4	2.31	1 (25%)	6,6,6	0.91	0
5	AGS	D	551	3,4	24,33,33	4.54	2 (8%)	28,52,52	1.22	3 (10%)
5	AGS	E	1	3,4	24,33,33	4.56	2 (8%)	28,52,52	1.29	2 (7%)
2	SO4	E	4005	-	4,4,4	2.10	1 (25%)	6,6,6	0.93	0
2	SO4	E	4006	-	4,4,4	2.25	1 (25%)	6,6,6	0.85	0
5	AGS	F	1	3,4	24,33,33	4.44	3 (12%)	28,52,52	1.11	2 (7%)
2	SO4	F	4004	-	4,4,4	2.14	1 (25%)	6,6,6	0.90	0
5	AGS	G	1	3,4	24,33,33	4.59	1 (4%)	28,52,52	1.22	3 (10%)
2	SO4	G	4002	-	4,4,4	2.24	1 (25%)	6,6,6	0.89	0
5	AGS	H	1	3,4	24,33,33	4.44	1 (4%)	28,52,52	1.24	3 (10%)
2	SO4	H	4017	-	4,4,4	2.26	1 (25%)	6,6,6	0.89	0
2	SO4	H	4018	-	4,4,4	2.25	1 (25%)	6,6,6	0.88	0
5	AGS	I	1	3,4	24,33,33	4.47	1 (4%)	28,52,52	1.21	3 (10%)
5	AGS	J	1	3,4	24,33,33	4.47	2 (8%)	28,52,52	1.07	1 (3%)
2	SO4	J	4019	-	4,4,4	2.25	1 (25%)	6,6,6	0.90	0
2	SO4	J	4020	-	4,4,4	2.26	1 (25%)	6,6,6	0.87	0
5	AGS	K	1	3,4	24,33,33	4.47	2 (8%)	28,52,52	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	K	4021	-	4,4,4	2.30	1 (25%)	6,6,6	0.86	0
2	SO4	K	4022	-	4,4,4	2.23	1 (25%)	6,6,6	0.89	0
5	AGS	L	1	3,4	24,33,33	4.42	1 (4%)	28,52,52	1.20	3 (10%)
2	SO4	L	4003	-	4,4,4	2.24	1 (25%)	6,6,6	0.91	0
5	AGS	M	1	3,4	24,33,33	4.44	1 (4%)	28,52,52	1.17	4 (14%)
2	SO4	M	4013	-	4,4,4	2.35	1 (25%)	6,6,6	0.88	0
2	SO4	M	4014	-	4,4,4	2.28	1 (25%)	6,6,6	0.86	0
5	AGS	N	1	3,4	24,33,33	4.48	1 (4%)	28,52,52	1.13	2 (7%)
2	SO4	N	4015	-	4,4,4	2.27	1 (25%)	6,6,6	0.88	0
2	SO4	N	4016	-	4,4,4	2.25	1 (25%)	6,6,6	0.88	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
5	AGS	A	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	A	4001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4007	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4008	-	-	0/0/0/0	0/0/0/0
5	AGS	B	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	B	4009	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4010	-	-	0/0/0/0	0/0/0/0
5	AGS	C	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	C	4011	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4012	-	-	0/0/0/0	0/0/0/0
5	AGS	D	551	3,4	-	0/15/38/38	0/3/3/3
5	AGS	E	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	E	4005	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4006	-	-	0/0/0/0	0/0/0/0
5	AGS	F	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	F	4004	-	-	0/0/0/0	0/0/0/0
5	AGS	G	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	G	4002	-	-	0/0/0/0	0/0/0/0
5	AGS	H	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	H	4017	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4018	-	-	0/0/0/0	0/0/0/0
5	AGS	I	1	3,4	-	0/15/38/38	0/3/3/3
5	AGS	J	1	3,4	-	0/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	J	4019	-	-	0/0/0/0	0/0/0/0
2	SO4	J	4020	-	-	0/0/0/0	0/0/0/0
5	AGS	K	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	K	4021	-	-	0/0/0/0	0/0/0/0
2	SO4	K	4022	-	-	0/0/0/0	0/0/0/0
5	AGS	L	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	L	4003	-	-	0/0/0/0	0/0/0/0
5	AGS	M	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	M	4013	-	-	0/0/0/0	0/0/0/0
2	SO4	M	4014	-	-	0/0/0/0	0/0/0/0
5	AGS	N	1	3,4	-	0/15/38/38	0/3/3/3
2	SO4	N	4015	-	-	0/0/0/0	0/0/0/0
2	SO4	N	4016	-	-	0/0/0/0	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-21.88	1.48	1.90
5	E	1	AGS	PG-S1G	-21.80	1.48	1.90
5	D	551	AGS	PG-S1G	-21.68	1.48	1.90
5	N	1	AGS	PG-S1G	-21.36	1.49	1.90
5	I	1	AGS	PG-S1G	-21.35	1.49	1.90
5	H	1	AGS	PG-S1G	-21.24	1.49	1.90
5	C	1	AGS	PG-S1G	-21.23	1.49	1.90
5	J	1	AGS	PG-S1G	-21.22	1.49	1.90
5	K	1	AGS	PG-S1G	-21.19	1.49	1.90
5	M	1	AGS	PG-S1G	-21.16	1.49	1.90
5	F	1	AGS	PG-S1G	-21.06	1.49	1.90
5	L	1	AGS	PG-S1G	-21.05	1.49	1.90
5	B	1	AGS	PG-S1G	-20.87	1.50	1.90
5	A	1	AGS	PG-S1G	-20.75	1.50	1.90
5	F	1	AGS	PG-O3G	-2.13	1.47	1.55
5	D	551	AGS	PG-O3G	-2.02	1.48	1.55
5	E	1	AGS	PG-O3G	-2.00	1.48	1.55
5	F	1	AGS	C2-N3	2.03	1.35	1.32
5	C	1	AGS	O4'-C1'	2.10	1.43	1.41
5	J	1	AGS	O4'-C1'	2.28	1.44	1.41
5	K	1	AGS	O4'-C1'	3.36	1.45	1.41
2	E	4005	SO4	O1-S	4.05	1.61	1.47
2	F	4004	SO4	O1-S	4.12	1.61	1.47
2	A	4007	SO4	O1-S	4.25	1.61	1.47
2	K	4022	SO4	O1-S	4.31	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4003	SO4	O1-S	4.31	1.61	1.47
2	G	4002	SO4	O1-S	4.34	1.62	1.47
2	A	4001	SO4	O1-S	4.34	1.62	1.47
2	A	4008	SO4	O1-S	4.35	1.62	1.47
2	N	4016	SO4	O1-S	4.35	1.62	1.47
