



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 07:58 AM EDT

PDB ID : 1KP8
Title : Structural Basis for GroEL-assisted Protein Folding from the Crystal Structure of (GroEL-KMgATP)₁₄ at 2.0 Å Resolution
Authors : Wang, J.
Deposited on : unknown
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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

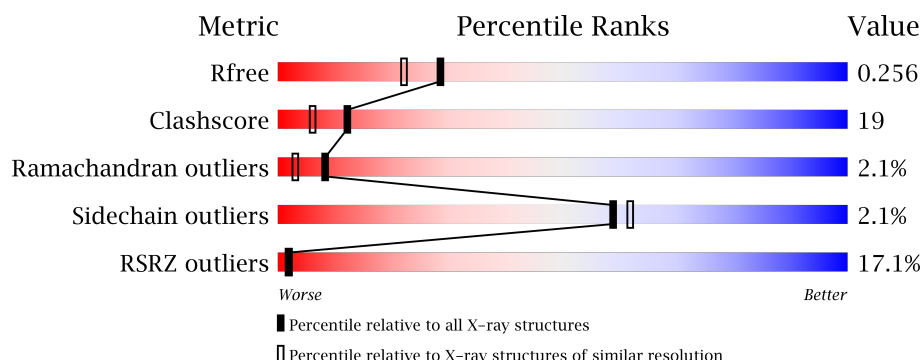
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 $\leq 5\%$. 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	<div> <div>13%</div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
1	B	547	<div> <div>23%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
1	C	547	<div> <div>21%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
1	D	547	<div> <div>6%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	E	547	<div> <div>18%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

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: O₄S).



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

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

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

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

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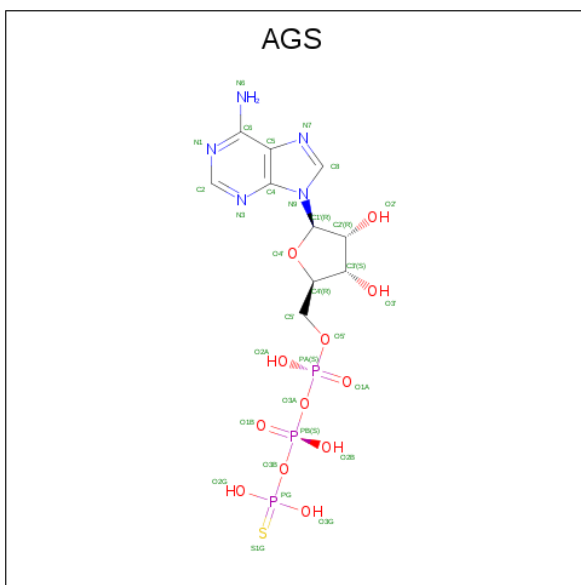
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0

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

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

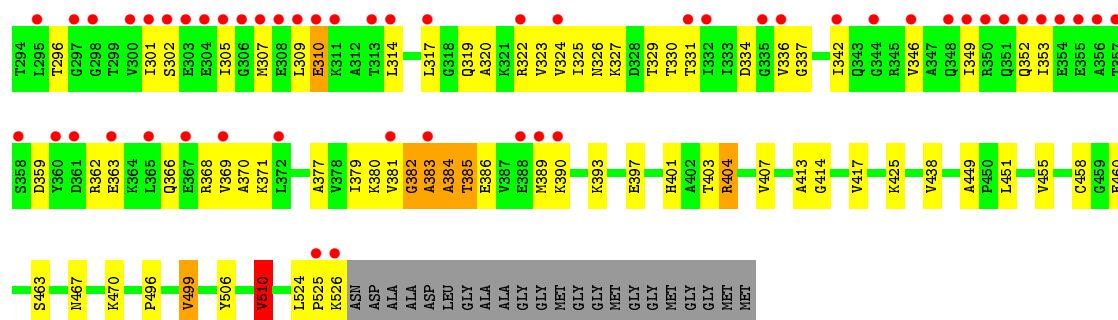
- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



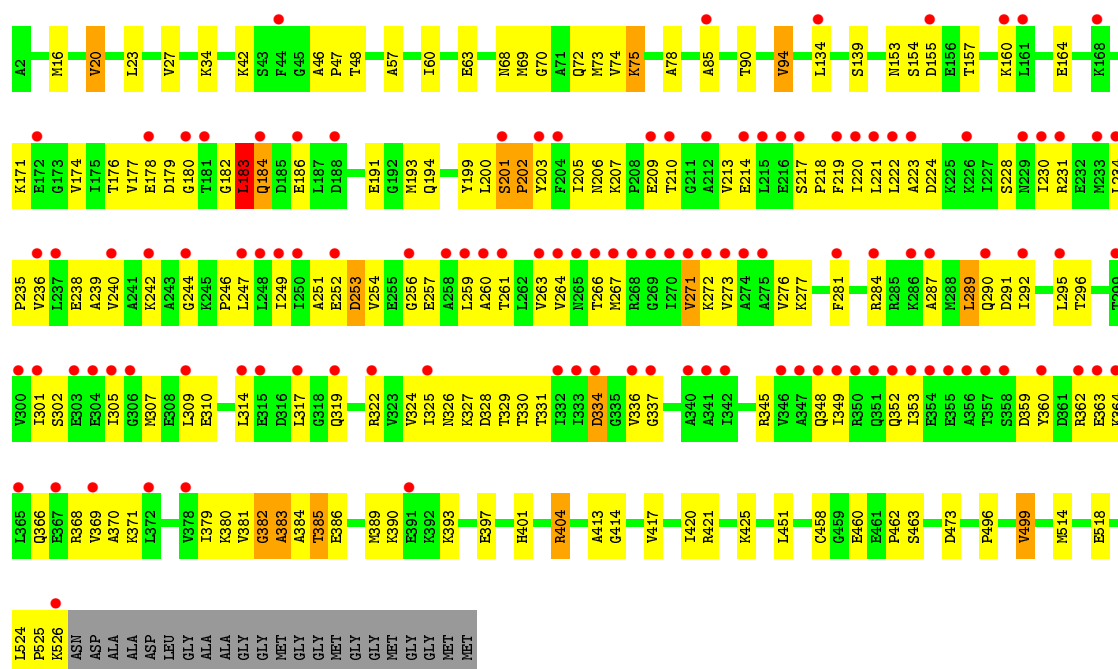
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	G	1	Total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

- Molecule 6 is water.

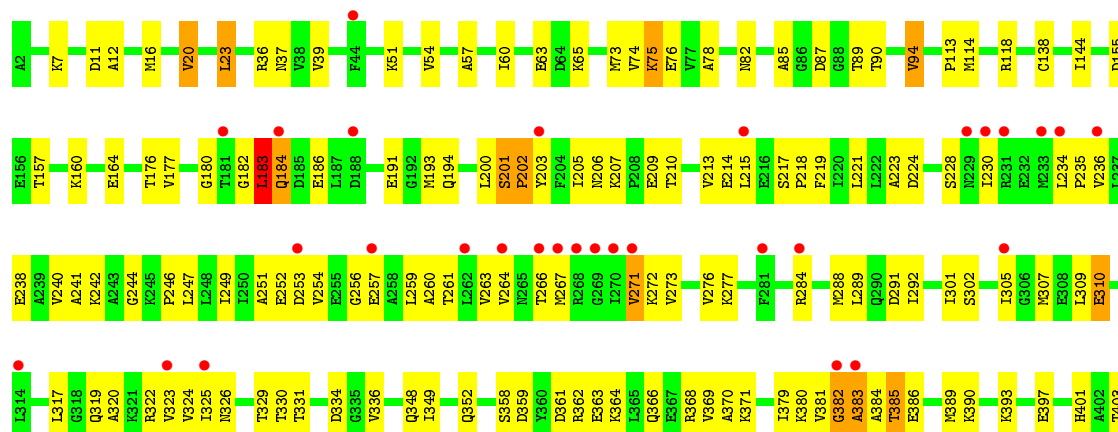
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total 156	O 156	0	0
6	B	214	Total 214	O 214	0	0
6	C	149	Total 149	O 149	0	0
6	D	261	Total 261	O 261	0	0
6	E	217	Total 217	O 217	0	0
6	F	200	Total 200	O 200	0	0
6	G	269	Total 269	O 269	0	0
6	H	204	Total 204	O 204	0	0
6	I	145	Total 145	O 145	0	0
6	J	139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

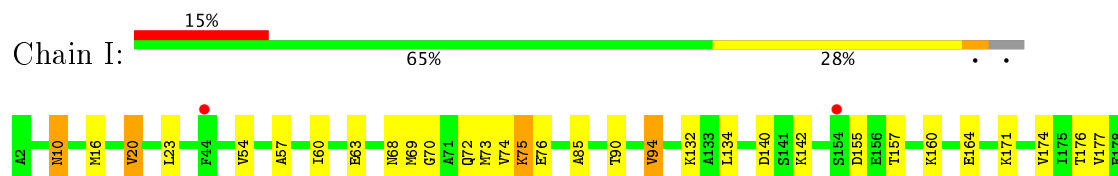
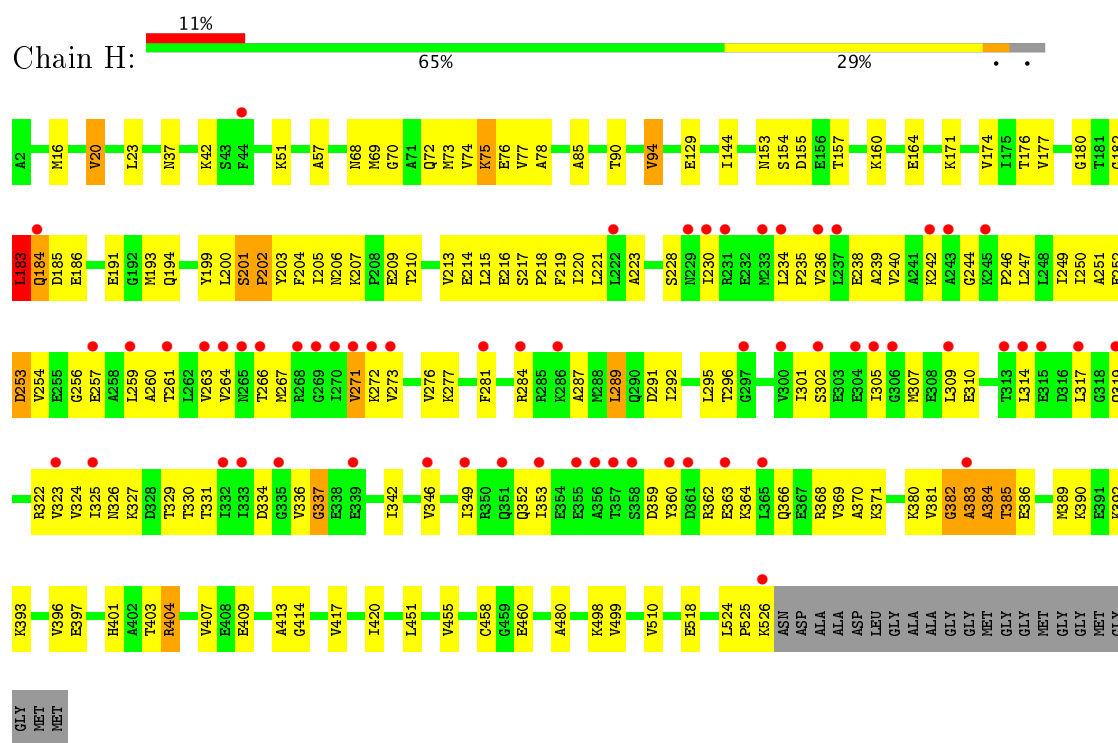
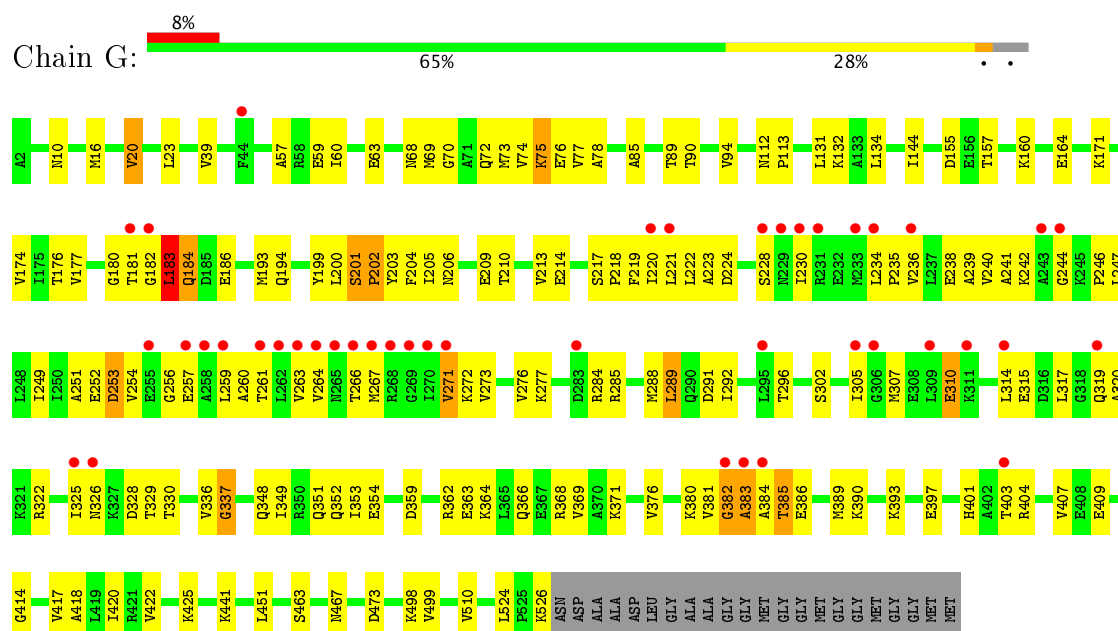