2	B	4009	SO4	O1-S	4.35	1.62	1.47
2	H	4017	SO4	O1-S	4.37	1.62	1.47
2	E	4006	SO4	O1-S	4.37	1.62	1.47
2	J	4020	SO4	O1-S	4.37	1.62	1.47
2	J	4019	SO4	O1-S	4.37	1.62	1.47
2	H	4018	SO4	O1-S	4.38	1.62	1.47
2	C	4011	SO4	O1-S	4.38	1.62	1.47
2	N	4015	SO4	O1-S	4.39	1.62	1.47
2	M	4014	SO4	O1-S	4.41	1.62	1.47
2	B	4010	SO4	O1-S	4.41	1.62	1.47
2	C	4012	SO4	O1-S	4.43	1.62	1.47
2	K	4021	SO4	O1-S	4.45	1.62	1.47
2	M	4013	SO4	O1-S	4.55	1.62	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1	AGS	C1'-N9-C4	-2.39	123.33	126.94
5	A	1	AGS	N3-C2-N1	-2.35	127.10	128.89
5	M	1	AGS	N3-C2-N1	-2.27	127.15	128.89
5	A	1	AGS	C1'-N9-C4	-2.21	123.61	126.94
5	L	1	AGS	C1'-N9-C4	-2.19	123.64	126.94
5	E	1	AGS	N3-C2-N1	-2.17	127.23	128.89
5	I	1	AGS	PB-O3B-PG	-2.17	125.38	132.67
5	D	551	AGS	N3-C2-N1	-2.16	127.24	128.89
5	C	1	AGS	N3-C2-N1	-2.14	127.26	128.89
5	B	1	AGS	N3-C2-N1	-2.11	127.28	128.89
5	D	551	AGS	C1'-N9-C4	-2.10	123.77	126.94
5	N	1	AGS	PB-O3B-PG	-2.10	125.63	132.67
5	G	1	AGS	C1'-N9-C4	-2.08	123.81	126.94
5	L	1	AGS	N3-C2-N1	-2.07	127.31	128.89
5	I	1	AGS	N3-C2-N1	-2.06	127.31	128.89
5	K	1	AGS	PB-O3B-PG	-2.06	125.76	132.67
5	M	1	AGS	PB-O3B-PG	-2.03	125.84	132.67
5	H	1	AGS	C1'-N9-C4	-2.03	123.87	126.94
5	G	1	AGS	PB-O3B-PG	-2.03	125.86	132.67
5	F	1	AGS	N3-C2-N1	-2.02	127.35	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	AGS	PB-O3B-PG	-2.02	125.89	132.67
5	H	1	AGS	PB-O3B-PG	-2.01	125.93	132.67
5	J	1	AGS	O4'-C1'-N9	2.37	113.06	108.10
5	N	1	AGS	O4'-C1'-N9	2.39	113.11	108.10
5	A	1	AGS	O4'-C1'-N9	2.44	113.21	108.10
5	F	1	AGS	O4'-C1'-N9	2.63	113.61	108.10
5	K	1	AGS	O4'-C1'-N9	2.86	114.09	108.10
5	M	1	AGS	O4'-C1'-N9	2.90	114.17	108.10
5	G	1	AGS	O4'-C1'-N9	2.92	114.22	108.10
5	D	551	AGS	O4'-C1'-N9	2.95	114.28	108.10
5	I	1	AGS	O4'-C1'-N9	2.98	114.34	108.10
5	L	1	AGS	O4'-C1'-N9	3.07	114.53	108.10
5	H	1	AGS	O4'-C1'-N9	3.10	114.59	108.10
5	C	1	AGS	O4'-C1'-N9	3.15	114.68	108.10
5	B	1	AGS	O4'-C1'-N9	3.38	115.17	108.10
5	E	1	AGS	O4'-C1'-N9	3.61	115.64	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	AGS	3	0
5	B	1	AGS	4	0
5	C	1	AGS	3	0
5	D	551	AGS	4	0
5	E	1	AGS	4	0
2	E	4005	SO4	1	0
5	F	1	AGS	3	0
5	G	1	AGS	4	0
5	H	1	AGS	4	0
5	I	1	AGS	4	0
5	J	1	AGS	3	0
5	K	1	AGS	5	0
5	L	1	AGS	5	0
5	M	1	AGS	5	0
5	N	1	AGS	4	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	525/547 (95%)	0.80	79 (15%) 3 3	28, 64, 121, 132	0
1	B	525/547 (95%)	1.44	130 (24%) 1 1	24, 59, 149, 159	0
1	C	525/547 (95%)	1.24	124 (23%) 1 1	29, 71, 141, 152	0
1	D	525/547 (95%)	0.54	34 (6%) 22 23	25, 48, 99, 115	0
1	E	525/547 (95%)	1.08	105 (20%) 1 2	23, 55, 134, 145	0
1	F	525/547 (95%)	1.37	122 (23%) 1 1	27, 66, 150, 159	0
1	G	525/547 (95%)	0.66	50 (9%) 10 11	26, 50, 113, 126	0
1	H	525/547 (95%)	0.72	65 (12%) 5 6	26, 56, 118, 130	0
1	I	525/547 (95%)	1.04	85 (16%) 3 3	31, 69, 132, 143	0
1	J	525/547 (95%)	1.11	94 (17%) 2 2	31, 73, 138, 146	0
1	K	525/547 (95%)	1.54	142 (27%) 1 1	31, 78, 151, 159	0
1	L	525/547 (95%)	0.98	94 (17%) 2 2	29, 66, 136, 149	0
1	M	525/547 (95%)	1.45	141 (26%) 1 1	30, 77, 152, 160	0
1	N	525/547 (95%)	0.79	69 (13%) 5 5	28, 65, 118, 129	0
All	All	7350/7658 (95%)	1.05	1334 (18%) 2 2	23, 60, 140, 160	0

All (1334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ILE	14.2
1	F	309	LEU	13.3
1	K	270	ILE	12.8
1	K	271	VAL	12.8
1	K	305	ILE	12.4
1	B	349	ILE	12.2
1	M	270	ILE	12.0
1	K	349	ILE	11.9

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Mol	Chain	Res	Type	RSRZ
1	F	240	VAL	11.5
1	J	356	ALA	11.1
1	E	353	ILE	11.1
1	E	356	ALA	10.9
1	F	233	MET	10.8
1	J	271	VAL	10.8
1	B	233	MET	10.8
1	F	353	ILE	10.8
1	M	353	ILE	10.7
1	B	356	ALA	10.7
1	I	270	ILE	10.7
1	J	270	ILE	10.6
1	C	356	ALA	10.5
1	K	309	LEU	10.3
1	M	259	LEU	10.3
1	L	266	THR	10.3
1	F	314	LEU	10.1
1	B	230	ILE	10.0
1	B	353	ILE	10.0
1	N	349	ILE	9.9
1	K	260	ALA	9.9
1	K	259	LEU	9.8
1	E	271	VAL	9.8
1	E	309	LEU	9.8
1	M	233	MET	9.8
1	M	237	LEU	9.7
1	C	270	ILE	9.7
1	F	259	LEU	9.6
1	K	236	VAL	9.6
1	J	269	GLY	9.5
1	M	221	LEU	9.5
1	M	271	VAL	9.3
1	C	353	ILE	9.3
1	K	237	LEU	9.3
1	F	349	ILE	9.2
1	J	349	ILE	9.0
1	K	233	MET	9.0
1	B	264	VAL	9.0
1	M	223	ALA	8.9
1	D	271	VAL	8.8
1	M	240	VAL	8.8
1	M	314	LEU	8.7

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Mol	Chain	Res	Type	RSRZ
1	F	270	ILE	8.5
1	I	305	ILE	8.4
1	B	301	ILE	8.4
1	K	231	ARG	8.4
1	K	360	TYR	8.4
1	I	271	VAL	8.3
1	B	227	ILE	8.3
1	K	267	MET	8.3
1	M	309	LEU	8.3
1	J	268	ARG	8.2
1	J	357	THR	8.2
1	B	258	ALA	8.2
1	B	281	PHE	8.1
1	B	365	LEU	8.1
1	A	270	ILE	8.1
1	K	264	VAL	8.1
1	M	267	MET	8.1
1	K	356	ALA	8.1
1	M	349	ILE	7.9
1	J	233	MET	7.9
1	M	357	THR	7.9
1	F	360	TYR	7.9
1	M	272	LYS	7.9
1	L	271	VAL	7.8
1	M	268	ARG	7.8
1	B	268	ARG	7.7
1	H	309	LEU	7.6
1	I	264	VAL	7.6
1	M	356	ALA	7.6
1	J	309	LEU	7.6
1	M	266	THR	7.6
1	L	270	ILE	7.6
1	A	356	ALA	7.6
1	K	265	ASN	7.5
1	K	203	TYR	7.5
1	K	353	ILE	7.5
1	C	271	VAL	7.5
1	K	268	ARG	7.5
1	A	353	ILE	7.4
1	I	356	ALA	7.2
1	E	230	ILE	7.2
1	M	239	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	K	340	ALA	7.2
1	N	263	VAL	7.1
1	F	227	ILE	7.1
1	M	264	VAL	7.1
1	E	349	ILE	7.1
1	M	251	ALA	7.1
1	B	259	LEU	7.1
1	I	265	ASN	7.1
1	E	234	LEU	7.0
1	L	264	VAL	7.0
1	F	219	PHE	7.0
1	M	273	VAL	7.0
1	J	353	ILE	7.0
1	F	230	ILE	7.0
1	J	44	PHE	7.0
1	M	244	GLY	7.0
1	I	268	ARG	6.9
1	L	231	ARG	6.9
1	E	233	MET	6.9
1	B	271	VAL	6.9
1	J	317	LEU	6.9
1	C	268	ARG	6.8
1	F	357	THR	6.8
1	E	223	ALA	6.8
1	M	358	SER	6.8
1	K	240	VAL	6.8
1	F	203	TYR	6.7
1	K	227	ILE	6.7
1	F	268	ARG	6.7
1	I	349	ILE	6.7
1	N	270	ILE	6.7
1	F	272	LYS	6.7
1	J	264	VAL	6.7
1	F	267	MET	6.7
1	M	204	PHE	6.7
1	F	255	GLU	6.7
1	I	230	ILE	6.6
1	B	309	LEU	6.6
1	M	263	VAL	6.6
1	J	237	LEU	6.6
1	J	526	LYS	6.6
1	G	230	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	229	ASN	6.6
1	B	257	GLU	6.6
1	E	305	ILE	6.6
1	B	265	ASN	6.5
1	E	266	THR	6.5
1	B	355	GLU	6.5
1	C	342	ILE	6.5
1	E	268	ARG	6.5
1	L	305	ILE	6.5
1	K	204	PHE	6.5
1	E	270	ILE	6.5
1	L	383	ALA	6.4
1	K	230	ILE	6.4
1	I	353	ILE	6.4
1	J	266	THR	6.4
1	F	222	LEU	6.4
1	B	307	MET	6.4
1	M	305	ILE	6.3
1	K	232	GLU	6.3
1	F	342	ILE	6.3
1	C	263	VAL	6.3
1	B	357	THR	6.3
1	H	233	MET	6.3
1	N	230	ILE	6.3
1	F	305	ILE	6.3
1	N	264	VAL	6.2
1	B	270	ILE	6.2
1	E	300	VAL	6.2
1	M	336	VAL	6.2
1	F	271	VAL	6.2
1	C	249	ILE	6.2
1	J	305	ILE	6.1
1	F	237	LEU	6.1
1	F	317	LEU	6.1
1	K	256	GLY	6.1
1	L	230	ILE	6.1
1	B	286	LYS	6.1
1	L	269	GLY	6.1
1	C	266	THR	6.0
1	K	223	ALA	6.0
1	F	234	LEU	6.0
1	B	240	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	357	THR	6.0
1	F	231	ARG	6.0
1	K	219	PHE	6.0
1	C	369	VAL	5.9
1	I	266	THR	5.9
1	G	383	ALA	5.9
1	B	269	GLY	5.9
1	L	309	LEU	5.9
1	K	306	GLY	5.8
1	H	270	ILE	5.8
1	I	352	GLN	5.8
1	B	203	TYR	5.8
1	C	237	LEU	5.8
1	E	312	ALA	5.8
1	B	342	ILE	5.8
1	L	234	LEU	5.8
1	M	265	ASN	5.8
1	K	228	SER	5.8
1	G	44	PHE	5.7
1	L	268	ARG	5.7
1	J	263	VAL	5.7
1	M	249	ILE	5.7
1	K	269	GLY	5.7
1	B	236	VAL	5.7
1	B	251	ALA	5.7
1	C	259	LEU	5.7
1	I	526	LYS	5.7
1	B	305	ILE	5.7
1	J	358	SER	5.6
1	J	351	GLN	5.6
1	K	241	ALA	5.6
1	M	342	ILE	5.6
1	C	203	TYR	5.6
1	K	188	ASP	5.6
1	M	365	LEU	5.6
1	F	389	MET	5.6
1	I	360	TYR	5.6
1	E	272	LYS	5.5
1	F	245	LYS	5.5
1	F	44	PHE	5.5
1	M	335	GLY	5.5
1	G	271	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	203	TYR	5.5
1	K	234	LEU	5.5
1	J	229	ASN	5.5
1	I	234	LEU	5.5
1	I	272	LYS	5.5
1	M	203	TYR	5.5
1	C	261	THR	5.5
1	K	273	VAL	5.5
1	C	365	LEU	5.5
1	H	234	LEU	5.5
1	B	231	ARG	5.5
1	F	273	VAL	5.4
1	K	383	ALA	5.4
1	B	237	LEU	5.4
1	C	256	GLY	5.4
1	E	351	GLN	5.4
1	L	259	LEU	5.4
1	J	219	PHE	5.4
1	A	263	VAL	5.4
1	B	273	VAL	5.4
1	C	357	THR	5.4
1	C	44	PHE	5.4
1	K	281	PHE	5.4
1	E	203	TYR	5.4
1	F	264	VAL	5.4
1	H	243	ALA	5.4
1	F	263	VAL	5.4
1	C	295	LEU	5.3
1	M	219	PHE	5.3
1	C	230	ILE	5.3
1	K	44	PHE	5.3
1	F	355	GLU	5.3
1	I	355	GLU	5.3
1	C	264	VAL	5.3
1	B	234	LEU	5.3
1	B	351	GLN	5.3
1	F	241	ALA	5.3
1	L	258	ALA	5.3
1	M	317	LEU	5.3
1	K	272	LYS	5.3
1	L	227	ILE	5.3
1	M	260	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	306	GLY	5.3
1	A	349	ILE	5.2
1	H	526	LYS	5.2
1	C	244	GLY	5.2
1	A	44	PHE	5.2
1	G	270	ILE	5.2
1	I	231	ARG	5.2
1	J	231	ARG	5.2
1	K	275	ALA	5.2
1	B	262	LEU	5.2
1	C	372	LEU	5.2
1	D	270	ILE	5.2
1	E	301	ILE	5.2
1	H	353	ILE	5.2
1	I	267	MET	5.2
1	B	44	PHE	5.2
1	K	335	GLY	5.2
1	M	186	GLU	5.2
1	M	195	PHE	5.2
1	C	304	GLU	5.1
1	D	230	ILE	5.1
1	H	356	ALA	5.1
1	K	263	VAL	5.1
1	C	333	ILE	5.1
1	M	340	ALA	5.1
1	J	281	PHE	5.1
1	H	229	ASN	5.1
1	J	265	ASN	5.1
1	F	365	LEU	5.1
1	I	309	LEU	5.1
1	D	44	PHE	5.1
1	B	526	LYS	5.1
1	I	243	ALA	5.0
1	C	360	TYR	5.0
1	L	317	LEU	5.0
1	M	250	ILE	5.0
1	B	266	THR	5.0
1	H	268	ARG	5.0