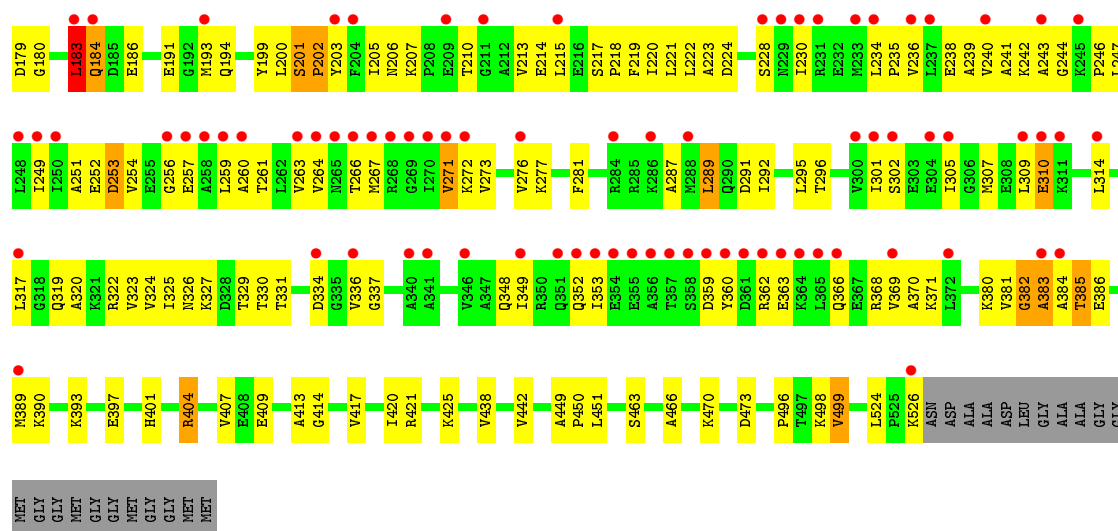
• Molecule 1: groEL protein



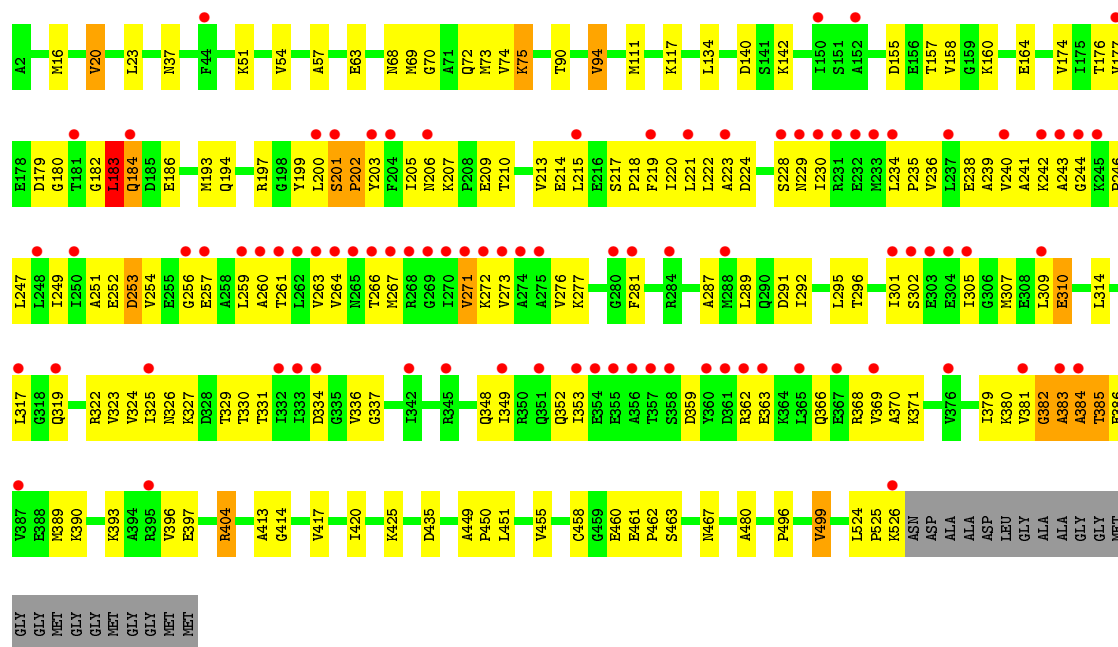
• Molecule 1: groEL protein



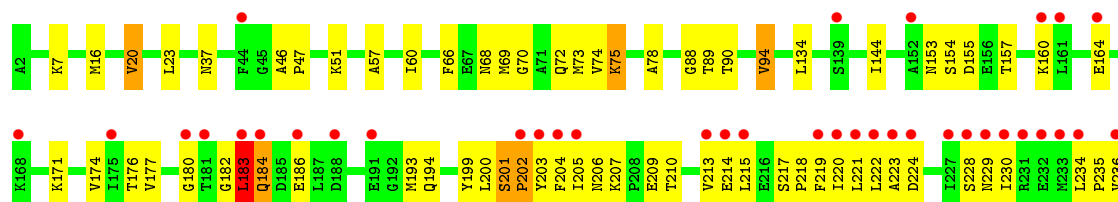


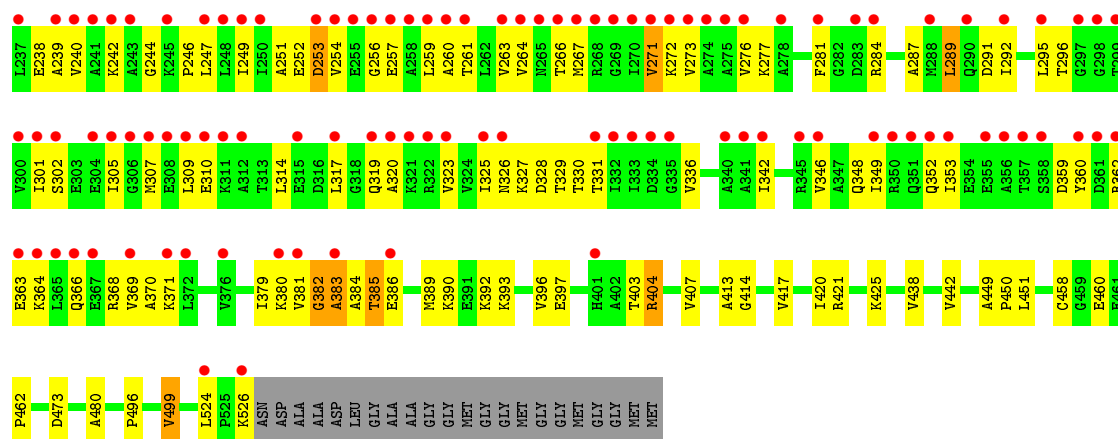


• Molecule 1: groEL protein

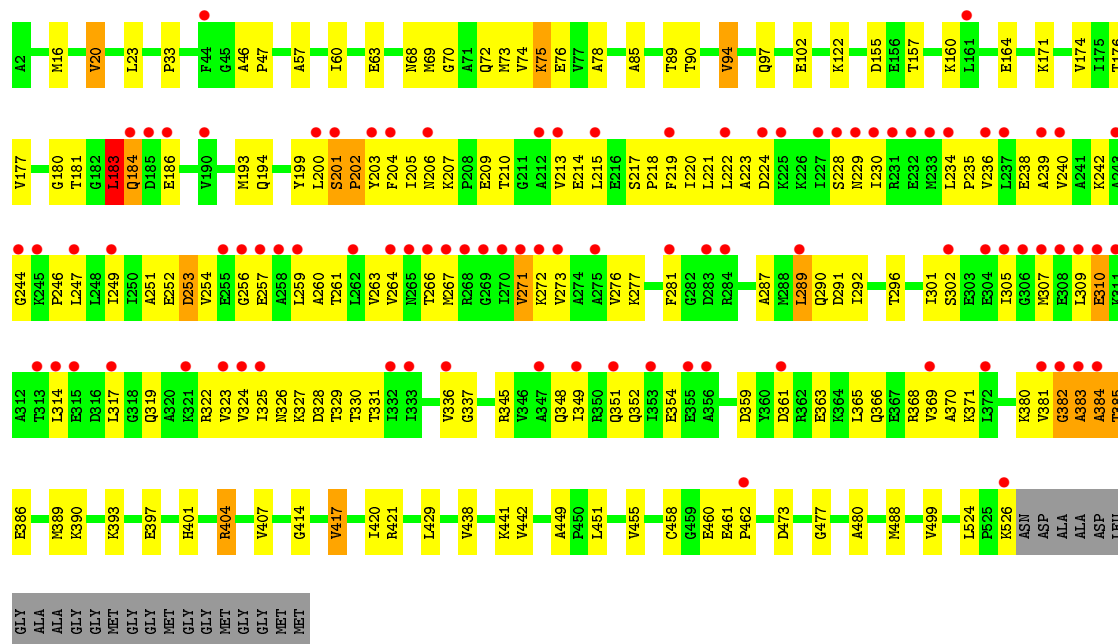


• Molecule 1: groEL protein

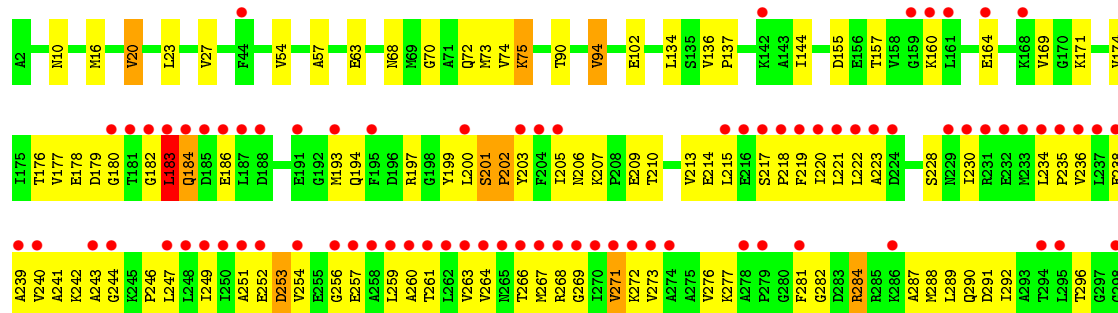


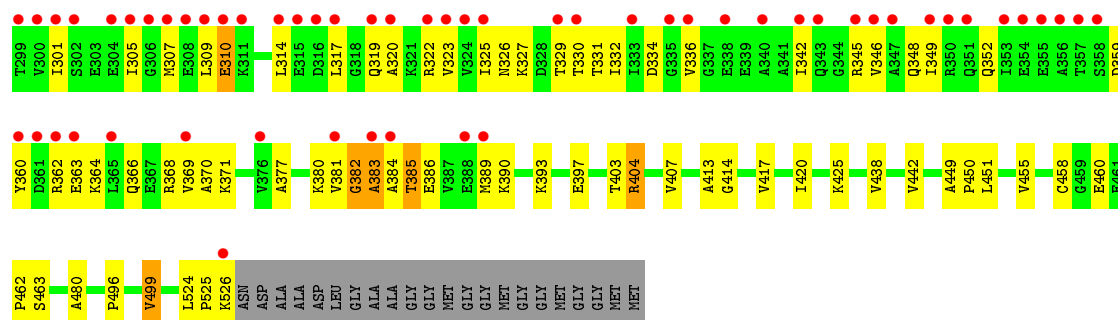


• Molecule 1: groEL protein

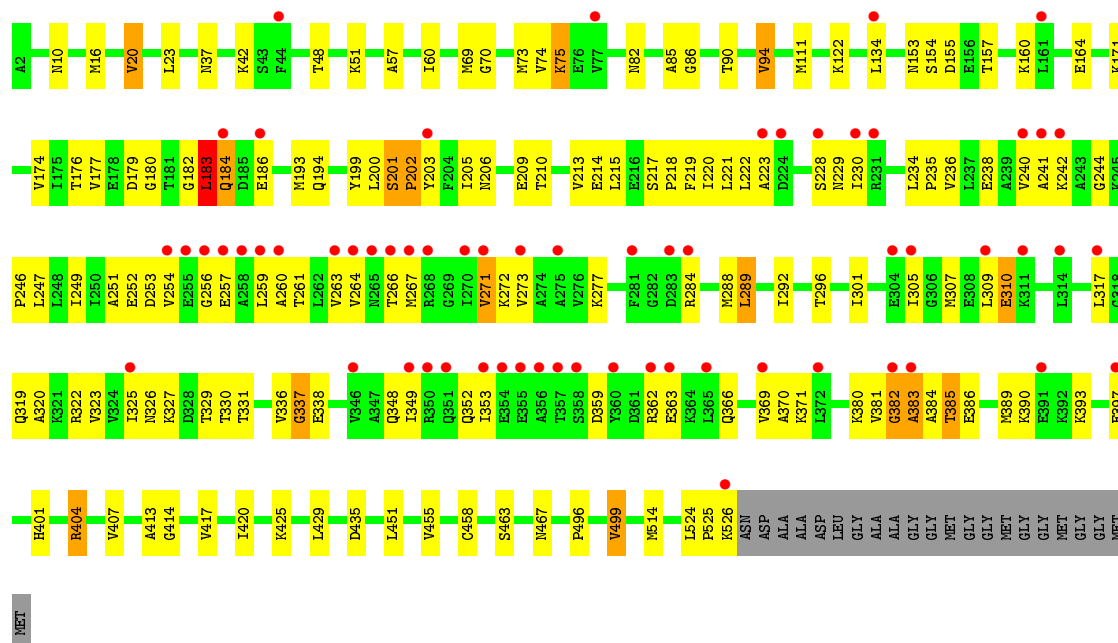


• Molecule 1: groEL protein





• Molecule 1: groEL protein



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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:S1G	5:H:1:AGS:PG	1.49	1.49
5:M:1:AGS:S1G	5:M:1:AGS:PG	1.49	1.48
5:D:551:AGS:PG	5:D:551:AGS:S1G	1.48	1.48
5:K:1:AGS:S1G	5:K:1:AGS:PG	1.49	1.48
5:F:1:AGS:PG	5:F:1:AGS:S1G	1.49	1.48
5:J:1:AGS:S1G	5:J:1:AGS:PG	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:C:1:AGS:PG	5:C:1:AGS:S1G	1.49	1.47
5:E:1:AGS:PG	5:E:1:AGS:S1G	1.48	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: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:N:183:LEU:H	1:N:383:ALA:HB3	1.17	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:A:235:PRO:HG3	1:A:310:GLU:HA	1.48	0.95
1:H:383:ALA:HB1	1:I:281:PHE:HZ	1.31	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:F:235:PRO:HG3	1:F:310:GLU:HA	1.49	0.94
1:J:383:ALA:HB1	1:K:281:PHE:HZ	1.33	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:E:218:PRO:HB3	1:E:246:PRO:HG2	1.49	0.91
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.53	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:F:218:PRO:HB3	1:F:246:PRO:HG2	1.51	0.89
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.55	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:H:289:LEU:HG	6:H:2938:HOH:O	1.77	0.82
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.60	0.82
1:J:57:ALA:O	1:J:75:LYS:HE2	1.80	0.82
1:B:86:GLY:HA3	1:B:401:HIS:CE1	2.15	0.82
1:I:183:LEU:N	1:I:383:ALA:HB3	1.93	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:B:200:LEU:HD21	1:B:277:LYS:HG3	1.64	0.80
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.64	0.80
1:N:57:ALA:O	1:N:75:LYS:HE2	1.80	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:359:ASP:O	1:C:363:GLU:HG2	1.83	0.79
1:C:463:SER:HB2	6:C:2549:HOH:O	1.82	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:I:359:ASP:O	1:I:363:GLU:HG2	1.86	0.76
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.68	0.76
1:F:414:GLY:O	1:F:417:VAL:HG13	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:M:381:VAL:HG21	1:M:393:LYS:HA	1.65	0.76
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.66	0.75
1:F:200:LEU:HD21	1:F:277:LYS:HG3	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:E:194:GLN:O	1:E:371:LYS:HE3	1.87	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: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
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.70	0.74
5:J:1:AGS:O3B	5:J:1:AGS:S1G	2.45	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
1:C:183:LEU:N	1:C:383:ALA:HB3	2.02	0.73
5:G:1:AGS:O3B	5:G:1:AGS:S1G	2.45	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:B:381:VAL:HG21	1:B:393:LYS:HA	1.71	0.73
1:I:381:VAL:HG21	1:I: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
1:A:57:ALA:O	1:A:75:LYS:HE2	1.89	0.72
5:N:1:AGS:O3G	5:N:1:AGS:S1G	2.46	0.72
1:F:263:VAL:O	1:F:267:MET:HB2	1.89	0.72
5:G:1:AGS:S1G	5:G:1:AGS:O3G	2.46	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
1:B:194:GLN:O	1:B:371:LYS:HE3	1.89	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:K:57:ALA:O	1:K:75:LYS:HE2	1.89	0.72
1:C:514:MET:HB3	6:C:2670:HOH:O	1.89	0.72
1:I:383:ALA:HB1	1:J:281:PHE:HZ	1.55	0.72
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.72	0.72
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.70	0.72
5:K:1:AGS:S1G	5:K:1:AGS:O3G	2.46	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: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:H:404:ARG:NH1	6:H:2827:HOH:O	2.24	0.71
1:L:57:ALA:O	1:L:75:LYS:HE2	1.89	0.71
1:G:177:VAL:HG21	1:G:397:GLU:CG	2.21	0.71
1:M:183:LEU:N	1:M:383:ALA:HB3	2.05	0.71
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.73	0.71
1:B:305:ILE:HD12	1:B:307:MET:HE2	1.72	0.71
5:F:1:AGS:S1G	5:F:1:AGS:O3B	2.48	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:D:420:ILE:HD12	1:D:451:LEU:HD13	1.72	0.70
1:K:414:GLY:O	1:K:417:VAL:HG13	1.91	0.70
1:I:183:LEU:H	1:I:383:ALA:CB	1.98	0.70
1:L:194:GLN:O	1:L:371:LYS:HE3	1.91	0.70
1:M:194:GLN:O	1:M: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: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
5:F:1:AGS:S1G	5:F:1:AGS:O3G	2.46	0.70
5:M:1:AGS:S1G	5:M:1:AGS:O3B	2.50	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: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:K:263:VAL:O	1:K:267:MET:HB2	1.92	0.69
1:L:183:LEU:H	1:L:383:ALA:CB	1.95	0.69
1:A:263:VAL:O	1:A:267:MET:HB2	1.91	0.69
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.74	0.69
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.23	0.69
5:D:551:AGS:S1G	5:D:551:AGS:O3G	2.45	0.69
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.74	0.69
5:J:1:AGS:O3G	5:J:1:AGS:S1G	2.47	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
1:C:525:PRO:HD3	6:C:1993:HOH:O	1.93	0.69
1:H:183:LEU:H	1:H:383:ALA:CB	1.98	0.69
5:I:1:AGS:S1G	5:I:1:AGS:O3G	2.45	0.69
1:M:414:GLY:O	1:M:417:VAL:HG13	1.92	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:D:213:VAL:HB	1:D:325:ILE:CG1	2.23	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
5:E:1:AGS:O3G	5:E:1:AGS:S1G	2.46	0.69
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.23	0.69
5:H:1:AGS:O3G	5:H:1:AGS:S1G	2.48	0.69
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.75	0.69
5:K:1:AGS:O3B	5:K:1:AGS:S1G	2.50	0.69
1:L:263:VAL:O	1:L:267:MET:HB2	1.93	0.69
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.74	0.69
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.75	0.68
1:H:183:LEU:HD23	1:H:384:ALA:HB2	1.76	0.68
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.23	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:J:183:LEU:H	1:J:383:ALA:CB	1.98	0.68
1:L:449:ALA:HB1	6:L:2642:HOH:O	1.93	0.68
1:B:263:VAL:O	1:B:267:MET:HB2	1.93	0.68
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.75	0.68
1:C:263:VAL:O	1:C:267:MET:HB2	1.93	0.68
1:H:305:ILE:HD12	1:H:307:MET:HE2	1.76	0.68
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.76	0.68
1:B:414:GLY:O	1:B:417:VAL:HG13	1.93	0.68
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.75	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:C:228:SER:O	1:C:257:GLU:HB3	1.95	0.67
1:H:177:VAL:HG21	1:H:397:GLU:CG	2.25	0.67
5:B:1:AGS:O3G	5:B:1:AGS:S1G	2.48	0.67
1:E:263:VAL:O	1:E:267:MET:HB2	1.94	0.67
1:J:384:ALA:HA	1:K:360:TYR:OH	1.95	0.67
1:D:160:LYS:O	1:D:164:GLU:HG3	1.95	0.66
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.76	0.66
1:N:305:ILE:HD12	1:N:307:MET:HE2	1.76	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
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:H:174:VAL:HG22	1:H:194:GLN:HE21	1.61	0.66
5:M:1:AGS:O3G	5:M:1:AGS:S1G	2.47	0.66
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.60	0.66
1:E:414:GLY:O	1:E:417:VAL:HG13	1.95	0.66
1:F:177:VAL:HG21	1:F:397:GLU:CG	2.26	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:N:183:LEU:HD23	1:N:384:ALA:HB2	1.78	0.66
1:A:194:GLN:O	1:A:371:LYS:HE3	1.94	0.66
1:B:183:LEU:HD23	1:B:384:ALA:HB2	1.77	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:I:160:LYS:O	1:I:164:GLU:HG3	1.96	0.66
1:L:183:LEU:HD23	1:L:384:ALA:HB2	1.78	0.66
1:E:392:LYS:HE3	6:E:2648:HOH:O	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:F:228:SER:O	1:F:257:GLU:HB3	1.95	0.66
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.77	0.66
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.78	0.65
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	0.65