1	J	204	PHE	5.0
1	J	256	GLY	5.0
1	F	243	ALA	4.9
1	F	336	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	274	ALA	4.9
1	B	317	LEU	4.9
1	L	233	MET	4.9
1	C	362	ARG	4.9
1	G	267	MET	4.9
1	E	355	GLU	4.9
1	I	363	GLU	4.9
1	K	358	SER	4.9
1	L	356	ALA	4.9
1	G	265	ASN	4.9
1	I	233	MET	4.9
1	B	250	ILE	4.9
1	F	269	GLY	4.9
1	K	247	LEU	4.8
1	C	233	MET	4.8
1	H	357	THR	4.8
1	M	355	GLU	4.8
1	F	306	GLY	4.8
1	B	243	ALA	4.8
1	G	259	LEU	4.8
1	K	160	LYS	4.8
1	H	44	PHE	4.8
1	E	264	VAL	4.8
1	B	372	LEU	4.8
1	M	222	LEU	4.8
1	F	258	ALA	4.8
1	F	356	ALA	4.8
1	A	182	GLY	4.8
1	C	346	VAL	4.8
1	E	44	PHE	4.8
1	E	263	VAL	4.8
1	B	295	LEU	4.8
1	E	247	LEU	4.8
1	M	351	GLN	4.8
1	L	203	TYR	4.8
1	E	358	SER	4.8
1	K	302	SER	4.8
1	E	273	VAL	4.7
1	K	357	THR	4.7
1	A	357	THR	4.7
1	A	361	ASP	4.7
1	F	315	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	223	ALA	4.7
1	M	218	PRO	4.7
1	I	357	THR	4.7
1	M	230	ILE	4.7
1	A	358	SER	4.7
1	E	384	ALA	4.7
1	G	258	ALA	4.7
1	B	300	VAL	4.7
1	J	262	LEU	4.7
1	A	268	ARG	4.7
1	B	383	ALA	4.6
1	D	305	ILE	4.6
1	A	271	VAL	4.6
1	E	231	ARG	4.6
1	H	383	ALA	4.6
1	N	281	PHE	4.6
1	I	351	GLN	4.6
1	B	221	LEU	4.6
1	F	236	VAL	4.6
1	G	306	GLY	4.6
1	K	283	ASP	4.6
1	L	255	GLU	4.6
1	D	526	LYS	4.6
1	C	292	ILE	4.6
1	F	242	LYS	4.6
1	J	260	ALA	4.6
1	K	362	ARG	4.6
1	B	358	SER	4.6
1	K	334	ASP	4.5
1	M	238	GLU	4.5
1	L	244	GLY	4.5
1	C	350	ARG	4.5
1	F	244	GLY	4.5
1	C	265	ASN	4.5
1	E	265	ASN	4.5
1	K	365	LEU	4.5
1	G	264	VAL	4.5
1	L	267	MET	4.5
1	B	363	GLU	4.5
1	F	249	ILE	4.5
1	H	305	ILE	4.5
1	B	260	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	4.5
1	B	261	THR	4.5
1	E	237	LEU	4.5
1	C	267	MET	4.5
1	C	355	GLU	4.4
1	E	383	ALA	4.4
1	F	346	VAL	4.4
1	K	346	VAL	4.4
1	C	284	ARG	4.4
1	M	231	ARG	4.4
1	B	180	GLY	4.4
1	F	266	THR	4.4
1	F	260	ALA	4.4
1	C	340	ALA	4.4
1	J	383	ALA	4.4
1	B	209	GLU	4.4
1	M	295	LEU	4.4
1	C	273	VAL	4.4
1	E	346	VAL	4.4
1	F	224	ASP	4.4
1	K	351	GLN	4.4
1	L	314	LEU	4.4
1	M	262	LEU	4.4
1	E	240	VAL	4.4
1	M	526	LYS	4.4
1	B	304	GLU	4.3
1	B	302	SER	4.3
1	L	526	LYS	4.3
1	J	362	ARG	4.3
1	M	44	PHE	4.3
1	M	258	ALA	4.3
1	J	257	GLU	4.3
1	F	369	VAL	4.3
1	F	351	GLN	4.3
1	B	354	GLU	4.3
1	C	351	GLN	4.3
1	F	358	SER	4.3
1	K	332	ILE	4.3
1	D	264	VAL	4.3
1	L	229	ASN	4.2
1	B	225	LYS	4.2
1	K	299	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	228	SER	4.2
1	J	360	TYR	4.2
1	H	349	ILE	4.2
1	I	384	ALA	4.2
1	J	333	ILE	4.2
1	E	354	GLU	4.2
1	F	261	THR	4.2
1	K	331	THR	4.2
1	F	225	LYS	4.2
1	B	311	LYS	4.2
1	I	44	PHE	4.2
1	A	187	LEU	4.2
1	M	161	LEU	4.2
1	C	231	ARG	4.2
1	D	268	ARG	4.2
1	H	265	ASN	4.2
1	C	161	LEU	4.2
1	F	221	LEU	4.2
1	F	256	GLY	4.2
1	E	360	TYR	4.2
1	I	184	GLN	4.2
1	J	203	TYR	4.2
1	D	266	THR	4.1
1	N	356	ALA	4.1
1	B	244	GLY	4.1
1	B	293	ALA	4.1
1	B	289	LEU	4.1
1	G	268	ARG	4.1
1	K	355	GLU	4.1
1	C	526	LYS	4.1
1	K	350	ARG	4.1
1	I	358	SER	4.1
1	H	355	GLU	4.1
1	E	295	LEU	4.1
1	K	258	ALA	4.0
1	L	311	LYS	4.0
1	B	219	PHE	4.0
1	M	269	GLY	4.0
1	B	224	ASP	4.0
1	K	301	ILE	4.0
1	M	347	ALA	4.0
1	C	219	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	L	44	PHE	4.0
1	K	307	MET	4.0
1	M	307	MET	4.0
1	I	269	GLY	4.0
1	M	180	GLY	4.0
1	J	367	GLU	4.0
1	J	365	LEU	4.0
1	F	381	VAL	4.0
1	J	342	ILE	4.0
1	J	355	GLU	4.0
1	C	181	THR	4.0
1	K	369	VAL	4.0
1	G	325	ILE	4.0
1	B	282	GLY	3.9
1	K	274	ALA	3.9
1	H	346	VAL	3.9
1	J	361	ASP	3.9
1	G	182	GLY	3.9
1	F	265	ASN	3.9
1	K	372	LEU	3.9
1	J	381	VAL	3.9
1	C	286	LYS	3.9
1	E	242	LYS	3.9
1	G	229	ASN	3.9
1	J	267	MET	3.9
1	C	309	LEU	3.9
1	C	347	ALA	3.9
1	L	224	ASP	3.9
1	K	181	THR	3.9
1	M	160	LYS	3.9
1	M	333	ILE	3.9
1	G	266	THR	3.9
1	E	255	GLU	3.9
1	E	257	GLU	3.9
1	I	211	GLY	3.9
1	H	264	VAL	3.9
1	K	250	ILE	3.9
1	F	396	VAL	3.9
1	G	233	MET	3.9
1	M	301	ILE	3.8
1	F	181	THR	3.8
1	M	350	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	241	ALA	3.8
1	K	266	THR	3.8
1	L	239	ALA	3.8
1	A	183	LEU	3.8
1	F	248	LEU	3.8
1	N	256	GLY	3.8
1	L	353	ILE	3.8
1	B	314	LEU	3.8
1	E	345	ARG	3.8
1	K	276	VAL	3.8
1	M	254	VAL	3.8
1	A	261	THR	3.8
1	M	261	THR	3.8
1	E	220	ILE	3.8
1	F	214	GLU	3.8
1	I	237	LEU	3.8
1	I	204	PHE	3.8
1	J	273	VAL	3.8
1	N	258	ALA	3.8
1	L	219	PHE	3.8
1	I	369	VAL	3.7
1	M	236	VAL	3.7
1	G	262	LEU	3.7
1	J	280	GLY	3.7
1	K	222	LEU	3.7
1	F	340	ALA	3.7
1	B	191	GLU	3.7
1	K	304	GLU	3.7
1	J	319	GLN	3.7
1	K	311	LYS	3.7
1	C	204	PHE	3.7
1	C	281	PHE	3.7
1	J	243	ALA	3.7
1	A	265	ASN	3.7
1	J	272	LYS	3.7
1	L	186	GLU	3.7
1	H	266	THR	3.7
1	B	275	ALA	3.7
1	K	215	LEU	3.7
1	B	238	GLU	3.7
1	F	232	GLU	3.7
1	A	237	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	185	ASP	3.7
1	F	251	ALA	3.7
1	I	240	VAL	3.6
1	K	213	VAL	3.6
1	M	188	ASP	3.6
1	C	229	ASN	3.6
1	H	259	LEU	3.6
1	L	222	LEU	3.6
1	F	178	GLU	3.6
1	L	228	SER	3.6
1	A	203	TYR	3.6
1	F	215	LEU	3.6
1	F	372	LEU	3.6
1	M	384	ALA	3.6
1	B	263	VAL	3.6
1	L	275	ALA	3.6
1	L	247	LEU	3.6
1	L	349	ILE	3.6
1	N	44	PHE	3.6
1	I	263	VAL	3.6
1	M	346	VAL	3.6
1	C	212	ALA	3.6
1	I	258	ALA	3.6
1	K	243	ALA	3.6
1	M	383	ALA	3.6
1	K	221	LEU	3.6
1	A	231	ARG	3.6
1	H	242	LYS	3.6
1	A	276	VAL	3.6
1	B	249	ILE	3.5
1	C	332	ILE	3.5
1	B	360	TYR	3.5
1	K	352	GLN	3.5
1	F	180	GLY	3.5
1	N	266	THR	3.5
1	A	381	VAL	3.5
1	C	300	VAL	3.5
1	F	300	VAL	3.5
1	K	152	ALA	3.5
1	D	325	ILE	3.5
1	F	337	GLY	3.5
1	N	365	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	345	ARG	3.5
1	J	261	THR	3.5
1	M	286	LYS	3.5
1	C	240	VAL	3.5
1	B	298	GLY	3.5
1	M	300	VAL	3.5
1	N	526	LYS	3.5
1	B	222	LEU	3.5
1	E	215	LEU	3.5
1	K	342	ILE	3.5
1	G	181	THR	3.5
1	C	223	ALA	3.5
1	E	284	ARG	3.5
1	M	168	LYS	3.5
1	H	263	VAL	3.5
1	K	376	VAL	3.5
1	C	358	SER	3.5
1	A	266	THR	3.5
1	K	191	GLU	3.5
1	A	204	PHE	3.5
1	E	219	PHE	3.5
1	K	202	PRO	3.4
1	K	310	GLU	3.4
1	M	235	PRO	3.4
1	M	217	SER	3.4
1	N	363	GLU	3.4
1	C	306	GLY	3.4
1	E	267	MET	3.4
1	L	307	MET	3.4
1	M	229	ASN	3.4
1	M	389	MET	3.4
1	H	360	TYR	3.4
1	A	284	ARG	3.4
1	D	281	PHE	3.4
1	A	365	LEU	3.4
1	E	342	ILE	3.4
1	B	346	VAL	3.4
1	C	186	GLU	3.4
1	E	229	ASN	3.4
1	I	259	LEU	3.4
1	H	361	ASP	3.4
1	K	224	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	358	SER	3.4
1	L	310	GLU	3.4
1	M	354	GLU	3.4
1	K	297	GLY	3.4
1	A	188	ASP	3.4
1	L	324	VAL	3.4
1	J	248	LEU	3.4
1	I	340	ALA	3.4
1	M	320	ALA	3.4
1	B	525	PRO	3.4
1	C	322	ARG	3.4
1	M	322	ARG	3.4
1	N	231	ARG	3.4
1	F	361	ASP	3.4
1	D	236	VAL	3.4
1	J	240	VAL	3.4
1	I	245	LYS	3.4
1	M	343	GLN	3.4
1	A	260	ALA	3.4
1	I	215	LEU	3.4
1	M	360	TYR	3.4
1	C	319	GLN	3.3
1	J	242	LYS	3.3
1	A	264	VAL	3.3
1	K	300	VAL	3.3
1	G	305	ILE	3.3
1	H	230	ILE	3.3
1	J	354	GLU	3.3
1	J	363	GLU	3.3
1	D	323	VAL	3.3
1	I	336	VAL	3.3
1	L	381	VAL	3.3
1	D	383	ALA	3.3
1	K	214	GLU	3.3
1	M	181	THR	3.3
1	K	242	LYS	3.3
1	K	245	LYS	3.3
1	I	383	ALA	3.3
1	B	187	LEU	3.3
1	E	304	GLU	3.3
1	K	139	SER	3.3
1	K	255	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	322	ARG	3.3
1	C	242	LYS	3.3
1	A	355	GLU	3.3
1	A	363	GLU	3.3
1	F	332	ILE	3.3
1	L	382	GLY	3.3
1	F	384	ALA	3.3
1	M	224	ASP	3.3
1	M	323	VAL	3.3
1	A	304	GLU	3.3
1	F	186	GLU	3.3
1	D	231	ARG	3.3
1	L	272	LYS	3.2
1	N	325	ILE	3.2
1	A	384	ALA	3.2
1	C	260	ALA	3.2
1	F	354	GLU	3.2
1	C	317	LEU	3.2
1	F	161	LEU	3.2
1	C	180	GLY	3.2
1	B	361	ASP	3.2
1	L	206	ASN	3.2
1	E	292	ILE	3.2
1	H	351	GLN	3.2
1	C	341	ALA	3.2
1	K	320	ALA	3.2
1	N	203	TYR	3.2
1	B	215	LEU	3.2
1	N	357	THR	3.2
1	B	256	GLY	3.2
1	E	184	GLN	3.2
1	E	382	GLY	3.2
1	A	181	THR	3.2
1	M	369	VAL	3.2
1	C	272	LYS	3.2
1	M	247	LEU	3.2
1	N	362	ARG	3.2
1	C	363	GLU	3.2
1	F	347	ALA	3.2
1	G	257	GLU	3.2
1	K	288	MET	3.2
1	A	273	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	236	VAL	3.2
1	B	352	GLN	3.2
1	F	352	GLN	3.2
1	L	302	SER	3.2
1	B	284	ARG	3.2
1	B	254	VAL	3.2
1	K	381	VAL	3.2
1	J	234	LEU	3.2
1	I	302	SER	3.1
1	L	249	ILE	3.1
1	N	351	GLN	3.1
1	K	361	ASP	3.1
1	A	281	PHE	3.1
1	F	204	PHE	3.1
1	F	295	LEU	3.1
1	G	231	ARG	3.1
1	K	308	GLU	3.1
1	A	382	GLY	3.1
1	G	311	LYS	3.1
1	B	267	MET	3.1
1	F	155	ASP	3.1
1	H	325	ILE	3.1
1	L	265	ASN	3.1
1	C	222	LEU	3.1
1	C	247	LEU	3.1
1	E	526	LYS	3.1
1	H	300	VAL	3.1
1	A	388	GLU	3.1
1	K	257	GLU	3.1
1	C	305	ILE	3.1
1	K	312	ALA	3.1
1	K	341	ALA	3.1
1	M	243	ALA	3.1
1	M	304	GLU	3.1
1	C	301	ILE	3.1
1	N	257	GLU	3.1
1	D	269	GLY	3.1
1	F	362	ARG	3.1
1	E	258	ALA	3.1
1	E	274	ALA	3.1
1	B	248	LEU	3.1
1	L	161	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	313	THR	3.1
1	C	220	ILE	3.1
1	H	286	LYS	3.1
1	L	325	ILE	3.1
1	G	243	ALA	3.0
1	K	323	VAL	3.0
1	L	240	VAL	3.0
1	N	346	VAL	3.0
1	N	354	GLU	3.0
1	A	245	LYS	3.0
1	N	284	ARG	3.0
1	B	332	ILE	3.0
1	C	315	GLU	3.0
1	H	304	GLU	3.0
1	J	250	ILE	3.0
1	F	319	GLN	3.0
1	H	271	VAL	3.0
1	H	314	LEU	3.0
1	I	314	LEU	3.0
1	K	380	LYS	3.0
1	B	188	ASP	3.0