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:228:SER:O	1:H:257:GLU:HB3	1.97	0.65
1:I:414:GLY:O	1:I:417:VAL:HG13	1.96	0.65
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.78	0.65
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.79	0.65
1:H:404:ARG:CG	1:H:404:ARG:HH11	2.08	0.65
1:D:326:ASN:HD22	1:D:329:THR:HB	1.61	0.65
1:F:178:GLU:OE2	1:F:322:ARG:HD3	1.96	0.65
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.77	0.65
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.27	0.65
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.26	0.65
1:L:228:SER:O	1:L:257:GLU:HB3	1.97	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:G:242:LYS:C	1:G:244:GLY:H	1.98	0.65
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.78	0.65
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.78	0.65
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.79	0.65
1:C:221:LEU:HD23	1:C:249:ILE:HD12	1.79	0.65
1:H:281:PHE:CZ	1:N:383:ALA:HB1	2.28	0.65
1:B:91:THR:O	1:B:94:VAL:HG22	1.96	0.65
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.79	0.65
1:H:42:LYS:HB2	6:H:2847:HOH:O	1.96	0.65
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.77	0.65
1:K:228:SER:O	1:K:257:GLU:HB3	1.97	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:E:177:VAL:HG21	1:E:397:GLU:HG3	1.79	0.64
1:G:228:SER:O	1:G:257:GLU:HB3	1.97	0.64
1:H:69:MET:O	1:H:73:MET:HG3	1.96	0.64
1:F:194:GLN:O	1:F:371:LYS:HE3	1.97	0.64
1:H:414:GLY:O	1:H:417:VAL:HG13	1.98	0.64
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.79	0.64
1:A:349:ILE:HA	1:A:352:GLN:CG	2.27	0.64
1:B:160:LYS:O	1:B:164:GLU:HG3	1.97	0.64
1:F:183:LEU:HD23	1:F:384:ALA:HB2	1.80	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:I:383:ALA:HB1	1:J:281:PHE:CZ	2.32	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:B:176:THR:HG21	1:B:322:ARG:HH12	1.63	0.64
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:219:PHE:HB3	1:B:317:LEU:HD23	1.80	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:J:177:VAL:HG21	1:J:397:GLU:HG3	1.80	0.64
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.63	0.64
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.80	0.64
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.28	0.64
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.28	0.64
1:A:268:ARG:O	1:B:257:GLU:HG3	1.97	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:177:VAL:HG21	1:A:397:GLU:HG3	1.80	0.63
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.28	0.63
1:K:183:LEU:H	1:K:383:ALA:CB	2.03	0.63
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.79	0.63
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.80	0.63
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.79	0.63
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.80	0.63
1:K:194:GLN:O	1:K:371:LYS:HE3	1.98	0.63
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.80	0.63
1:M:326:ASN:HD22	1:M:329:THR:HB	1.64	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:A:186:GLU:HB2	1:A:380:LYS:HB2	1.80	0.63
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.81	0.63
1:C:90:THR:O	1:C:94:VAL:HG13	1.98	0.63
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	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:B:247:LEU:HB3	1:B:273:VAL:HG22	1.80	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: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:D:193:MET:HE2	1:D:292:ILE:HG12	1.80	0.63
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.79	0.63
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.29	0.63
1:J:54:VAL:HG23	6:J:2067:HOH:O	1.98	0.63
1:G:194:GLN:O	1:G:371:LYS:HE3	1.99	0.62
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.81	0.62
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.64	0.62
1:G:305:ILE:HD12	1:G:307:MET:HE2	1.81	0.62
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.81	0.62
1:M:228:SER:O	1:M:257:GLU:HB3	1.99	0.62
1:N:228:SER:O	1:N:257:GLU:HB3	1.99	0.62
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.80	0.62
1:C:139:SER:HB3	6:C:2796:HOH:O	2.00	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:K:200:LEU:O	1:K:201:SER:HB3	1.99	0.62
5:L:1:AGS:S1G	5:L:1:AGS:O3G	2.49	0.62
1:E:228:SER:O	1:E:257:GLU:HB3	1.99	0.62
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.82	0.62
1:F:160:LYS:O	1:F:164:GLU:HG3	2.00	0.62
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.81	0.62
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.81	0.62
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.27	0.62
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.63	0.62
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.81	0.62
1:A:360:TYR:OH	1:G:384:ALA:HA	2.00	0.62
1:C:404:ARG:HH11	1:C:404:ARG:HG2	1.63	0.62
1:D:82:ASN:HA	6:D:2757:HOH:O	1.98	0.62
1:B:68:ASN:O	1:B:72:GLN:HG2	1.98	0.62
1:C:200:LEU:O	1:C:201:SER:HB3	1.99	0.62
1:N:183:LEU:H	1:N:383:ALA:CB	2.02	0.62
1:D:200:LEU:O	1:D:201:SER:HB3	2.00	0.62
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.81	0.62
1:F:413:ALA:HB3	1:F:417:VAL:HG22	1.82	0.62
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.80	0.62
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.00	0.62
1:N:272:LYS:HD2	1:N:272:LYS:N	2.15	0.62
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.80	0.62
1:F:219:PHE:HB3	1:F: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:J:221:LEU:HD23	1:J:249:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:205:ILE:HA	1:K:213:VAL:HG22	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: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:N:414:GLY:O	1:N:417:VAL:HG13	2.00	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:G:291:ASP:OD2	1:G:368:ARG:HD2	2.01	0.61
1:J:177:VAL:HG21	1:J:397:GLU:CG	2.30	0.61
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.82	0.61
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.83	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:E:78:ALA:HB3	6:E:2338:HOH:O	2.00	0.61
1:G:78:ALA:HB3	6:G:1724:HOH:O	1.98	0.61
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.82	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:E:291:ASP:OD2	1:E:368:ARG:HD2	2.00	0.61
1:M:268:ARG:O	1:N:257:GLU:HG3	1.99	0.61
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.83	0.61
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.83	0.61
1:J:160:LYS:O	1:J:164:GLU:HG3	2.01	0.61
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.83	0.61
1:A:69:MET:O	1:A:73:MET:HG3	2.00	0.61
1:G:183:LEU:O	1:G:184:GLN:HB2	2.00	0.61
1:C:183:LEU:HD12	1:C:184:GLN:HG3	1.83	0.61
1:C:272:LYS:HD2	1:C:272:LYS:N	2.16	0.61
1:M:177:VAL:HG21	1:M:397:GLU:CG	2.30	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:C:177:VAL:HG21	1:C:397:GLU:CG	2.31	0.60
1:D:39:VAL:HG12	1:E:69:MET:HE2	1.83	0.60
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.01	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:213:VAL:HB	1:M:325:ILE:HG12	1.82	0.60
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.81	0.60
1:M:362:ARG:O	1:M:366:GLN:HG3	2.02	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:C:247:LEU:HB3	1:C:273:VAL:HG22	1.83	0.60
1:B:425:LYS:HB2	6:B:2916:HOH:O	2.01	0.60
1:A:46:ALA:CB	1:B:76:GLU:HG3	2.31	0.60
1:M:200:LEU:O	1:M:201:SER:HB3	1.99	0.60
1:D:272:LYS:HD2	1:D:272:LYS:N	2.17	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:228:SER:O	1:D:257:GLU:HB3	2.01	0.60
1:A:177:VAL:HG21	1:A:397:GLU:CG	2.31	0.60
1:B:57:ALA:O	1:B:75:LYS:HE2	2.01	0.60
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.83	0.60
1:J:228:SER:O	1:J:257:GLU:HB3	2.02	0.60
1:N:194:GLN:O	1:N:371:LYS:HE3	2.00	0.60
1:F:383:ALA:O	1:F:384:ALA:HB3	2.01	0.59
1:J:272:LYS:N	1:J:272:LYS:HD2	2.17	0.59
1:J:349:ILE:HA	1:J:352:GLN:CG	2.31	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:A:23:LEU:HD22	1:A:74:VAL:HG13	1.85	0.59
1:D:242:LYS:C	1:D:244:GLY:H	2.03	0.59
1:E:183:LEU:HD23	1:E:384:ALA:HB2	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:J:218:PRO:CB	1:J:246:PRO:HG2	2.28	0.59