1	G	269	GLY	3.0
1	H	269	GLY	3.0
1	I	310	GLU	3.0
1	D	229	ASN	3.0
1	D	267	MET	3.0
1	E	224	ASP	3.0
1	G	234	LEU	3.0
1	H	363	GLU	3.0
1	N	369	VAL	3.0
1	K	205	ILE	3.0
1	M	299	THR	3.0
1	C	221	LEU	3.0
1	I	257	GLU	3.0
1	M	216	GLU	3.0
1	E	251	ALA	3.0
1	F	223	ALA	3.0
1	B	390	LYS	3.0
1	B	280	GLY	3.0
1	M	182	GLY	3.0
1	B	255	GLU	3.0
1	H	365	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	308	GLU	3.0
1	G	384	ALA	3.0
1	M	363	GLU	2.9
1	E	250	ILE	2.9
1	F	385	THR	2.9
1	C	336	VAL	2.9
1	K	317	LEU	2.9
1	L	336	VAL	2.9
1	A	301	ILE	2.9
1	C	250	ILE	2.9
1	M	220	ILE	2.9
1	C	352	GLN	2.9
1	J	184	GLN	2.9
1	F	238	GLU	2.9
1	I	365	LEU	2.9
1	N	360	TYR	2.9
1	B	274	ALA	2.9
1	C	226	LYS	2.9
1	I	260	ALA	2.9
1	C	172	GLU	2.9
1	L	308	GLU	2.9
1	K	220	ILE	2.9
1	B	228	SER	2.9
1	A	346	VAL	2.9
1	B	336	VAL	2.9
1	K	526	LYS	2.9
1	N	304	GLU	2.9
1	A	362	ARG	2.9
1	M	362	ARG	2.9
1	E	188	ASP	2.9
1	I	361	ASP	2.9
1	B	183	LEU	2.9
1	B	252	GLU	2.9
1	E	307	MET	2.9
1	L	273	VAL	2.9
1	N	265	ASN	2.9
1	N	283	ASP	2.9
1	K	325	ILE	2.9
1	L	333	ILE	2.9
1	N	353	ILE	2.9
1	A	295	LEU	2.9
1	H	237	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	248	LEU	2.9
1	N	309	LEU	2.9
1	D	203	TYR	2.9
1	K	164	GLU	2.9
1	A	184	GLN	2.8
1	A	250	ILE	2.8
1	B	205	ILE	2.8
1	J	301	ILE	2.8
1	G	314	LEU	2.8
1	I	229	ASN	2.8
1	K	295	LEU	2.8
1	C	334	ASP	2.8
1	A	305	ILE	2.8
1	E	249	ILE	2.8
1	I	250	ILE	2.8
1	B	348	GLN	2.8
1	D	262	LEU	2.8
1	L	184	GLN	2.8
1	N	241	ALA	2.8
1	M	279	PRO	2.8
1	I	284	ARG	2.8
1	F	250	ILE	2.8
1	J	303	GLU	2.8
1	L	304	GLU	2.8
1	M	234	LEU	2.8
1	C	299	THR	2.8
1	L	313	THR	2.8
1	A	256	GLY	2.8
1	C	269	GLY	2.8
1	J	177	VAL	2.8
1	N	382	GLY	2.8
1	A	209	GLU	2.8
1	E	232	GLU	2.8
1	C	248	LEU	2.8
1	A	300	VAL	2.8
1	E	381	VAL	2.8
1	M	319	GLN	2.8
1	H	315	GLU	2.8
1	M	193	MET	2.8
1	B	272	LYS	2.8
1	K	253	ASP	2.8
1	C	367	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	350	ARG	2.8
1	G	309	LEU	2.8
1	L	284	ARG	2.8
1	M	183	LEU	2.8
1	M	205	ILE	2.8
1	M	376	VAL	2.8
1	N	254	VAL	2.8
1	I	209	GLU	2.7
1	I	304	GLU	2.7
1	H	317	LEU	2.7
1	B	381	VAL	2.7
1	I	389	MET	2.7
1	I	256	GLY	2.7
1	F	281	PHE	2.7
1	N	311	LYS	2.7
1	M	315	GLU	2.7
1	A	259	LEU	2.7
1	D	234	LEU	2.7
1	I	301	ILE	2.7
1	M	215	LEU	2.7
1	F	343	GLN	2.7
1	L	462	PRO	2.7
1	J	387	VAL	2.7
1	H	297	GLY	2.7
1	H	335	GLY	2.7
1	E	361	ASP	2.7
1	F	350	ARG	2.7
1	C	215	LEU	2.7
1	I	154	SER	2.7
1	B	335	GLY	2.7
1	B	186	GLU	2.7
1	E	339	GLU	2.7
1	L	315	GLU	2.7
1	C	85	ALA	2.7
1	H	261	THR	2.7
1	L	232	GLU	2.7
1	E	317	LEU	2.7
1	E	318	GLY	2.7
1	L	200	LEU	2.7
1	M	256	GLY	2.7
1	B	239	ALA	2.7
1	G	261	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	286	LYS	2.7
1	C	209	GLU	2.7
1	D	257	GLU	2.7
1	N	267	MET	2.7
1	D	382	GLY	2.7
1	K	180	GLY	2.7
1	L	262	LEU	2.6
1	B	322	ARG	2.6
1	N	305	ILE	2.6
1	J	275	ALA	2.6
1	A	242	LYS	2.6
1	I	183	LEU	2.6
1	I	372	LEU	2.6
1	F	333	ILE	2.6
1	E	352	GLN	2.6
1	M	184	GLN	2.6
1	J	288	MET	2.6
1	M	298	GLY	2.6
1	C	354	GLU	2.6
1	J	232	GLU	2.6
1	L	281	PHE	2.6
1	C	217	SER	2.6
1	F	239	ALA	2.6
1	F	339	GLU	2.6
1	G	236	VAL	2.6
1	I	276	VAL	2.6
1	C	337	GLY	2.6
1	F	359	ASP	2.6
1	C	391	GLU	2.6
1	E	214	GLU	2.6
1	E	261	THR	2.6
1	J	334	ASP	2.6
1	K	261	THR	2.6
1	M	330	THR	2.6
1	J	152	ALA	2.6
1	J	332	ILE	2.6
1	K	175	ILE	2.6
1	H	236	VAL	2.6
1	C	160	LYS	2.6
1	H	245	LYS	2.6
1	J	304	GLU	2.6
1	M	361	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	365	LEU	2.6
1	G	221	LEU	2.6
1	J	181	THR	2.6
1	K	248	LEU	2.6
1	L	215	LEU	2.6
1	L	306	GLY	2.6
1	M	200	LEU	2.6
1	J	384	ALA	2.6
1	N	260	ALA	2.6
1	K	333	ILE	2.6
1	H	284	ARG	2.6
1	N	268	ARG	2.6
1	L	283	ASP	2.6
1	J	228	SER	2.5
1	K	321	LYS	2.5
1	B	303	GLU	2.5
1	B	367	GLU	2.5
1	E	299	THR	2.5
1	F	363	GLU	2.5
1	H	313	THR	2.5
1	N	259	LEU	2.5
1	C	236	VAL	2.5
1	M	324	VAL	2.5
1	G	283	ASP	2.5
1	M	316	ASP	2.5
1	J	302	SER	2.5
1	M	159	GLY	2.5
1	L	351	GLN	2.5
1	L	384	ALA	2.5
1	A	354	GLU	2.5
1	L	332	ILE	2.5
1	N	77	VAL	2.5
1	M	302	SER	2.5
1	K	284	ARG	2.5
1	B	308	GLU	2.5
1	C	287	ALA	2.5
1	L	204	PHE	2.5
1	M	185	ASP	2.5
1	J	215	LEU	2.5
1	K	161	LEU	2.5
1	D	184	GLN	2.5
1	F	285	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	300	VAL	2.5
1	M	381	VAL	2.5
1	G	382	GLY	2.5
1	H	306	GLY	2.5
1	M	311	LYS	2.5
1	M	232	GLU	2.5
1	M	329	THR	2.5
1	J	200	LEU	2.5
1	N	317	LEU	2.5
1	A	286	LYS	2.5
1	B	344	GLY	2.5
1	C	214	GLU	2.5
1	E	338	GLU	2.5
1	L	256	GLY	2.5
1	B	292	ILE	2.5
1	C	155	ASP	2.5
1	H	273	VAL	2.5
1	H	333	ILE	2.5
1	I	346	VAL	2.5
1	F	157	THR	2.5
1	I	288	MET	2.5
1	I	362	ARG	2.5
1	K	239	ALA	2.5
1	K	326	ASN	2.5
1	M	187	LEU	2.5
1	N	161	LEU	2.5
1	I	334	ASP	2.5
1	L	361	ASP	2.5
1	B	369	VAL	2.5
1	C	184	GLN	2.5
1	C	325	ILE	2.5
1	J	150	ILE	2.5
1	K	249	ILE	2.5
1	K	290	GLN	2.5
1	M	325	ILE	2.5
1	B	285	ARG	2.5
1	D	284	ARG	2.5
1	H	272	LYS	2.5
1	K	364	LYS	2.5
1	M	164	GLU	2.4
1	L	347	ALA	2.4
1	B	204	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	289	LEU	2.4
1	N	314	LEU	2.4
1	E	225	LYS	2.4
1	E	286	LYS	2.4
1	M	310	GLU	2.4
1	N	240	VAL	2.4
1	J	274	ALA	2.4
1	B	310	GLU	2.4
1	C	168	LYS	2.4
1	J	245	LYS	2.4
1	A	360	TYR	2.4
1	B	247	LEU	2.4
1	G	295	LEU	2.4
1	L	237	LEU	2.4
1	C	378	VAL	2.4
1	N	273	VAL	2.4
1	E	287	ALA	2.4
1	E	341	ALA	2.4
1	I	354	GLU	2.4
1	N	350	ARG	2.4
1	A	262	LEU	2.4
1	C	234	LEU	2.4
1	J	221	LEU	2.4
1	K	183	LEU	2.4
1	I	364	LYS	2.4
1	A	322	ARG	2.4
1	G	244	GLY	2.4
1	N	358	SER	2.4
1	J	325	ILE	2.4
1	M	274	ALA	2.4
1	N	275	ALA	2.4
1	E	168	LYS	2.4
1	A	200	LEU	2.4
1	K	184	GLN	2.4
1	A	240	VAL	2.4
1	C	258	ALA	2.4
1	F	213	VAL	2.4
1	G	263	VAL	2.4
1	J	369	VAL	2.4
1	K	278	ALA	2.4
1	N	383	ALA	2.4
1	M	191	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLN	2.4
1	C	201	SER	2.4
1	E	222	LEU	2.4
1	E	256	GLY	2.4
1	L	257	GLU	2.4
1	M	388	GLU	2.4
1	C	275	ALA	2.3
1	I	359	ASP	2.3
1	J	376	VAL	2.3
1	L	190	VAL	2.3
1	H	332	ILE	2.3
1	K	322	ARG	2.3
1	A	244	GLY	2.3
1	G	228	SER	2.3
1	K	371	LYS	2.3
1	D	181	THR	2.3
1	F	288	MET	2.3
1	A	359	ASP	2.3
1	N	224	ASP	2.3
1	C	290	GLN	2.3
1	J	345	ARG	2.3
1	L	236	VAL	2.3
1	A	311	LYS	2.3
1	H	339	GLU	2.3
1	A	288	MET	2.3
1	D	233	MET	2.3
1	E	334	ASP	2.3
1	E	350	ARG	2.3
1	H	231	ARG	2.3
1	D	314	LEU	2.3
1	I	317	LEU	2.3
1	I	311	LYS	2.3
1	K	367	GLU	2.3
1	E	227	ILE	2.3
1	F	297	GLY	2.3
1	G	220	ILE	2.3
1	K	229	ASN	2.3
1	K	292	ILE	2.3
1	L	201	SER	2.3
1	B	288	MET	2.3
1	B	389	MET	2.3
1	E	193	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	288	MET	2.3
1	K	386	GLU	2.3
1	N	186	GLU	2.3
1	F	183	LEU	2.3
1	J	223	ALA	2.3
1	B	297	GLY	2.3
1	C	188	ASP	2.3
1	K	366	GLN	2.3
1	M	306	GLY	2.3
1	A	236	VAL	2.3
1	E	238	GLU	2.3
1	F	257	GLU	2.3
1	L	213	VAL	2.3
1	L	369	VAL	2.3
1	N	271	VAL	2.3
1	F	321	LYS	2.3
1	L	225	LYS	2.3
1	B	331	THR	2.3
1	E	239	ALA	2.3
1	L	289	LEU	2.3
1	J	395	ARG	2.3
1	K	319	GLN	2.3
1	E	363	GLU	2.3
1	M	281	PHE	2.3
1	N	255	GLU	2.3
1	I	228	SER	2.3
1	J	244	GLY	2.3
1	N	242	LYS	2.3
1	B	324	VAL	2.3
1	I	236	VAL	2.3
1	K	254	VAL	2.3
1	I	193	MET	2.3
1	B	181	THR	2.3
1	C	216	GLU	2.3
1	A	526	LYS	2.3
1	D	188	ASP	2.3
1	H	319	GLN	2.3
1	K	363	GLU	2.3
1	N	184	GLN	2.3
1	G	326	ASN	2.3
1	L	212	ALA	2.3
1	E	372	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	372	LEU	2.3
1	A	339	GLU	2.2
1	F	310	GLU	2.2
1	K	186	GLU	2.2
1	L	355	GLU	2.2
1	F	160	LYS	2.2
1	M	294	THR	2.2
1	M	278	ALA	2.2
1	J	259	LEU	2.2
1	C	303	GLU	2.2
1	N	391	GLU	2.2
1	A	207	LYS	2.2
1	C	348	GLN	2.2
1	F	316	ASP	2.2
1	F	313	THR	2.2
1	J	230	ILE	2.2
1	E	43	SER	2.2
1	N	228	SER	2.2
1	I	341	ALA	2.2
1	C	134	LEU	2.2
1	E	259	LEU	2.2
1	F	247	LEU	2.2
1	H	222	LEU	2.2
1	I	248	LEU	2.2
1	J	284	ARG	2.2
1	N	134	LEU	2.2
1	E	336	VAL	2.2
1	H	323	VAL	2.2
1	L	323	VAL	2.2
1	E	160	LYS	2.2
1	K	168	LYS	2.2
1	L	245	LYS	2.2
1	A	350	ARG	2.2
1	N	223	ALA	2.2
1	C	314	LEU	2.2
1	D	215	LEU	2.2
1	A	267	MET	2.2
1	C	178	GLU	2.2
1	H	257	GLU	2.2
1	C	210	THR	2.2
1	F	364	LYS	2.2
1	G	403	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	281	PHE	2.2
1	E	297	GLY	2.2
1	E	306	GLY	2.2
1	D	253	ASP	2.2
1	I	249	ILE	2.2
1	L	243	ALA	2.2
1	J	206	ASN	2.2
1	N	355	GLU	2.2
1	E	366	GLN	2.2
1	H	302	SER	2.2
1	M	338	GLU	2.2
1	B	290	GLN	2.1
1	K	401	HIS	2.1
1	K	524	LEU	2.1
1	N	372	LEU	2.1
1	F	308	GLU	2.1
1	G	255	GLU	2.1
1	J	201	SER	2.1
1	K	298	GLY	2.1
1	A	258	ALA	2.1
1	D	273	VAL	2.1
1	E	340	ALA	2.1
1	G	240	VAL	2.1
1	M	345	ARG	2.1
1	B	220	ILE	2.1
1	B	388	GLU	2.1
1	K	315	GLU	2.1
1	E	183	LEU	2.1
1	F	290	GLN	2.1
1	I	219	PHE	2.1
1	I	366	GLN	2.1
1	C	252	GLU	2.1
1	C	381	VAL	2.1
1	F	188	ASP	2.1
1	M	142	LYS	2.1
1	L	183	LEU	2.1
1	N	234	LEU	2.1
1	G	319	GLN	2.1
1	H	184	GLN	2.1
1	M	252	GLU	2.1
1	C	364	LYS	2.1
1	C	384	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	341	ALA	2.1
1	J	235	PRO	2.1
1	N	361	ASP	2.1
1	E	369	VAL	2.1