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.03	0.59
1:F:90:THR:O	1:F:94:VAL:HG13	2.02	0.59
1:K:177:VAL:HG21	1:K:397:GLU:CG	2.32	0.59
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.02	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:M:206:ASN:HD21	1:M:214:GLU:H	1.51	0.59
1:M:349:ILE:HA	1:M:352:GLN:CG	2.32	0.59
1:B:114:MET:HB3	6:B:2278:HOH:O	2.02	0.59
1:B:449:ALA:HB1	6:B:2545:HOH:O	2.02	0.59
1:I:272:LYS:N	1:I:272:LYS:HD2	2.18	0.59
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.83	0.59
1:M:160:LYS:O	1:M:164:GLU:HG3	2.03	0.59
1:C:362:ARG:O	1:C:366:GLN:HG3	2.03	0.59
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.84	0.59
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.84	0.59
1:E:272:LYS:HD2	1:E:272:LYS:N	2.17	0.59
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.85	0.59
1:L:90:THR:O	1:L:94:VAL:HG13	2.03	0.59
1:A:272:LYS:HD2	1:A:272:LYS:N	2.18	0.58
1:A:362:ARG:O	1:A:366:GLN:HG3	2.03	0.58
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.83	0.58
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:F:386:GLU:O	1:F:390:LYS:HG2	2.03	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:J:174:VAL:HG22	1:J:194:GLN:HE21	1.68	0.58
1:D:362:ARG:O	1:D:366:GLN:HG3	2.03	0.58
1:K:272:LYS:HD2	1:K:272:LYS:N	2.18	0.58
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.69	0.58
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.84	0.58
1:F:362:ARG:O	1:F:366:GLN:HG3	2.04	0.58
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.85	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:A:404:ARG:NH1	6:A:2654:HOH:O	2.36	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:H:183:LEU:O	1:H:184:GLN:HB2	2.03	0.58
1:I:183:LEU:HD12	1:I:184:GLN:HG3	1.85	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: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: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: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: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: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:B:272:LYS:N	1:B:272:LYS:HD2	2.19	0.57
1:D:463:SER:HB2	6:D:2645:HOH:O	2.03	0.57
1:L:272:LYS:HD2	1:L:272:LYS:N	2.19	0.57
1:L:349:ILE:HA	1:L:352:GLN:CG	2.34	0.57
1:L:383:ALA:O	1:L:384:ALA:HB3	2.04	0.57
1:A:420:ILE:HD12	1:A:451:LEU:HD13	1.87	0.57
1:E:183:LEU:H	1:E:383:ALA:CB	2.05	0.57
1:G:213:VAL:HB	1:G:325:ILE:HG13	1.86	0.57
1:G:382:GLY:O	1:G:389:MET:HG2	2.04	0.57
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.27	0.57
1:J:206:ASN:HD21	1:J:214:GLU:H	1.51	0.57
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.87	0.57
1:D:11:ASP:CB	6:D:2704:HOH:O	2.52	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:I:205:ILE:HA	1:I:213:VAL:HG22	1.85	0.57
1:N:183:LEU:HD12	1:N:184:GLN:HG3	1.87	0.57
1:A:326:ASN:HD22	1:A:329:THR:HB	1.70	0.57
1:D:90:THR:O	1:D:94:VAL:HG13	2.05	0.57
1:H:360:TYR:OH	1:N:384:ALA:HA	2.04	0.57
1:I:349:ILE:HA	1:I:352:GLN:CG	2.33	0.57
1:K:183:LEU:HD12	1:K:184:GLN:HG3	1.87	0.57
1:L:386:GLU:O	1:L:390:LYS:HG2	2.04	0.57
1:N:183:LEU:CD1	1:N:184:GLN:HG3	2.34	0.57
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.86	0.57
1:N:362:ARG:O	1:N:366:GLN:HG3	2.05	0.57
1:A:218:PRO:CB	1:A:246:PRO:HG2	2.32	0.57
1:A:235:PRO:CG	1:A:310:GLU:HA	2.29	0.57
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.57
1:I:183:LEU:O	1:I:184:GLN:HB2	2.05	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:B:382:GLY:O	1:B:389:MET:HG2	2.05	0.57
1:K:206:ASN:HD21	1:K:214:GLU:H	1.51	0.57
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.85	0.57
1:A:16:MET:O	1:A:20:VAL:HG13	2.04	0.57
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.85	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: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:281:PHE:HZ	1:G:383:ALA:CB	2.15	0.57
1:D:160:LYS:NZ	1:D:160:LYS:HB2	2.20	0.57
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.29	0.57
1:F:404:ARG:HG2	1:F:404:ARG:HH11	1.70	0.57
1:K:326:ASN:HD22	1:K:329:THR:HB	1.70	0.57
1:L:193:MET:CE	1:L:292:ILE:HG12	2.35	0.57
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.86	0.57
1:A:155:ASP:OD1	1:A:157:THR:HB	2.04	0.56
1:A:200:LEU:O	1:A:201:SER:HB3	2.04	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:N:183:LEU:O	1:N:184:GLN:HB2	2.05	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: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:L:183:LEU:O	1:L:184:GLN:HB2	2.06	0.56
1:A:183:LEU:O	1:A:184:GLN:HB2	2.06	0.56
1:D:386:GLU:O	1:D:390:LYS:HG2	2.05	0.56
1:J:383:ALA:O	1:J:384:ALA:HB3	2.05	0.56
1:L:384:ALA:HA	1:M:360:TYR:OH	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:M:220:ILE:HD12	1:M:296:THR:HG21	1.88	0.56
1:N:242:LYS:C	1:N:244:GLY:H	2.07	0.56
1:B:183:LEU:HD12	1:B:184:GLN:HG3	1.86	0.56
1:E:71:ALA:O	1:E:75:LYS:HB2	2.05	0.56
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.88	0.56
1:A:282:GLY:HA3	1:G:181:THR:O	2.05	0.56
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.46	0.56
1:H:68:ASN:O	1:H:72:GLN:HG2	2.04	0.56
1:L:155:ASP:OD1	1:L:157:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:M:272:LYS:N	1:M:272:LYS:HD2	2.19	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:B:349:ILE:HA	1:B:352:GLN:CG	2.34	0.56
1:E:300:VAL:HG22	6:E:2717:HOH:O	2.04	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:E:242:LYS:C	1:E:244:GLY:H	2.08	0.56
1:E:301:ILE:HG21	1:E:309:LEU:HD23	1.88	0.56
1:F:54:VAL:HG23	6:F:2017:HOH:O	2.06	0.56
1:H:242:LYS:C	1:H:244:GLY:H	2.09	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:I:193:MET:HE1	1:I:292:ILE:HG12	1.88	0.56
1:I:362:ARG:O	1:I:366:GLN:HG3	2.06	0.56
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.35	0.56
1:C:183:LEU:H	1:C:383:ALA:CB	2.08	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: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: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:176:THR:HG21	1:G:322:ARG:HH12	1.72	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: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:J:326:ASN:HD22	1:J:329:THR:HB	1.71	0.55
1:K:242:LYS:C	1:K:244:GLY:H	2.08	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:C:193:MET:CE	1:C:292:ILE:HG12	2.37	0.55
1:I:266:THR:CG2	1:I:273:VAL:H	2.19	0.55
1:J:180:GLY:HA3	1:J:381:VAL:O	2.07	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:218:PRO:CB	1:F:246:PRO:HG2	2.31	0.54
1:J:176:THR:HG21	1:J:322:ARG:HH12	1.71	0.54
1:N:382:GLY:O	1:N:389:MET:HG2	2.07	0.54
1:B:218:PRO:CB	1:B:246:PRO:HG2	2.29	0.54
1:C:183:LEU:CD1	1:C:184:GLN:HG3	2.38	0.54
1:H:160:LYS:O	1:H:164:GLU:HG3	2.06	0.54
1:I:305:ILE:HB	1:I:307:MET:HE2	1.89	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:K:383:ALA:O	1:K:384:ALA:HB3	2.08	0.54
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.07	0.54
1:E:489:ILE:HD13	1:E:494:LEU:CD2	2.38	0.54
1:G:236:VAL:O	1:G:240:VAL:HG23	2.07	0.54
1:H:16:MET:O	1:H:20:VAL:HG13	2.07	0.54
1:H:193:MET:CE	1:H:292:ILE:HG12	2.38	0.54
1:H:200:LEU:O	1:H:201:SER:HB3	2.07	0.54
1:J:183:LEU:O	1:J:184:GLN:HB2	2.08	0.54
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.90	0.54
1:N:218:PRO:CB	1:N:246:PRO:HG2	2.34	0.54
1:H:305:ILE:O	1:H:305:ILE:HG22	2.08	0.54
1:I:16:MET:O	1:I:20:VAL:HG13	2.08	0.54
1:J:259:LEU:O	1:J:263:VAL:HG23	2.08	0.54
1:B:206:ASN:HD21	1:B:214:GLU:H	1.56	0.54
1:C:382:GLY:O	1:C:389:MET:HG2	2.08	0.54
1:D:85:ALA:HB1	6:D:2188:HOH:O	2.07	0.54
1:E:382:GLY:O	1:E:389:MET:HG2	2.08	0.54
1:F:160:LYS:NZ	1:F:160:LYS:HB2	2.23	0.54
1:F:242:LYS:C	1:F:244:GLY:H	2.10	0.54
1:J:305:ILE:O	1:J:305:ILE:HG22	2.08	0.54
1:M:183:LEU:HD12	1:M:184:GLN:HG3	1.90	0.54
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.88	0.54
1:H:176:THR:HG22	1:H:177:VAL:N	2.22	0.54
1:G:266:THR:CG2	1:G:273:VAL:H	2.21	0.54
1:I:183:LEU:CD1	1:I:184:GLN:HG3	2.38	0.54
1:J:236:VAL:O	1:J:240:VAL:HG23	2.08	0.54
1:M:183:LEU:O	1:M:184:GLN:HB2	2.08	0.54
1:B:242:LYS:C	1:B:244:GLY:H	2.11	0.53
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

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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:H:382:GLY:O	1:H:389:MET:HG2	2.08	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:A:281:PHE:CZ	1:G:383:ALA:CB	2.89	0.53
1:D:16:MET:O	1:D:20:VAL:HG13	2.08	0.53
1:F:176:THR:HG22	1:F:177:VAL:N	2.23	0.53
1:G:218:PRO:CB	1:G:246:PRO:HG2	2.32	0.53
1:H:73:MET:O	1:H:76:GLU:HB2	2.09	0.53
1:I:90:THR:O	1:I:94:VAL:HG13	2.08	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:A:305:ILE:O	1:A:305:ILE:HG22	2.08	0.53
1:C:383:ALA:O	1:C:384:ALA:HB3	2.08	0.53
1:H:183:LEU:HD12	1:H:184:GLN:HG3	1.91	0.53
1:H:319:GLN:O	1:H:336:VAL:HG23	2.08	0.53
1:I:174:VAL:HG22	1:I:194:GLN:HE21	1.73	0.53
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.88	0.53
1:K:183:LEU:CD1	1:K:184:GLN:HG3	2.38	0.53
1:K:319:GLN:O	1:K:336:VAL:HG23	2.08	0.53
1:M:176:THR:HG22	1:M:177:VAL:N	2.24	0.53
1:M:183:LEU:CD1	1:M:184:GLN:HG3	2.38	0.53
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.88	0.53
1:A:301:ILE:HG21	1:A:309:LEU:HD23	1.90	0.53
1:G:206:ASN:HD21	1:G:214:GLU:H	1.56	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:I:242:LYS:C	1:I:244:GLY:H	2.11	0.53
1:G:155:ASP:OD1	1:G:157:THR:HB	2.08	0.53
1:J:310:GLU:N	1:J:310:GLU:OE1	2.41	0.53
1:A:202:PRO:O	1:A:203:TYR:HB2	2.08	0.53
1:B:219:PHE:O	1:B:247:LEU:HD12	2.08	0.53
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.90	0.53
1:M:219:PHE:O	1:M:247:LEU:HD12	2.09	0.53
1:M:301:ILE:HG21	1:M:309:LEU:HD23	1.90	0.53
1:A:252:GLU:O	1:A:253:ASP:HB2	2.09	0.53
1:B:183:LEU:CD1	1:B:184:GLN:HG3	2.38	0.53
1:C:235:PRO:CG	1:C:310:GLU:HA	2.32	0.53
1:E:362:ARG:O	1:E:366:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:THR:OG1	5:I:1:AGS:S1G	2.65	0.53
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.74	0.53
1:L:319:GLN:O	1:L:336:VAL:HG23	2.09	0.53
1:M:155:ASP:OD1	1:M:157:THR:HB	2.08	0.53
1:M:183:LEU:H	1:M:383:ALA:CB	2.10	0.53
1:N:23:LEU:CD2	1:N:74:VAL:HG13	2.38	0.53
1:N:326:ASN:HD22	1:N:329:THR:HB	1.74	0.53
1:B:239:ALA:O	1:B:314:LEU:HD11	2.09	0.53
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.91	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:247:LEU:HD21	1:D:249:ILE:HD11	1.90	0.53
1:E:386:GLU:O	1:E:390:LYS:HG2	2.09	0.53
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.89	0.53
1:C:176:THR:HG22	1:C:177:VAL:N	2.23	0.53
1:D:383:ALA:O	1:D:384:ALA:HB3	2.09	0.53
1:G:183:LEU:HD12	1:G:184:GLN:HG3	1.90	0.53
1:G:325:ILE:HG22	1:G:330:THR:HA	1.91	0.53
1:J:155:ASP:OD1	1:J:157:THR:HB	2.09	0.53
1:K:16:MET:O	1:K:20:VAL:HG13	2.09	0.53
1:K:239:ALA:O	1:K:314:LEU:HD11	2.08	0.53
1:L:183:LEU:CD1	1:L:184:GLN:HG3	2.39	0.53
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.74	0.53
1:B:310:GLU:OE1	1:B:310:GLU:N	2.42	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:F:183:LEU:CD1	1:F:184:GLN:HG3	2.39	0.53
1:G:16:MET:O	1:G:20:VAL:HG13	2.09	0.53
1:G:193:MET:CE	1:G:292:ILE:HG12	2.39	0.53
1:H:266:THR:CG2	1:H:273:VAL:H	2.22	0.53
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.39	0.53
1:B:176:THR:HG22	1:B:177:VAL:N	2.24	0.52
1:E:180:GLY:HA3	1:E:381:VAL:O	2.09	0.52
1:E:383:ALA:O	1:E:384:ALA:HB3	2.09	0.52
1:F:272:LYS:N	1:F:272:LYS:HD2	2.24	0.52
1:G:160:LYS:O	1:G:164:GLU:HG3	2.09	0.52
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.10	0.52
1:I:382:GLY:O	1:I:389:MET:HG2	2.08	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:K:193:MET:CE	1:K:292:ILE:HG12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.92	0.52
1:M:383:ALA:O	1:M:384:ALA:HB3	2.09	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.39	0.52
1:H:383:ALA:O	1:H:384:ALA:HB3	2.09	0.52
1:K:524:LEU:O	1:K:526:LYS:N	2.41	0.52
1:N:219:PHE:O	1:N:247:LEU:HD12	2.08	0.52
1:A:242:LYS:C	1:A:244:GLY:H	2.12	0.52
1:C:305:ILE:O	1:C:305:ILE:HG22	2.09	0.52
1:G:235:PRO:CG	1:G:310:GLU:HA	2.32	0.52
1:K:90:THR:O	1:K:94:VAL:HG13	2.09	0.52
1:C:242:LYS:C	1:C:244:GLY:H	2.11	0.52
1:G:160:LYS:HB2	1:G:160:LYS:NZ	2.25	0.52
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.92	0.52
1:I:310:GLU:OE1	1:I:310:GLU:N	2.42	0.52
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.90	0.52
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.10	0.52
1:B:90:THR:OG1	5:B:1:AGS:S1G	2.67	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:H:183:LEU:CD1	1:H:184:GLN:HG3	2.40	0.52
1:L:193:MET:HE2	1:L:292:ILE:HG12	1.90	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:K:254:VAL:HG12	1:K:259:LEU:HB2	1.92	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:J:496:PRO:HB2	1:J:499:VAL:CG1	2.40	0.52
1:N:193:MET:CE	1:N:292:ILE:HG12	2.39	0.52
1:E:310:GLU:OE1	1:E:310:GLU:N	2.43	0.52
1:F:271:VAL:HG12	1:F:273:VAL:HG23	1.92	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:M:134:LEU:HD21	1:M:425:LYS:NZ	2.25	0.52
1:M:90:THR:O	1:M:94:VAL:HG13	2.10	0.52
1:E:69:MET:O	1:E:73:MET:HG3	2.09	0.52
1:I:235:PRO:CG	1:I:310:GLU:HA	2.33	0.52
1:J:386:GLU:O	1:J:390:LYS:HG2	2.10	0.52
1:C:160:LYS:O	1:C:164:GLU:HG3	2.10	0.52
1:C:180:GLY:HA3	1:C:381:VAL:O	2.10	0.52
1:E:193:MET:HE2	1:E:292:ILE:HG12	1.92	0.52
1:E:252:GLU:O	1:E:253:ASP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.92	0.52
1:E:319:GLN:O	1:E:336:VAL:HG23	2.10	0.52
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.92	0.52
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.51
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.10	0.51
1:G:305:ILE:O	1:G:305:ILE:HG22	2.10	0.51
1:I:305:ILE:HG22	1:I:305:ILE:O	2.10	0.51
1:K:235:PRO:CG	1:K:310:GLU:HA	2.35	0.51
1:M:284:ARG:NH1	1:M:364:LYS:NZ	2.58	0.51
1:M:305:ILE:O	1:M:305:ILE:HG22	2.09	0.51
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.51
1:C:160:LYS:HB2	1:C:160:LYS:NZ	2.24	0.51
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.92	0.51
1:E:524:LEU:O	1:E:526:LYS:N	2.43	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:I:68:ASN:O	1:I:72:GLN:HG2	2.10	0.51
1:A:310:GLU:N	1:A:310:GLU:OE1	2.44	0.51
1:B:193:MET:CE	1:B:292:ILE:HG12	2.40	0.51
1:C:134:LEU:HD21	1:C:425:LYS:NZ	2.25	0.51
1:C:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:E:174:VAL:HG22	1:E:194:GLN:HE21	1.74	0.51
1:F:382:GLY:O	1:F:389:MET:HG2	2.10	0.51
1:I:239:ALA:O	1:I:314:LEU:HD11	2.10	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:A:54:VAL:HG23	6:A:2015:HOH:O	2.10	0.51
1:C:384:ALA:O	1:C:385:THR:HG23	2.11	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:F:223:ALA:O	1:F:251:ALA:HA	2.10	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:160:LYS:HB2	1:A:160:LYS:NZ	2.26	0.51
1:E:305:ILE:HG22	1:E:305:ILE:O	2.10	0.51
1:A:193:MET:CE	1:A:292:ILE:HG12	2.41	0.51
1:B:305:ILE:O	1:B:305:ILE:HG22	2.11	0.51
1:F:239:ALA:O	1:F:314:LEU:HD11	2.10	0.51
1:I:176:THR:HG22	1:I:177:VAL:N	2.25	0.51
1:L:266:THR:CG2	1:L:273:VAL:H	2.24	0.51
1:L:305:ILE:O	1:L:305:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:287:ALA:HB1	1:M:368:ARG:NH1	2.25	0.51
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.92	0.51
1:I:386:GLU:O	1:I:390:LYS:HG2	2.11	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:M:252:GLU:O	1:M:253:ASP:HB2	2.10	0.51
1:A:200:LEU:HG	1:A:276:VAL:HA	1.93	0.51
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.51	0.51
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.92	0.51
1:E:183:LEU:HD12	1:E:184:GLN:HG3	1.93	0.51
1:E:271:VAL:HG12	1:E:273:VAL:HG23	1.93	0.51
1:A:176:THR:HG22	1:A:177:VAL:N	2.25	0.51
1:D:155:ASP:OD1	1:D:157:THR:HB	2.11	0.51
1:F:193:MET:CE	1:F:292:ILE:HG12	2.41	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:N:266:THR:HG22	1:N:271:VAL:O	2.11	0.51
1:N:383:ALA:O	1:N:384:ALA:HB3	2.10	0.51
1:D:305:ILE:O	1:D:305:ILE:HG22	2.10	0.51
1:F:310:GLU:OE1	1:F:310:GLU:N	2.44	0.51
1:J:202:PRO:O	1:J:203:TYR:HB2	2.11	0.51
1:K:183:LEU:O	1:K:184:GLN:HB2	2.11	0.51
1:K:252:GLU:O	1:K:253:ASP:HB2	2.11	0.51
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.93	0.50
1:B:271:VAL:HG12	1:B:273:VAL:HG23	1.93	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:G:90:THR:O	1:G:94:VAL:HG13	2.11	0.50
1:H:78:ALA:HB3	6:H:2660:HOH:O	2.11	0.50
1:M:310:GLU:N	1:M:310:GLU:OE1	2.44	0.50
1:N:496:PRO:HD2	6:N:2145:HOH:O	2.10	0.50
1:C:85:ALA:O	1:C:401:HIS:HE1	1.94	0.50
1:E:383:ALA:HB1	1:F:281:PHE:HZ	1.75	0.50
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.92	0.50
1:I:54:VAL:HG23	6:I:2135:HOH:O	2.11	0.50
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.93	0.50
1:N:305:ILE:O	1:N:305:ILE:HG22	2.11	0.50
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.93	0.50
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.26	0.50
1:G:441:LYS:HE2	6:G:1481:HOH:O	2.11	0.50
1:H:301:ILE:HG21	1:H:309:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:496:PRO:HB2	1:M:499:VAL:CG1	2.41	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:G:326:ASN:HD22	1:G:329:THR:HB	1.75	0.50
1:J:271:VAL:HG12	1:J:273:VAL:HG23	1.92	0.50
1:K:223:ALA:O	1:K:251:ALA:HA	2.12	0.50
1:K:193:MET:HE2	1:K:292:ILE:HG12	1.93	0.50
1:N:202:PRO:O	1:N:203:TYR:HB2	2.11	0.50
1:N:319:GLN:O	1:N:336:VAL:HG23	2.12	0.50
1:C:325:ILE:HG22	1:C:330:THR:HA	1.92	0.50
1:D:183:LEU:CD1	1:D:184:GLN:HG3	2.40	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:L:183:LEU:HD12	1:L:184:GLN:HG3	1.93	0.50
1:N:514:MET:SD	6:N:2800:HOH:O	2.60	0.50
1:D:260:ALA:O	1:D:264:VAL:HG23	2.11	0.50
1:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.50
1:I:206:ASN:OD1	1:I:207:LYS:HG3	2.11	0.50
1:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.50
1:L:174:VAL:HG22	1:L:194:GLN:HE21	1.75	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:F:301:ILE:HG21	1:F:309:LEU:HD23	1.93	0.50
1:H:252:GLU:O	1:H:253:ASP:HB2	2.12	0.50
1:M:209:GLU:OE1	1:M:209:GLU:N	2.44	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:K:271:VAL:HG12	1:K:273:VAL:HG23	1.93	0.50
1:K:310:GLU:OE1	1:K:310:GLU:N	2.44	0.50
1:L:180:GLY:HA3	1:L:381:VAL:O	2.11	0.50
1:M:266:THR:CG2	1:M:273:VAL:H	2.25	0.50
1:N:310:GLU:OE1	1:N:310:GLU:N	2.45	0.50
1:F:236:VAL:O	1:F:240:VAL:HG23	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: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:A:287:ALA:HB1	1:A:368:ARG:NH1	2.26	0.49
1:E:239:ALA:O	1:E:314:LEU:HD11	2.12	0.49
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.75	0.49
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.94	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:M:413:ALA:HB3	1:M:417:VAL:HG22	1.94	0.49
1:A:319:GLN:O	1:A:336:VAL:HG23	2.12	0.49
1:B:183:LEU:HD13	1:B:184:GLN:N	2.26	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:G:205:ILE:HA	1:G:213:VAL:HG22	1.94	0.49
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.94	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:C:193:MET:HE1	1:C:292:ILE:HG12	1.93	0.49
1:D:78:ALA:HB1	1:D:89:THR:HB	1.94	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.92	0.49
1:E:236:VAL:O	1:E:240:VAL:HG23	2.12	0.49
1:F:174:VAL:HG22	1:F:194:GLN:HE21	1.77	0.49
1:G:202:PRO:O	1:G:203:TYR:HB2	2.12	0.49
1:H:325:ILE:HG22	1:H:330:THR:HA	1.95	0.49
1:L:252:GLU:O	1:L:253:ASP:HB2	2.11	0.49
1:N:348:GLN:O	1:N:352:GLN:HG2	2.13	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:H:176:THR:HG21	1:H:322:ARG:HH12	1.76	0.49
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.94	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.11	0.49
1:C:68:ASN:O	1:C:72:GLN:HG2	2.12	0.49
1:E:90:THR:OG1	5:E:1:AGS:S1G	2.66	0.49
1:A:229:ASN:ND2	1:G:244:GLY:HA3	2.28	0.49
1:H:310:GLU:N	1:H:310:GLU:OE1	2.45	0.49
1:H:413:ALA:HB3	1:H:417:VAL:HG22	1.93	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:E:171:LYS:HB2	1:E:407:VAL:HG11	1.93	0.49
1:L:202:PRO:O	1:L:203:TYR:HB2	2.12	0.49
1:A:266:THR:CG2	1:A:273:VAL:H	2.26	0.49
1:B:202:PRO:O	1:B:203:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:PRO:O	1:D:203:TYR:HB2	2.12	0.49
1:K:69:MET:O	1:K:73:MET:HG3	2.12	0.49
1:L:223:ALA:O	1:L:251:ALA:HA	2.12	0.49
1:B:326:ASN:HD22	1:B:329:THR:HB	1.76	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.13	0.49
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.95	0.49
1:L:524:LEU:O	1:L:526:LYS:N	2.45	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:B:5:ASP:HB2	1:B:524:LEU:HD12	1.95	0.49
1:C:319:GLN:O	1:C:336:VAL:HG23	2.13	0.49
6:C:2466:HOH:O	1:D:518:GLU:HG2	2.12	0.49
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.42	0.49
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.27	0.49
1:I:252:GLU:O	1:I:253:ASP:HB2	2.12	0.49
1:J:382:GLY:O	1:J:389:MET:HG2	2.13	0.49
1:N:218:PRO:HD2	1:N:320:ALA:O	2.13	0.49
1:A:271:VAL:HG12	1:A:273:VAL:HG23	1.94	0.49
1:A:60:ILE:O	1:A:75:LYS:HE3	2.13	0.49
1:C:63:GLU:OE2	1:D:526:LYS:HE2	2.13	0.49
1:E:287:ALA:HB1	1:E:368:ARG:NH1	2.27	0.49
1:H:202:PRO:O	1:H:203:TYR:HB2	2.11	0.49
1:J:63:GLU:OE2	1:K:526:LYS:HE2	2.12	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.95	0.49
1:N:234:LEU:O	1:N:238:GLU:HG3	2.13	0.49
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:F:235:PRO:CG	1:F:310:GLU:HA	2.31	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:K:202:PRO:O	1:K:203:TYR:HB2	2.12	0.48
1:M:223:ALA:O	1:M:251:ALA:HA	2.13	0.48
1:B:179:ASP:HB3	1:B:389:MET:CE	2.44	0.48
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.78	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:E:202:PRO:O	1:E:203:TYR:HB2	2.13	0.48
1:G:259:LEU:O	1:G:263:VAL:HG23	2.13	0.48
1:G:69:MET:O	1:G:73:MET:HG3	2.13	0.48
1:H:384:ALA:O	1:H:385:THR:HG23	2.13	0.48
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:LEU:CD2	1:L:74:VAL:HG13	2.42	0.48
1:L:326:ASN:HD22	1:L:329:THR:HB	1.77	0.48
1:L:69:MET:O	1:L:73:MET:HG3	2.13	0.48
1:M:202:PRO:O	1:M:203:TYR:HB2	2.13	0.48
1:N:413:ALA:HB3	1:N:417:VAL:HG22	1.94	0.48
1:C:183:LEU:O	1:C:184:GLN:HB2	2.14	0.48
1:E:404:ARG:NH1	6:E:2208:HOH:O	2.45	0.48
1:F:319:GLN:O	1:F:336:VAL:HG23	2.12	0.48
1:F:73:MET:O	1:F:76:GLU:HB2	2.13	0.48
1:H:234:LEU:O	1:H:238:GLU:HG3	2.13	0.48
1:J:496:PRO:O	1:J:499:VAL:HG13	2.12	0.48
1:A:234:LEU:O	1:A:238:GLU:HG3	2.13	0.48
1:A:239:ALA:O	1:A:314:LEU:HD11	2.13	0.48
1:B:153:ASN:O	1:B:154:SER:HB2	2.14	0.48
1:B:252:GLU:O	1:B:253:ASP:HB2	2.13	0.48
1:B:77:VAL:HG11	1:B:510:VAL:CG2	2.43	0.48
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.96	0.48
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.95	0.48
1:C:310:GLU:N	1:C:310:GLU:OE1	2.46	0.48
1:C:524:LEU:O	1:C:526:LYS:N	2.45	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:G:425:LYS:NZ	6:G:2070:HOH:O	2.45	0.48
1:I:73:MET:O	1:I:76:GLU:HB2	2.13	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:K:160:LYS:O	1:K:164:GLU:HG3	2.12	0.48
1:L:176:THR:HG22	1:L:177:VAL:N	2.28	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:M:193:MET:CE	1:M:292:ILE:HG12	2.43	0.48
1:A:266:THR:HG22	1:A:271:VAL:O	2.13	0.48
1:B:236:VAL:O	1:B:240:VAL:HG23	2.12	0.48
1:E:235:PRO:CG	1:E:310:GLU:HA	2.32	0.48
1:H:223:ALA:O	1:H:251:ALA:HA	2.12	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:N:499:VAL:HG11	6:N:2145:HOH:O	2.13	0.48
1:A:260:ALA:O	1:A:264:VAL:HG23	2.13	0.48
1:D:384:ALA:O	1:D:385:THR:HG23	2.14	0.48
1:D:63:GLU:OE2	1:E:526:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ASN:O	1:E:154:SER:HB2	2.13	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.48
1:I:524:LEU:O	1:I:526:LYS:N	2.46	0.48
1:J:413:ALA:HB3	1:J:417:VAL:HG22	1.95	0.48
1:L:174:VAL:HG22	1:L:194:GLN:NE2	2.28	0.48
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.95	0.48
1:N:222:LEU:HB3	1:N:289:LEU:CD2	2.43	0.48
1:A:206:ASN:OD1	1:A:207:LYS:HG3	2.13	0.48
1:A:176:THR:HG21	1:A:322:ARG:HH12	1.79	0.48
1:A:46:ALA:HB2	1:B:76:GLU:HG2	1.93	0.48
1:B:200:LEU:HG	1:B:276:VAL:HA	1.96	0.48
1:G:266:THR:HG22	1:G:271:VAL:O	2.14	0.48
1:G:362:ARG:HD2	6:G:1728:HOH:O	2.13	0.48
1:L:219:PHE:O	1:L:247:LEU:HD12	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:B:144:ILE:HG23	1:B:403:THR:CG2	2.44	0.48
1:E:353:ILE:HD13	1:E:366:GLN:HG2	1.96	0.48
1:J:319:GLN:O	1:J:336:VAL:HG23	2.14	0.48
1:K:384:ALA:O	1:K:385:THR:HG23	2.14	0.48
1:L:209:GLU:OE1	1:L:209:GLU:N	2.47	0.48
1:M:174:VAL:HG22	1:M:194:GLN:HE21	1.77	0.48
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.95	0.48
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.95	0.48
1:N:325:ILE:HG22	1:N:330:THR:HA	1.96	0.48
1:B:185:ASP:OD1	1:B:382:GLY:N	2.47	0.48
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	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:E:259:LEU:O	1:E:263:VAL:HG23	2.14	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: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:I:199:TYR:CZ	1:I:327:LYS:HA	2.49	0.48
1:K:325:ILE:HG22	1:K:330:THR:HA	1.96	0.48
1:N:223:ALA:O	1:N:251:ALA:HA	2.14	0.48
1:N:386:GLU:O	1:N:390:LYS:HG2	2.14	0.48
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.48
1:F:222:LEU:HB3	1:F:289:LEU:CD2	2.44	0.48