1	G	323	VAL	2.1
1	H	240	VAL	2.1
1	H	298	GLY	2.1
1	N	336	VAL	2.1
1	F	229	ASN	2.1
1	A	205	ILE	2.1
1	J	220	ILE	2.1
1	M	257	GLU	2.1
1	N	397	GLU	2.1
1	L	321	LYS	2.1
1	C	289	LEU	2.1
1	E	248	LEU	2.1
1	L	238	GLU	2.1
1	F	323	VAL	2.1
1	F	324	VAL	2.1
1	M	352	GLN	2.1
1	J	175	ILE	2.1
1	A	309	LEU	2.1
1	B	235	PRO	2.1
1	G	308	GLU	2.1
1	I	255	GLU	2.1
1	B	368	ARG	2.1
1	D	258	ALA	2.1
1	G	219	PHE	2.1
1	C	190	VAL	2.1
1	C	361	ASP	2.1
1	H	367	GLU	2.0
1	A	342	ILE	2.0
1	J	249	ILE	2.0
1	A	395	ARG	2.0
1	C	246	PRO	2.0
1	E	462	PRO	2.0
1	J	289	LEU	2.0
1	A	180	GLY	2.0
1	M	344	GLY	2.0
1	C	254	VAL	2.0
1	E	321	LYS	2.0
1	K	199	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	284	ARG	2.0
1	A	335	GLY	2.0
1	B	182	GLY	2.0
1	C	227	ILE	2.0
1	I	332	ILE	2.0
1	D	183	LEU	2.0
1	N	237	LEU	2.0
1	A	233	MET	2.0
1	A	383	ALA	2.0
1	B	312	ALA	2.0
1	E	209	GLU	2.0
1	H	258	ALA	2.0
1	M	167	ASP	2.0
1	A	366	GLN	2.0
1	L	300	VAL	2.0
1	F	279	PRO	2.0
1	G	525	PRO	2.0
1	G	138	CYS	2.0
1	F	292	ILE	2.0
1	G	526	LYS	2.0
1	I	333	ILE	2.0
1	M	242	LYS	2.0
1	N	332	ILE	2.0
1	N	233	MET	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
2	SO4	K	4021	5/5	0.55	0.44	15.81	137,138,139,139	0
2	SO4	F	4004	5/5	0.84	0.32	12.50	137,138,138,138	0
2	SO4	N	4015	5/5	0.85	0.27	12.12	132,133,133,133	0
2	SO4	B	4009	5/5	0.86	0.28	12.02	118,119,119,120	0
2	SO4	C	4011	5/5	0.83	0.29	9.95	137,137,137,138	0
2	SO4	J	4019	5/5	0.89	0.23	9.62	123,124,124,124	0
2	SO4	A	4007	5/5	0.84	0.27	8.79	128,129,129,129	0
2	SO4	E	4005	5/5	0.87	0.34	8.18	140,141,141,141	0
2	SO4	H	4017	5/5	0.68	0.33	6.73	145,146,146,146	0
2	SO4	L	4003	5/5	0.75	0.24	4.60	130,131,132,132	0
2	SO4	G	4002	5/5	0.82	0.27	4.55	128,128,129,129	0
2	SO4	A	4001	5/5	0.86	0.24	4.49	119,120,120,120	0
2	SO4	M	4013	5/5	0.81	0.23	4.37	126,126,127,127	0
4	K	I	549	1/1	0.99	0.18	1.25	43,43,43,43	0
5	AGS	D	551	31/31	0.94	0.16	1.21	25,31,39,41	0
4	K	H	549	1/1	0.98	0.15	0.93	41,41,41,41	0
4	K	M	549	1/1	0.99	0.14	0.93	45,45,45,45	0
5	AGS	C	1	31/31	0.96	0.14	0.60	37,41,49,52	0
4	K	J	549	1/1	0.99	0.14	0.60	47,47,47,47	0
5	AGS	J	1	31/31	0.95	0.13	0.54	39,42,53,54	0
4	K	G	549	1/1	0.98	0.15	0.52	39,39,39,39	0
5	AGS	N	1	31/31	0.96	0.14	0.51	35,39,47,48	0
5	AGS	M	1	31/31	0.95	0.14	0.49	38,42,50,52	0
5	AGS	L	1	31/31	0.95	0.14	0.43	34,37,45,48	0
5	AGS	G	1	31/31	0.95	0.14	0.31	25,32,40,41	0
5	AGS	K	1	31/31	0.95	0.13	0.27	37,40,51,54	0
5	AGS	E	1	31/31	0.96	0.12	0.21	27,30,34,37	0
5	AGS	H	1	31/31	0.96	0.13	0.14	30,34,38,42	0
4	K	D	549	1/1	0.98	0.14	0.08	34,34,34,34	0
5	AGS	A	1	31/31	0.96	0.12	0.02	35,38,42,44	0
5	AGS	F	1	31/31	0.95	0.14	0.01	34,37,44,45	0
5	AGS	B	1	31/31	0.96	0.12	-0.08	31,37,48,50	0
4	K	N	549	1/1	0.96	0.12	-0.11	41,41,41,41	0
5	AGS	I	1	31/31	0.96	0.14	-0.34	37,41,48,51	0
4	K	C	549	1/1	0.97	0.12	-0.45	45,45,45,45	0
4	K	K	549	1/1	0.97	0.12	-0.46	46,46,46,46	0
4	K	L	549	1/1	0.99	0.14	-0.48	39,39,39,39	0
4	K	A	549	1/1	0.99	0.12	-0.53	40,40,40,40	0
4	K	F	549	1/1	0.99	0.11	-0.59	41,41,41,41	0
4	K	B	549	1/1	0.98	0.12	-0.68	38,38,38,38	0
4	K	E	4007	1/1	0.99	0.11	-1.39	36,36,36,36	0
4	K	D	1	1/1	0.99	0.12	-1.75	30,30,30,30	0
4	K	E	549	1/1	0.99	0.08	-2.48	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	N	4016	5/5	0.83	0.26	-	137,137,137,138	0
3	MG	B	550	1/1	0.95	0.14	-	31,31,31,31	0
3	MG	G	550	1/1	0.97	0.18	-	29,29,29,29	0
2	SO4	M	4014	5/5	0.75	0.24	-	142,142,143,143	0
3	MG	I	550	1/1	0.97	0.17	-	34,34,34,34	0
3	MG	E	550	1/1	0.98	0.10	-	24,24,24,24	0
3	MG	C	550	1/1	0.99	0.15	-	36,36,36,36	0
2	SO4	H	4018	5/5	0.75	0.33	-	125,125,126,126	0
2	SO4	K	4022	5/5	0.84	0.27	-	145,146,146,146	0
3	MG	F	550	1/1	0.97	0.13	-	30,30,30,30	0
3	MG	L	550	1/1	0.93	0.12	-	31,31,31,31	0
2	SO4	B	4010	5/5	0.84	0.29	-	137,137,137,138	0
2	SO4	C	4012	5/5	0.70	0.27	-	141,141,141,142	0
3	MG	N	550	1/1	0.97	0.20	-	34,34,34,34	0
3	MG	H	550	1/1	0.98	0.15	-	26,26,26,26	0
3	MG	A	550	1/1	0.97	0.18	-	31,31,31,31	0
2	SO4	J	4020	5/5	0.75	0.47	-	160,160,160,160	0
3	MG	D	550	1/1	0.97	0.14	-	29,29,29,29	0
2	SO4	E	4006	5/5	0.75	0.33	-	118,119,119,120	0
3	MG	K	550	1/1	0.98	0.12	-	35,35,35,35	0
3	MG	J	550	1/1	0.98	0.13	-	37,37,37,37	0
2	SO4	A	4008	5/5	0.77	0.36	-	150,150,150,150	0
3	MG	M	550	1/1	0.98	0.19	-	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.