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.50	0.47
1:A:209:GLU:N	1:A:209:GLU:OE1	2.44	0.47
1:A:231:ARG:NH1	1:G:242:LYS:HG2	2.28	0.47
1:B:206:ASN:OD1	1:B:207:LYS:HG3	2.13	0.47
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	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:H:239:ALA:O	1:H:314:LEU:HD11	2.15	0.47
1:L:78:ALA:HB1	1:L:89:THR:HB	1.97	0.47
1:M:524:LEU:O	1:M:526:LYS:N	2.46	0.47
1:N:160:LYS:HB2	1:N:160:LYS:NZ	2.29	0.47
1:A:305:ILE:HB	1:A:307:MET:HE2	1.95	0.47
1:B:383:ALA:HB1	1:C:281:PHE:CE2	2.49	0.47
1:C:301:ILE:HG21	1:C:309:LEU:HD23	1.95	0.47
1:D:89:THR:HG23	6:D:2757:HOH:O	2.13	0.47
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.96	0.47
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.95	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:A:183:LEU:CD2	1:A:384:ALA:HB2	2.44	0.47
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.96	0.47
1:D:12:ALA:N	6:D:2704:HOH:O	2.47	0.47
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.95	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:J:176:THR:HG22	1:J:177:VAL:N	2.29	0.47
1:L:366:GLN:HA	1:L:369:VAL:HG22	1.95	0.47
1:N:183:LEU:HD13	1:N:184:GLN:N	2.29	0.47
1:D:252:GLU:O	1:D:253:ASP:HB2	2.15	0.47
1:I:206:ASN:ND2	1:I:214:GLU:H	2.12	0.47
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.47
1:I:272:LYS:NZ	1:J:229:ASN:OD1	2.47	0.47
1:J:266:THR:HG22	1:J:271:VAL:O	2.15	0.47
1:J:369:VAL:HG23	1:J:370:ALA:N	2.30	0.47
1:L:234:LEU:N	1:L:235:PRO:HD2	2.30	0.47
1:M:206:ASN:OD1	1:M:207:LYS:HG3	2.14	0.47
1:M:260:ALA:O	1:M:264:VAL:HG23	2.15	0.47
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.50	0.47
1:A:134:LEU:HD21	1:A:425:LYS:NZ	2.30	0.47
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.96	0.47
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.50	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:E:70:GLY:HA2	1:E:73:MET:HE3	1.97	0.47
1:F:206:ASN:OD1	1:F:207:LYS:HG3	2.14	0.47
1:H:185:ASP:OD1	1:H:382:GLY:N	2.46	0.47
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.97	0.47
1:J:525:PRO:HD3	6:J:2970:HOH:O	2.14	0.47
1:K:183:LEU:CD2	1:K:384:ALA:HB2	2.43	0.47
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.96	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:C:183:LEU:HD13	1:C:184:GLN:N	2.30	0.47
1:C:252:GLU:O	1:C:253:ASP:HB2	2.14	0.47
1:E:260:ALA:O	1:E:264:VAL:HG23	2.15	0.47
1:E:90:THR:O	1:E:94:VAL:HG13	2.14	0.47
1:J:111:MET:HG2	1:J:435:ASP:OD1	2.15	0.47
1:K:160:LYS:HB2	1:K:160:LYS:NZ	2.30	0.47
1:L:236:VAL:O	1:L:240:VAL:HG23	2.15	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:A:236:VAL:O	1:A:240:VAL:HG23	2.15	0.47
1:C:23:LEU:CD2	1:C:74:VAL:HG13	2.45	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:D:206:ASN:HD21	1:D:214:GLU:H	1.63	0.47
1:D:302:SER:H	1:D:307:MET:HE1	1.80	0.47
1:J:234:LEU:O	1:J:238:GLU:HG3	2.13	0.47
1:L:271:VAL:HG12	1:L:273:VAL:HG23	1.96	0.47
1:M:90:THR:OG1	5:M:1:AGS:S1G	2.63	0.47
1:M:269:GLY:O	1:N:229:ASN:OD1	2.33	0.47
1:A:73:MET:O	1:A:76:GLU:HB2	2.15	0.46
1:D:238:GLU:O	1:D:241:ALA:HB3	2.15	0.46
1:F:234:LEU:O	1:F:238:GLU:HG3	2.14	0.46
1:F:384:ALA:O	1:F:385:THR:HG23	2.14	0.46
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.96	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:L:242:LYS:C	1:L:244:GLY:N	2.69	0.46
1:A:169:VAL:HG13	1:A:377:ALA:HB2	1.97	0.46
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.98	0.46
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.81	0.46
1:C:60:ILE:O	1:C:75:LYS:HE3	2.15	0.46
1:G:384:ALA:O	1:G:385:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:I:260:ALA:O	1:I:264:VAL:HG23	2.14	0.46
1:I:325:ILE:HG22	1:I:330:THR:HA	1.98	0.46
1:M:63:GLU:OE2	1:N:526:LYS:HE2	2.15	0.46
1:N:155:ASP:OD1	1:N:157:THR:HB	2.14	0.46
1:C:234:LEU:N	1:C:235:PRO:HD2	2.30	0.46
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.50	0.46
1:E:451:LEU:HD23	1:E:451:LEU:C	2.35	0.46
5:G:1:AGS:O2G	5:G:1:AGS:S1G	2.53	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.46
1:G:78:ALA:HB1	1:G:89:THR:HB	1.96	0.46
1:I:463:SER:HB2	6:I:2586:HOH:O	2.14	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:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.46
1:B:325:ILE:HG22	1:B:330:THR:HA	1.96	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:F:353:ILE:HD13	1:F:366:GLN:HG2	1.98	0.46
1:F:381:VAL:O	1:F:382:GLY:O	2.33	0.46
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.46
1:G:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.98	0.46
1:K:183:LEU:HD13	1:K:184:GLN:N	2.30	0.46
1:N:122:LYS:HE2	1:N:429:LEU:HD11	1.97	0.46
1:A:90:THR:O	1:A:94:VAL:HG13	2.14	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:325:ILE:HA	1:K:329:THR:O	2.15	0.46
1:K:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.46
1:K:60:ILE:O	1:K:75:LYS:HE3	2.16	0.46
1:L:455:VAL:O	1:L:458:CYS:HB2	2.14	0.46
1:M:234:LEU:N	1:M:235:PRO:HD2	2.30	0.46
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.96	0.46
1:A:182:GLY:HA2	1:A:383:ALA:HB3	1.97	0.46
1:C:209:GLU:N	1:C:209:GLU:OE1	2.45	0.46
1:D:235:PRO:CG	1:D:310:GLU:HA	2.34	0.46
1:E:10:ASN:HB2	6:E:1989:HOH:O	2.14	0.46
1:E:223:ALA:O	1:E:251:ALA:HA	2.16	0.46
1:F:234:LEU:N	1:F:235:PRO:HD2	2.30	0.46
1:F:200:LEU:HG	1:F:276:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ALA:O	1:F:384:ALA:CB	2.63	0.46
1:H:250:ILE:HG22	6:H:2938:HOH:O	2.15	0.46
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.71	0.46
1:J:234:LEU:N	1:J:235:PRO:HD2	2.31	0.46
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.96	0.46
1:M:234:LEU:O	1:M:238:GLU:HG3	2.14	0.46
1:A:199:TYR:CZ	1:A:327:LYS:HA	2.51	0.46
1:A:366:GLN:O	1:A:369:VAL:HG22	2.15	0.46
1:D:266:THR:CG2	1:D:273:VAL:H	2.28	0.46
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.97	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:M:10:ASN:HA	6:M:2195:HOH:O	2.15	0.46
1:A:78:ALA:HB3	6:A:2430:HOH:O	2.15	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:E:420:ILE:HG13	1:E:448:GLU:HG2	1.96	0.46
1:F:217:SER:N	1:F:218:PRO:HD3	2.31	0.46
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.30	0.46
1:H:217:SER:N	1:H:218:PRO:CD	2.79	0.46
1:I:217:SER:N	1:I:218:PRO:CD	2.79	0.46
1:J:223:ALA:O	1:J:251:ALA:HA	2.15	0.46
1:J:219:PHE:O	1:J:247:LEU:HD12	2.15	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.16	0.46
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.98	0.46
1:M:325:ILE:HA	1:M:329:THR:O	2.16	0.46
1:M:438:VAL:O	1:M:442:VAL:HG23	2.16	0.46
1:N:234:LEU:N	1:N:235:PRO:HD2	2.31	0.46
1:B:180:GLY:HA3	1:B:381:VAL:O	2.15	0.46
1:C:290:GLN:HB3	1:C:345:ARG:NH2	2.31	0.46
1:E:234:LEU:N	1:E:235:PRO:HD2	2.31	0.46
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.97	0.46
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.98	0.46
1:H:353:ILE:HD13	1:H:366:GLN:HG2	1.98	0.46
1:H:183:LEU:CD2	1:H:384:ALA:HB2	2.45	0.46
1:I:301:ILE:HG21	1:I:309:LEU:HD23	1.97	0.46
1:J:319:GLN:HB3	1:J:336:VAL:HG21	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:A:325:ILE:HG22	1:A:330:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:O	1:A:526:LYS:N	2.48	0.46
1:I:69:MET:O	1:I:73:MET:HG3	2.15	0.46
1:K:210:THR:HG22	1:K:210:THR:O	2.16	0.46
1:K:234:LEU:N	1:K:235:PRO:HD2	2.31	0.46
1:A:101:THR:HG23	6:A:2971:HOH:O	2.16	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:F:458:CYS:SG	1:F:480:ALA:HB1	2.57	0.45
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.98	0.45
1:K:177:VAL:HA	1:K:379:ILE:O	2.16	0.45
1:K:302:SER:H	1:K:307:MET:HE1	1.81	0.45
1:L:171:LYS:HB2	1:L:407:VAL:HG11	1.98	0.45
1:B:183:LEU:CD2	1:B:384:ALA:HB2	2.43	0.45
1:C:324:VAL:O	1:C:331:THR:HG22	2.16	0.45
1:D:319:GLN:O	1:D:336:VAL:HG23	2.17	0.45
1:G:234:LEU:O	1:G:238:GLU:HG3	2.17	0.45
1:H:235:PRO:CG	1:H:310:GLU:HA	2.35	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:J:183:LEU:HD13	1:J:184:GLN:N	2.30	0.45
1:J:260:ALA:O	1:J:264:VAL:HG23	2.16	0.45
1:K:369:VAL:HG23	1:K:370:ALA:N	2.31	0.45
1:N:271:VAL:HG12	1:N:273:VAL:HG23	1.97	0.45
1:N:215:LEU:HB2	1:N:323:VAL:CG2	2.47	0.45
1:A:182:GLY:HA2	1:A:383:ALA:CB	2.46	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:E:206:ASN:ND2	1:E:214:GLU:H	2.11	0.45
1:E:219:PHE:O	1:E:247:LEU:HD12	2.16	0.45
1:E:325:ILE:HG22	1:E:330:THR:HA	1.97	0.45
1:F:160:LYS:HB2	1:F:160:LYS:HZ2	1.81	0.45
1:F:217:SER:N	1:F:218:PRO:CD	2.79	0.45
1:F:193:MET:HE2	1:F:292:ILE:HG12	1.99	0.45
1:I:60:ILE:O	1:I:75:LYS:HE3	2.16	0.45
1:J:325:ILE:HA	1:J:329:THR:O	2.16	0.45
1:J:524:LEU:O	1:J:526:LYS:N	2.49	0.45
1:M:325:ILE:HG22	1:M:330:THR:HA	1.97	0.45
1:N:266:THR:HG21	1:N:273:VAL:H	1.80	0.45
1:A:384:ALA:O	1:A:385:THR:HG23	2.16	0.45
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.99	0.45
1:C:413:ALA:HB3	1:C:417:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:LEU:HD21	1:I:425:LYS:NZ	2.31	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
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.32	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:M:169:VAL:HG13	1:M:377:ALA:HB2	1.99	0.45
1:N:10:ASN:ND2	6:N:2158:HOH:O	2.49	0.45
1:E:182:GLY:O	1:E:183:LEU:O	2.35	0.45
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.99	0.45
1:E:369:VAL:HG23	1:E:370:ALA:N	2.30	0.45
1:F:219:PHE:O	1:F:247:LEU:HD12	2.16	0.45
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.98	0.45
1:I:183:LEU:CD2	1:I:384:ALA:HB2	2.45	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:N:254:VAL:HG12	1:N:259:LEU:HB2	1.99	0.45
1:A:185:ASP:OD1	1:A:382:GLY:N	2.48	0.45
1:D:90:THR:OG1	5:D:551:AGS:S1G	2.68	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.79	0.45
1:H:524:LEU:O	1:H:526:LYS:N	2.49	0.45
1:I:183:LEU:HD13	1:I:184:GLN:N	2.31	0.45
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.98	0.45
1:L:438:VAL:O	1:L:442:VAL:HG23	2.17	0.45
1:M:217:SER:N	1:M:218:PRO:HD3	2.32	0.45
1:A:369:VAL:HG23	1:A:370:ALA:N	2.32	0.45
1:A:39:VAL:HG12	1:B:69:MET:CE	2.47	0.45
1:C:206:ASN:OD1	1:C:207:LYS:HG3	2.17	0.45
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.17	0.45
1:D:87:ASP:N	6:D:2757:HOH:O	2.49	0.45
1:E:158:VAL:HG22	6:E:2648:HOH:O	2.16	0.45
1:G:238:GLU:O	1:G:241:ALA:HB3	2.16	0.45
1:L:222:LEU:HB3	1:L:289:LEU:CD2	2.46	0.45
1:L:524:LEU:HA	1:L:524:LEU:HD12	1.87	0.45
1:M:222:LEU:HB3	1:M:289:LEU:CD2	2.47	0.45
1:E:210:THR:HG22	1:E:210:THR:O	2.17	0.45
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.47	0.45
1:F:325:ILE:HG22	1:F:330:THR:HA	1.98	0.45
1:F:366:GLN:O	1:F:369:VAL:HG22	2.16	0.45
1:G:463:SER:O	1:G:467:ASN:HB2	2.17	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:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.45
1:N:174:VAL:HG22	1:N:194:GLN:HE21	1.82	0.45
1:N:238:GLU:O	1:N:241:ALA:HB3	2.17	0.45
1:N:252:GLU:O	1:N:253:ASP:HB2	2.16	0.45
1:N:90:THR:O	1:N:94:VAL:HG13	2.16	0.45
1:A:217:SER:N	1:A:218:PRO:CD	2.80	0.45
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.29	0.45
1:B:210:THR:HG22	1:B:210:THR:O	2.16	0.45
1:B:217:SER:N	1:B:218:PRO:HD3	2.32	0.45
1:C:239:ALA:C	1:C:314:LEU:HD21	2.38	0.45
1:D:242:LYS:C	1:D:244:GLY:N	2.67	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:239:ALA:O	1:J:314:LEU:HD11	2.16	0.45
1:J:272:LYS:NZ	1:K:229:ASN:OD1	2.50	0.45
1:K:174:VAL:HG22	1:K:194:GLN:NE2	2.32	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: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:L:325:ILE:HG22	1:L:330:THR:HG23	1.98	0.45
1:L:369:VAL:HG23	1:L:370:ALA:N	2.32	0.45
1:N:242:LYS:C	1:N:244:GLY:N	2.69	0.45
1:A:217:SER:N	1:A:218:PRO:HD3	2.32	0.45
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.45
1:B:342:ILE:O	1:B:346:VAL:HG23	2.17	0.45
1:B:39:VAL:HG12	1:C:69:MET:CE	2.47	0.45
1:C:210:THR:HG22	1:C:210:THR:O	2.17	0.45
1:E:141:SER:HB3	6:E:2603:HOH:O	2.17	0.45
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.57	0.45
1:J:183:LEU:CD2	1:J:384:ALA:HB2	2.44	0.45
1:L:90:THR:OG1	5:L:1:AGS:S1G	2.65	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.98	0.45
1:M:238:GLU:O	1:M:241:ALA:HB3	2.17	0.45
1:C:182:GLY:HA2	1:C:383:ALA:HB3	1.97	0.44
1:C:305:ILE:HB	1:C:307:MET:HE2	1.98	0.44
1:C:381:VAL:O	1:C:382:GLY:O	2.36	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
1:J:37:ASN:HD21	1:J:51:LYS:HE3	1.80	0.44

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:VAL:HG23	1:C:370:ALA:N	2.32	0.44
1:D:218:PRO:HD2	1:D:320:ALA:O	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:I:348:GLN:O	1:I:352:GLN:HG2	2.18	0.44
1:J:217:SER:N	1:J:218:PRO:HD3	2.32	0.44
1:J:324:VAL:O	1:J:331:THR:HG22	2.18	0.44
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.44
1:K:134:LEU:HD21	1:K:425:LYS:NZ	2.32	0.44
5:K:1:AGS:O2G	5:K:1:AGS:S1G	2.55	0.44
1:K:413:ALA:HB3	1:K:417:VAL:HG22	1.98	0.44
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.99	0.44
1:M:290:GLN:HB3	1:M:345:ARG:NH2	2.31	0.44
1:M:73:MET:HB3	6:M:2221:HOH:O	2.18	0.44
1:N:193:MET:HE2	1:N:292:ILE:HG12	1.99	0.44
1:N:384:ALA:O	1:N:385:THR:HG23	2.17	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:C:325:ILE:HA	1:C:329:THR:O	2.17	0.44
1:D:413:ALA:HB3	1:D:417:VAL:HG22	1.98	0.44
1:E:384:ALA:O	1:E:385:THR:HG23	2.17	0.44
1:F:210:THR:O	1:F:210:THR:HG22	2.17	0.44
1:F:369:VAL:HG23	1:F:370:ALA:N	2.32	0.44
1:F:183:LEU:CD2	1:F:384:ALA:HB2	2.47	0.44
1:A:69:MET:CE	1:G:39:VAL:HG12	2.47	0.44
1:H:176:THR:HG22	1:H:177:VAL:H	1.82	0.44
1:H:215:LEU:HB2	1:H:323:VAL:HG22	2.00	0.44
1:J:217:SER:N	1:J:218:PRO:CD	2.81	0.44
1:J:68:ASN:O	1:J:72:GLN:HG2	2.17	0.44
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.99	0.44
1:L:253:ASP:OD1	1:L:277:LYS:HE2	2.18	0.44
1:M:182:GLY:HA2	1:M:383:ALA:HB3	2.00	0.44
1:A:218:PRO:HD2	1:A:320:ALA:O	2.17	0.44
1:C:16:MET:O	1:C:20:VAL:HG13	2.17	0.44
1:C:217:SER:N	1:C:218:PRO:CD	2.81	0.44
1:D:234:LEU:N	1:D:235:PRO:HD2	2.33	0.44
1:H:392:LYS:O	1:H:396:VAL:HG23	2.18	0.44
1:I:384:ALA:O	1:I:385:THR:HG23	2.18	0.44
1:I:496:PRO:O	1:I:499:VAL:HG13	2.17	0.44
1:J:224:ASP:HB3	1:J:302:SER:HB3	2.00	0.44
1:N:153:ASN:O	1:N:154:SER:HB2	2.18	0.44
1:C:179:ASP:HB3	1:C:389:MET:CE	2.48	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:E:242:LYS:C	1:E:244:GLY:N	2.71	0.44
1:F:389:MET:N	6:F:2746:HOH:O	2.50	0.44
1:G:336:VAL:O	1:G:337:GLY:C	2.55	0.44
1:K:242:LYS:C	1:K:244:GLY:N	2.71	0.44
1:M:369:VAL:HG23	1:M:370:ALA:N	2.32	0.44
1:N:217:SER:N	1:N:218:PRO:CD	2.81	0.44
1:N:42:LYS:HE3	1:N:48:THR:OG1	2.18	0.44
1:B:217:SER:N	1:B:218:PRO:CD	2.80	0.43
1:B:259:LEU:O	1:B:263:VAL:HG23	2.18	0.43
1:B:325:ILE:HA	1:B:329:THR:O	2.18	0.43
1:B:413:ALA:HB3	1:B:417:VAL:HG22	2.00	0.43
1:D:200:LEU:HD13	1:D:254:VAL:HB	2.00	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:G:381:VAL:O	1:G:382:GLY:O	2.36	0.43
1:G:70:GLY:HA2	1:G:73:MET:HE3	2.01	0.43
1:H:217:SER:N	1:H:218:PRO:HD3	2.33	0.43
1:H:302:SER:H	1:H:307:MET:HE1	1.83	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.17	0.43
1:M:210:THR:HG22	1:M:210:THR:O	2.18	0.43
1:B:451:LEU:HD23	1:B:451:LEU:C	2.39	0.43
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.98	0.43
1:C:348:GLN:O	1:C:352:GLN:HG2	2.18	0.43
1:C:183:LEU:CD2	1:C:384:ALA:HB2	2.47	0.43
1:D:236:VAL:O	1:D:240:VAL:HG23	2.19	0.43
1:E:200:LEU:HG	1:E:276:VAL:HA	2.01	0.43
1:F:342:ILE:O	1:F:346:VAL:HG23	2.18	0.43
1:G:260:ALA:O	1:G:264: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:J:242:LYS:C	1:J:244:GLY:N	2.71	0.43
1:L:199:TYR:CZ	1:L:327:LYS:HA	2.53	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:L:421:ARG:CZ	1:L:473:ASP:HA	2.48	0.43
1:A:348:GLN:O	1:A:352:GLN:HG2	2.17	0.43
1:B:242:LYS:O	1:B:243:ALA:HB3	2.19	0.43
1:E:73:MET:O	1:E:76:GLU:HB2	2.18	0.43
1:G:351:GLN:HA	1:G:354:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:ALA:O	1:H:264:VAL:HG23	2.18	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
1:N:210:THR:HG22	1:N:210:THR:O	2.18	0.43
1:N:217:SER:N	1:N:218:PRO:HD3	2.33	0.43
1:N:525:PRO:HD3	6:N:2033:HOH:O	2.18	0.43
1:A:210:THR:HG22	1:A:210:THR:O	2.18	0.43
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.19	0.43
1:I:409:GLU:OE2	1:I:498:LYS:HG3	2.19	0.43
1:N:171:LYS:HB2	1:N:407:VAL:HG11	2.01	0.43
1:A:191:GLU:O	1:A:334:ASP:HA	2.18	0.43
1:B:218:PRO:HD2	1:B:320:ALA:O	2.18	0.43
1:B:266:THR:HG22	1:B:271:VAL:O	2.19	0.43
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.01	0.43
1:G:224:ASP:HB3	1:G:302:SER:HB3	2.00	0.43
1:H:384:ALA:C	1:H:385:THR:HG23	2.39	0.43
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.54	0.43
1:J:69:MET:O	1:J:73:MET:HG3	2.19	0.43
1:M:217:SER:N	1:M:218:PRO:CD	2.82	0.43
1:N:284:ARG:O	1:N:288:MET:HG3	2.19	0.43
1:N:366:GLN:O	1:N:369:VAL:HG22	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: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:D:325:ILE:HG22	1:D:330:THR:HG23	1.99	0.43
1:F:178:GLU:OE2	1:F:322:ARG:NH1	2.51	0.43
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.00	0.43
1:H:183:LEU:HD13	1:H:184:GLN:N	2.33	0.43
1:H:409:GLU:OE2	1:H:498:LYS:HG3	2.19	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:J:240:VAL:HG11	1:J:247:LEU:HB2	1.99	0.43
1:J:449:ALA:HB3	1:J:450:PRO:HD3	2.01	0.43
1:K:205:ILE:CA	1:K:213:VAL:HG22	2.49	0.43
1:M:259:LEU:O	1:M:263:VAL:HG23	2.19	0.43
1:N:37:ASN:HD21	1:N:51:LYS:HE3	1.84	0.43
1:N:82:ASN:O	1:N:86:GLY:N	2.49	0.43
1:A:194:GLN:OE1	1:A:329:THR:HG21	2.18	0.43
1:A:384:ALA:O	1:A:385:THR:OG1	2.33	0.43
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:O	1:B:238:GLU:HG3	2.18	0.43
1:E:176:THR:HG22	1:E:177:VAL:N	2.33	0.43
1:E:218:PRO:HD2	1:E:320:ALA:O	2.19	0.43
1:F:383:ALA:HA	6:F:2746:HOH:O	2.19	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:J:209:GLU:N	1:J:209:GLU:OE1	2.47	0.43
1:L:85:ALA:O	1:L:401:HIS:HE1	2.01	0.43
1:A:69:MET:HE2	1:G:39:VAL:HG12	2.01	0.43
1:B:215:LEU:HB2	1:B:323:VAL:CG2	2.48	0.43
1:B:463:SER:O	1:B:467:ASN:HB2	2.19	0.43
1:C:272:LYS:NZ	1:D:228:SER:HB2	2.34	0.43
1:D:349:ILE:CG2	1:D:369:VAL:HG13	2.48	0.43
1:E:324:VAL:O	1:E:331:THR:HG22	2.17	0.43
1:G:223:ALA:O	1:G:251:ALA:HA	2.19	0.43
1:H:37:ASN:ND2	1:H:51:LYS:HE3	2.34	0.43
1:I:259:LEU:O	1:I:263:VAL:HG23	2.18	0.43
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.49	0.43
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.00	0.43
1:L:239:ALA:O	1:L:314:LEU:HD11	2.18	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:F:209:GLU:OE1	1:F:209:GLU:N	2.49	0.43
1:F:348:GLN:O	1:F:352:GLN:HG2	2.18	0.43
1:F:420:ILE:CD1	1:F:451:LEU:HD13	2.49	0.43
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.43
1:L:217:SER:N	1:L:218:PRO:CD	2.82	0.43
1:L:381:VAL:O	1:L:382:GLY:O	2.37	0.43
1:M:68:ASN:O	1:M:72:GLN:HG2	2.18	0.43
1:N:222:LEU:HB3	1:N:289:LEU:HD21	2.01	0.43
1:A:417:VAL:HG11	1:A:488:MET:HG3	2.00	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.43
1:B:384:ALA:C	1:B:385:THR:HG23	2.38	0.43
1:B:241:ALA:HB1	1:C:231:ARG:NH1	2.33	0.43
1:D:234:LEU:O	1:D:238:GLU:HG3	2.18	0.43
1:D:65:LYS:HG2	6:D:1200:HOH:O	2.19	0.43
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.99	0.43
1:I:496:PRO:HB2	1:I:499:VAL:CG1	2.49	0.43
1:K:220:ILE:CD1	1:K:296:THR:HG21	2.49	0.43
1:L:217:SER:N	1:L:218:PRO:HD3	2.33	0.43
1:N:524:LEU:O	1:N:526:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:HG22	6:A:2839:HOH:O	2.18	0.42
1:B:353:ILE:HD13	1:B:366:GLN:HG2	2.01	0.42
1:C:421:ARG:CZ	1:C:473:ASP:HA	2.49	0.42
1:E:177:VAL:HA	1:E:379:ILE:O	2.19	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.42
1:F:191:GLU:O	1:F:334:ASP:HA	2.18	0.42
1:J:179:ASP:HB3	1:J:389:MET:CE	2.48	0.42
1:K:182:GLY:HA2	1:K:383:ALA:CB	2.49	0.42
1:K:70:GLY:HA2	1:K:73:MET:HE3	2.01	0.42
1:L:383:ALA:O	1:L:384:ALA:CB	2.66	0.42
1:L:60:ILE:O	1:L:75:LYS:HE3	2.19	0.42
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.00	0.42
1:M:284:ARG:HH11	1:M:364:LYS:CE	2.32	0.42
5:N:1:AGS:O2G	5:N:1:AGS:S1G	2.54	0.42
1:A:366:GLN:HA	1:A:369:VAL:HG22	2.00	0.42
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.00	0.42
1:G:302:SER:H	1:G:307:MET:HE1	1.83	0.42
1:I:466:ALA:O	1:I:470:LYS:HG3	2.19	0.42
1:J:222:LEU:HB3	1:J:289:LEU:CD2	2.50	0.42
1:K:319:GLN:HB3	1:K:336:VAL:HG21	2.00	0.42
1:K:384:ALA:C	1:K:385:THR:HG23	2.39	0.42
1:M:496:PRO:O	1:M:499:VAL:HG13	2.19	0.42
1:A:253:ASP:OD1	1:A:277:LYS:HE2	2.19	0.42
1:B:193:MET:HE3	1:B:292:ILE:HG12	2.02	0.42
1:C:496:PRO:O	1:C:499:VAL:HG13	2.19	0.42
1:D:284:ARG:O	1:D:288:MET:HG3	2.19	0.42
1:D:37:ASN:HD21	1:D:51:LYS:HE3	1.84	0.42
1:E:220:ILE:CD1	1:E:296:THR:HG21	2.48	0.42
1:I:238:GLU:O	1:I:241:ALA:HB3	2.19	0.42
1:I:496:PRO:HD2	1:I:499:VAL:CG1	2.49	0.42
1:J:200:LEU:HG	1:J:276:VAL:HA	2.01	0.42
1:K:421:ARG:CZ	1:K:473:ASP:HA	2.49	0.42
1:K:438:VAL:O	1:K:442:VAL:HG23	2.18	0.42
1:L:324:VAL:O	1:L:331:THR:HG22	2.19	0.42
1:N:272:LYS:CD	1:N:272:LYS:N	2.83	0.42
1:N:336:VAL:O	1:N:337:GLY:C	2.58	0.42
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	0.42
1:A:8:PHE:HB3	6:A:1960:HOH:O	2.20	0.42
1:B:169:VAL:HG13	1:B:377:ALA:HB2	2.00	0.42
1:C:271:VAL:HG12	1:C:273:VAL:HG23	2.00	0.42
1:D:206:ASN:OD1	1:D:207:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:GLN:O	1:E:352:GLN:HG2	2.19	0.42
1:D:36:ARG:HG3	1:E:518:GLU:HG2	2.00	0.42
1:F:253:ASP:OD1	1:F:277:LYS:HE2	2.19	0.42
1:F:384:ALA:C	1:F:385:THR:HG23	2.40	0.42
1:G:85:ALA:O	1:G:401:HIS:HE1	2.02	0.42
1:G:524:LEU:O	1:G:526:LYS:N	2.52	0.42
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.42
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.02	0.42
1:L:94:VAL:HB	6:L:2642:HOH:O	2.20	0.42
1:M:288:MET:HA	1:M:291:ASP:OD2	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:N:193:MET:HE1	1:N:292:ILE:HG12	2.01	0.42
1:A:183:LEU:HD13	1:A:184:GLN:N	2.34	0.42
1:A:240:VAL:HG11	1:A:247:LEU:HB2	2.00	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:D:445:ARG:HD3	6:D:2123:HOH:O	2.19	0.42
1:F:183:LEU:HD13	1:F:184:GLN:N	2.34	0.42
1:F:60:ILE:O	1:F:75:LYS:HE3	2.19	0.42
1:G:134:LEU:HD22	6:G:2213:HOH:O	2.19	0.42
1:H:342:ILE:O	1:H:346:VAL:HG23	2.19	0.42
6:I:2009:HOH:O	1:J:117:LYS:HE3	2.18	0.42
1:J:238:GLU:O	1:J:241:ALA:HB3	2.20	0.42
1:J:215:LEU:HB2	1:J:323:VAL:CG2	2.50	0.42
1:L:183:LEU:HD13	1:L:184:GLN:N	2.34	0.42
1:L:202:PRO:O	1:L:204:PHE:N	2.46	0.42
1:M:284:ARG:HH11	1:M:364:LYS:NZ	2.18	0.42
1:D:404:ARG:HH11	1:D:404:ARG:CG	2.27	0.42
1:E:209:GLU:OE1	1:E:209:GLU:N	2.49	0.42
1:E:266:THR:HG22	1:E:271:VAL:O	2.19	0.42
1:F:319:GLN:HB3	1:F:336:VAL:HG21	2.02	0.42
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.91	0.42
1:G:242:LYS:O	1:G:244:GLY:N	2.52	0.42
1:G:266:THR:HG21	1:G:273:VAL:H	1.84	0.42
1:G:131:LEU:HD13	1:G:422:VAL:HG21	2.02	0.42
1:H:160:LYS:HB2	1:H:160:LYS:HZ3	1.84	0.42
1:J:348:GLN:O	1:J:352:GLN:HG2	2.19	0.42
1:J:182:GLY:HA2	1:J:383:ALA:HB3	2.02	0.42
6:C:2549:HOH:O	1:J:463:SER:HB2	2.19	0.42
1:K:460:GLU:O	1:K:462:PRO:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.60	0.42
1:L:259:LEU:O	1:L:263:VAL:HG23	2.19	0.42
1:M:220:ILE:CD1	1:M:296:THR:HG21	2.48	0.42
1:N:194:GLN:HG3	1:N:331:THR:HB	2.00	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.02	0.42
1:N:259:LEU:O	1:N:263:VAL:HG23	2.20	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: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:336:VAL:O	1:I:337:GLY:C	2.58	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:K:496:PRO:O	1:K:499:VAL:HG13	2.19	0.42
1:M:242:LYS:O	1:M:243:ALA:HB3	2.20	0.42
1:N:111:MET:HG2	1:N:435:ASP:OD1	2.19	0.42
1:A:302:SER:O	1:A:307:MET:HE3	2.20	0.42
1:B:140:ASP:O	1:B:144:ILE:HG13	2.20	0.42
1:B:197:ARG:HD2	1:B:277:LYS:HB2	2.01	0.42
1:F:206:ASN:ND2	1:F:214:GLU:H	2.16	0.42
1:G:193:MET:HE2	1:G:292:ILE:HG12	2.00	0.42
1:H:210:THR:O	1:H:210:THR:HG22	2.20	0.42
1:H:319:GLN:HB3	1:H:336:VAL:HG21	2.01	0.42
1:H:325:ILE:HA	1:H:329:THR:O	2.19	0.42
1:H:381:VAL:O	1:H:382:GLY:O	2.38	0.42
1:I:266:THR:HG21	1:I:273:VAL:H	1.84	0.42
1:J:305:ILE:HB	1:J:307:MET:HE2	2.01	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:M:179:ASP:HB3	1:M:389:MET:CE	2.50	0.42
1:M:524:LEU:HA	1:M:524:LEU:HD12	1.87	0.42
1:B:324:VAL:O	1:B:331:THR:HG22	2.20	0.42
1:B:77:VAL:HG11	1:B:506:TYR:O	2.18	0.42
1:A:4:LYS:HG3	1:G:59:GLU:O	2.19	0.42
1:I:366:GLN:HA	1:I:369:VAL:HG22	2.01	0.42
1:L:206:ASN:ND2	1:L:214:GLU:H	2.18	0.42
1:L:382:GLY:O	1:L:389:MET:HG2	2.20	0.42
1:M:348:GLN:O	1:M:352:GLN:HG2	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: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:D:223:ALA:O	1:D:251:ALA:HA	2.20	0.42
1:E:76:GLU:HG3	6:E:2322:HOH:O	2.20	0.42
1:F:259:LEU:O	1:F:263:VAL:HG23	2.19	0.42
1:G:219:PHE:O	1:G:247:LEU:HD12	2.19	0.42
1:H:240:VAL:HG11	1:H:247:LEU:HB2	2.01	0.42
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.91	0.42
1:L:33:PRO:CG	1:L:480:ALA:HB3	2.50	0.42
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.35	0.42
1:A:336:VAL:O	1:A:337:GLY:C	2.59	0.41
1:B:305:ILE:HB	1:B:307:MET:HE2	2.02	0.41
1:C:222:LEU:HB3	1:C:289:LEU:CD2	2.50	0.41
1:D:191:GLU:O	1:D:334:ASP:HA	2.20	0.41
1:F:242:LYS:C	1:F:244:GLY:N	2.73	0.41
1:F:510:VAL:CG2	6:F:2556:HOH:O	2.67	0.41
1:G:417:VAL:HG13	6:G:2394:HOH:O	2.20	0.41
1:H:220:ILE:HD12	1:H:296:THR:HG21	2.02	0.41
1:I:177:VAL:HG21	1:I:397:GLU:HG2	1.99	0.41
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.34	0.41
1:N:325:ILE:HA	1:N:329:THR:O	2.18	0.41
1:N:183:LEU:CD2	1:N:384:ALA:HB2	2.49	0.41
1:A:176:THR:HG22	1:A:177:VAL:H	1.84	0.41
1:B:366:GLN:HA	1:B:369:VAL:HG22	2.02	0.41
1:C:200:LEU:HG	1:C:276:VAL:HA	2.02	0.41
1:D:160:LYS:HZ2	1:D:160:LYS:HB2	1.84	0.41
1:D:177:VAL:HA	1:D:379:ILE:O	2.20	0.41
1:F:487:ASN:O	1:F:491:MET:HG3	2.20	0.41
1:G:353:ILE:HD13	1:G:366:GLN:HG2	2.02	0.41
1:G:409:GLU:OE2	1:G:498:LYS:HG3	2.20	0.41
5:L:1:AGS:O2G	5:L:1:AGS:S1G	2.55	0.41
1:L:97:GLN:HG2	6:L:2018:HOH:O	2.19	0.41
1:M:242:LYS:C	1:M:244:GLY:N	2.72	0.41
1:M:171:LYS:HB2	1:M:407:VAL:HG11	2.02	0.41
1:M:496:PRO:HB2	1:M:499:VAL:HG12	2.02	0.41
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.21	0.41
1:A:153:ASN:O	1:A:154:SER:HB2	2.19	0.41
1:A:220:ILE:HD12	1:A:296:THR:HG21	2.02	0.41
1:B:194:GLN:OE1	1:B:329:THR:HG21	2.20	0.41
1:B:222:LEU:HB3	1:B:289:LEU:CD2	2.49	0.41
1:C:224:ASP:HB3	1:C:302:SER:HB3	2.02	0.41
1:C:353:ILE:HD13	1:C:366:GLN:HG2	2.01	0.41
1:D:217:SER:N	1:D:218:PRO:HD3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:GLU:O	1:E:334:ASP:HA	2.20	0.41
1:E:238:GLU:O	1:E:241:ALA:HB3	2.19	0.41
1:E:183:LEU:CD2	1:E:384:ALA:HB2	2.50	0.41
1:F:182:GLY:HA2	1:F:383:ALA:HB3	2.01	0.41
1:G:222:LEU:HB3	1:G:289:LEU:CD2	2.50	0.41
1:G:384:ALA:C	1:G:385:THR:HG23	2.40	0.41
1:J:336:VAL:O	1:J:337:GLY:C	2.58	0.41
1:K:239:ALA:C	1:K:314:LEU:HD21	2.41	0.41
1:L:210:THR:O	1:L:210:THR:HG22	2.20	0.41
1:L:122:LYS:HE2	1:L:429:LEU:HD11	2.02	0.41
1:M:193:MET:HE2	1:M:292:ILE:HG12	2.02	0.41
1:N:209:GLU:N	1:N:209:GLU:OE1	2.48	0.41
1:N:524:LEU:HA	1:N:524:LEU:HD12	1.91	0.41
1:N:69:MET:O	1:N:73:MET:HG3	2.19	0.41
1:B:240:VAL:HG11	1:B:247:LEU:HB2	2.01	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:H:16:MET:HE3	6:H:2854:HOH:O	2.21	0.41
1:I:217:SER:HA	1:I:320:ALA:O	2.20	0.41
1:J:177:VAL:HA	1:J:379:ILE:O	2.20	0.41
1:J:295:LEU:HD13	1:J:295:LEU:O	2.20	0.41
1:K:366:GLN:HA	1:K:369:VAL:HG22	2.01	0.41
1:K:171:LYS:HB2	1:K:407:VAL:HG11	2.02	0.41
1:N:176:THR:HG22	1:N:177:VAL:N	2.35	0.41
1:A:182:GLY:O	1:A:183:LEU:O	2.39	0.41
1:A:219:PHE:O	1:A:247:LEU:HD12	2.20	0.41
1:B:325:ILE:HG22	1:B:330:THR:HG23	2.03	0.41
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.87	0.41
1:C:177:VAL:HA	1:C:379:ILE:O	2.20	0.41
1:C:460:GLU:O	1:C:462:PRO:HD3	2.21	0.41
1:D:284:ARG:NH1	1:D:364:LYS:NZ	2.67	0.41
1:D:182:GLY:HA2	1:D:383:ALA:HB3	2.03	0.41
1:E:182:GLY:HA2	1:E:383:ALA:HB3	2.02	0.41
1:E:325:ILE:HG22	1:E:330:THR:HG23	2.02	0.41
1:E:178:GLU:OE1	1:E:378:VAL:HG11	2.20	0.41
1:E:28:LYS:HD2	1:E:453:GLN:NE2	2.36	0.41
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.50	0.41
1:H:153:ASN:O	1:H:154:SER:HB2	2.20	0.41
1:H:295:LEU:C	1:H:295:LEU:HD13	2.41	0.41
1:J:134:LEU:HD21	1:J:425:LYS:NZ	2.35	0.41
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.91	0.41
1:M:54:VAL:HG23	6:M:2164:HOH:O	2.20	0.41
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.50	0.41
1:N:463:SER:O	1:N:467:ASN:HB2	2.19	0.41
1:B:193:MET:HE1	1:B:292:ILE:HG12	2.02	0.41
1:B:336:VAL:O	1:B:337:GLY:C	2.59	0.41
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.85	0.41
1:C:182:GLY:HA2	1:C:383:ALA:CB	2.50	0.41
1:D:200:LEU:HG	1:D:276:VAL:HA	2.01	0.41
1:D:210:THR:HG22	1:D:210:THR:O	2.19	0.41
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.41
1:H:85:ALA:O	1:H:401:HIS:HE1	2.03	0.41
1:I:324:VAL:O	1:I:331:THR:HG22	2.21	0.41
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.56	0.41
1:K:204:PHE:C	1:K:213:VAL:HG22	2.41	0.41
1:K:295:LEU:HD13	1:K:295:LEU:O	2.20	0.41
1:K:366:GLN:O	1:K:369:VAL:HG22	2.20	0.41
1:L:477:GLY:CA	6:L:2905:HOH:O	2.68	0.41
1:M:136:VAL:HA	1:M:137:PRO:HD3	1.87	0.41
1:M:215:LEU:HB2	1:M:323:VAL:HG22	2.03	0.41
1:A:231:ARG:NH1	1:G:242:LYS:HA	2.35	0.41
1:A:242:LYS:C	1:A:244:GLY:N	2.73	0.41
1:A:266:THR:HG21	1:A:273:VAL:H	1.86	0.41
1:B:69:MET:O	1:B:73:MET:HG3	2.20	0.41
1:E:305:ILE:HB	1:E:307:MET:HE2	2.02	0.41
1:N:455:VAL:O	1:N:458:CYS:HB2	2.21	0.41
1:B:302:SER:H	1:B:307:MET:HE1	1.85	0.41
1:D:201:SER:O	1:D:202:PRO:O	2.39	0.41
1:D:324:VAL:HB	1:D:331:THR:CG2	2.51	0.41
1:D:348:GLN:O	1:D:352:GLN:HG2	2.21	0.41
1:E:336:VAL:O	1:E:337:GLY:C	2.58	0.41
1:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:E:85:ALA:O	1:E:401:HIS:HE1	2.03	0.41
1:F:238:GLU:O	1:F:241:ALA:HB3	2.20	0.41
1:G:202:PRO:C	1:G:204:PHE:H	2.23	0.41
1:G:266:THR:HG22	1:G:273:VAL:H	1.86	0.41
1:G:183:LEU:CD2	1:G:384:ALA:HB2	2.48	0.41
1:I:242:LYS:O	1:I:243:ALA:HB3	2.20	0.41
1:J:140:ASP:OD2	1:J:142:LYS:HB3	2.21	0.41
1:K:153:ASN:O	1:K:154:SER:HB2	2.20	0.41
1:K:381:VAL:O	1:K:382:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:194:GLN:HG3	1:L:331:THR:HB	2.03	0.41
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.61	0.41
1:N:260:ALA:O	1:N:264:VAL:HG23	2.21	0.41
1:A:194:GLN:HG3	1:A:331:THR:HB	2.02	0.41
1:B:194:GLN:HG3	1:B:331:THR:HB	2.03	0.41
1:B:177:VAL:HA	1:B:379:ILE:O	2.21	0.41
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.41
1:C:496:PRO:HB2	1:C:499:VAL:CG1	2.50	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.50	0.41
1:F:421:ARG:CZ	1:F:473:ASP:HA	2.51	0.41
1:G:200:LEU:HG	1:G:276:VAL:HA	2.02	0.41
1:H:177:VAL:HG21	1:H:397:GLU:HG2	2.00	0.41
1:H:191:GLU:O	1:H:334:ASP:HA	2.19	0.41
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.60	0.41
1:I:63:GLU:HB2	1:J:524:LEU:CD2	2.50	0.41
1:J:182:GLY:HA2	1:J:383:ALA:CB	2.50	0.41
1:J:381:VAL:O	1:J:382:GLY:O	2.39	0.41
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.41
1:L:235:PRO:CG	1:L:310:GLU:HA	2.34	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: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:M:253:ASP:OD1	1:M:277:LYS:HE2	2.20	0.41
1:N:194:GLN:OE1	1:N:329:THR:HG21	2.21	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:E:160:LYS:HB2	1:E:160:LYS:NZ	2.36	0.41
1:E:366:GLN:HA	1:E:369:VAL:HG22	2.03	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:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	0.41
1:G:77:VAL:CG2	1:G:510:VAL:HG21	2.51	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
1:I:421:ARG:CZ	1:I:473:ASP:HA	2.51	0.41
1:J:242:LYS:O	1:J:243:ALA:HB3	2.20	0.41
1:K:353:ILE:HD13	1:K:366:GLN:HG2	2.01	0.41
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.34	0.41
1:L:200:LEU:HG	1:L:276:VAL:HA	2.02	0.41
1:L:290:GLN:HB3	1:L:345:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:477:GLY:HA2	6:L:2905:HOH:O	2.20	0.41
1:L:46:ALA:HA	1:L:47:PRO:HD3	1.93	0.41
1:M:449:ALA:HB3	1:M:450:PRO:HD3	2.03	0.41
1:N:134:LEU:HD21	1:N:425:LYS:NZ	2.35	0.41
1:N:85:ALA:O	1:N:401:HIS:HE1	2.03	0.41
1:A:325:ILE:HA	1:A:329:THR:O	2.20	0.41
1:C:153:ASN:O	1:C:154:SER:HB2	2.21	0.41
1:E:202:PRO:C	1:E:204:PHE:H	2.23	0.41
1:E:224:ASP:HB3	1:E:302:SER:HB3	2.01	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:F:23:LEU:CD2	1:F:74:VAL:HG13	2.51	0.41
1:M:102:GLU:HB2	1:M:442:VAL:HG13	2.03	0.41
1:N:193:MET:HG3	1:N:371:LYS:HB3	2.03	0.41
1:A:466:ALA:O	1:A:470:LYS:HG3	2.21	0.40
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.51	0.40
1:H:77:VAL:HG23	1:H:510:VAL:HG21	2.03	0.40
1:K:46:ALA:HA	1:K:47:PRO:HD3	1.88	0.40
1:L:160:LYS:NZ	1:L:160:LYS:HB2	2.36	0.40
1:M:205:ILE:CA	1:M:213:VAL:HG22	2.48	0.40
1:M:384:ALA:C	1:M:385:THR:HG23	2.42	0.40
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.03	0.40
1:C:284:ARG:HH12	1:C:364:LYS:NZ	2.19	0.40
1:D:224:ASP:HB3	1:D:302:SER:HB3	2.04	0.40
1:E:242:LYS:O	1:E:243:ALA:HB3	2.21	0.40
1:F:302:SER:O	1:F:307:MET:HE3	2.21	0.40
1:G:182:GLY:HA2	1:G:383:ALA:HB3	2.04	0.40
1:H:200:LEU:HG	1:H:276:VAL:HA	2.02	0.40
1:I:325:ILE:HG22	1:I:330:THR:HG23	2.02	0.40
1:I:496:PRO:HD2	1:I:499:VAL:HG11	2.03	0.40
1:J:366:GLN:O	1:J:369:VAL:HG22	2.20	0.40
1:K:215:LEU:HB2	1:K:323:VAL:CG2	2.51	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:CG	1:K:404:ARG:HH11	2.31	0.40
1:K:451:LEU:C	1:K:451:LEU:HD23	2.41	0.40
1:K:7:LYS:HE2	1:K:66:PHE:CE2	2.56	0.40
1:M:197:ARG:HD2	1:M:277:LYS:HB2	2.04	0.40
1:N:384:ALA:C	1:N:385:THR:HG23	2.41	0.40
1:A:342:ILE:O	1:A:346:VAL:HG23	2.21	0.40
1:C:174:VAL:HG22	1:C:194:GLN:HE21	1.87	0.40
1:C:295:LEU:O	1:C:295:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.56	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:H:455:VAL:HG13	1:H:460:GLU:HB2	2.02	0.40
1:I:242:LYS:C	1:I:244:GLY:N	2.73	0.40
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.02	0.40
1:I:295:LEU:HD13	1:I:295:LEU:C	2.42	0.40
1:K:284:ARG:HH12	1:K:364:LYS:NZ	2.20	0.40
1:M:183:LEU:HD13	1:M:184:GLN:N	2.35	0.40
1:M:342:ILE:O	1:M:346:VAL:HG23	2.22	0.40
1:A:295:LEU:HD13	1:A:295:LEU:C	2.42	0.40
1:B:253:ASP:OD1	1:B:277:LYS:HE2	2.21	0.40
1:B:111:MET:SD	1:B:438:VAL:HG21	2.62	0.40
1:C:160:LYS:HB2	1:C:160:LYS:HZ2	1.87	0.40
1:C:201:SER:O	1:C:202:PRO:O	2.40	0.40
1:C:266:THR:HG21	1:C:273:VAL:H	1.86	0.40
1:C:34:LYS:HG3	1:C:458:CYS:SG	2.62	0.40
1:C:46:ALA:HA	1:C:47:PRO:HD3	1.94	0.40
1:C:524:LEU:HD12	1:C:524:LEU:HA	1.92	0.40
1:D:118:ARG:HD2	1:D:436:GLN:NE2	2.36	0.40
1:D:369:VAL:HG23	1:D:370:ALA:N	2.36	0.40
1:E:384:ALA:C	1:E:385:THR:HG23	2.42	0.40
1:F:215:LEU:HB2	1:F:323:VAL:HG22	2.03	0.40
1:H:202:PRO:C	1:H:204:PHE:H	2.24	0.40
1:I:194:GLN:HG3	1:I:331:THR:HB	2.02	0.40
1:I:384:ALA:C	1:I:385:THR:HG23	2.41	0.40
1:I:438:VAL:O	1:I:442:VAL:HG23	2.21	0.40
1:I:524:LEU:HA	1:I:524:LEU:HD12	1.93	0.40
1:K:240:VAL:HG11	1:K:247:LEU:HB2	2.02	0.40
1:K:200:LEU:HG	1:K:276:VAL:HA	2.03	0.40
1:K:392:LYS:O	1:K:396:VAL:HG23	2.22	0.40
1:L:361:ASP:O	1:L:365:LEU:HG	2.20	0.40
1:N:10:ASN:HA	6:N:2143:HOH:O	2.21	0.40
1:N:179:ASP:HB3	1:N:389:MET:CE	2.51	0.40
1:N:182:GLY:O	1:N:183:LEU:O	2.40	0.40
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.95	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:D:404:ARG:HG2	1:D:404:ARG:NH1	2.33	0.40
1:G:174:VAL:HG12	1:G:376:VAL:HG13	2.04	0.40
1:H:182:GLY:HA2	1:H:383:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:GLU:C	1:H:218:PRO:HD3	2.41	0.40
1:H:266:THR:HG21	1:H:273:VAL:H	1.85	0.40
1:H:326:ASN:HD22	1:H:329:THR:HB	1.86	0.40
1:I:132:LYS:HE2	6:I:1912:HOH:O	2.21	0.40
1:I:85:ALA:O	1:I:401:HIS:HE1	2.04	0.40
1:J:253:ASP:OD1	1:J:277:LYS:HE2	2.22	0.40
1:K:217:SER:HA	1:K:320:ALA:O	2.21	0.40
1:K:302:SER:O	1:K:307:MET:HE3	2.22	0.40
1:K:194:GLN:HG3	1:K:331:THR:HB	2.03	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40
1:M:194:GLN:HG3	1:M:331:THR:HB	2.03	0.40
5:M:1:AGS:S1G	5:M:1:AGS:O2G	2.54	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	7	3
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	8	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%)	8	3
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	7	3
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	8	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	7	3
1	I	523/547 (96%)	486 (93%)	27 (5%)	10 (2%)	9	4
1	J	523/547 (96%)	486 (93%)	25 (5%)	12 (2%)	7	3
1	K	523/547 (96%)	484 (92%)	29 (6%)	10 (2%)	9	4
1	L	523/547 (96%)	488 (93%)	23 (4%)	12 (2%)	7	3
1	M	523/547 (96%)	487 (93%)	25 (5%)	11 (2%)	8	3
1	N	523/547 (96%)	487 (93%)	26 (5%)	10 (2%)	9	4
All	All	7322/7658 (96%)	6820 (93%)	350 (5%)	152 (2%)	8	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 ⓘ

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%)	53	54
1	B	404/413 (98%)	397 (98%)	7 (2%)	66	70
1	C	404/413 (98%)	396 (98%)	8 (2%)	60	64
1	D	404/413 (98%)	394 (98%)	10 (2%)	53	54
1	E	404/413 (98%)	397 (98%)	7 (2%)	66	70
1	F	404/413 (98%)	396 (98%)	8 (2%)	60	64
1	G	404/413 (98%)	395 (98%)	9 (2%)	57	60
1	H	404/413 (98%)	397 (98%)	7 (2%)	66	70
1	I	404/413 (98%)	395 (98%)	9 (2%)	57	60
1	J	404/413 (98%)	397 (98%)	7 (2%)	66	70
1	K	404/413 (98%)	396 (98%)	8 (2%)	60	64
1	L	404/413 (98%)	394 (98%)	10 (2%)	53	54
1	M	404/413 (98%)	396 (98%)	8 (2%)	60	64
1	N	404/413 (98%)	396 (98%)	8 (2%)	60	64
All	All	5656/5782 (98%)	5540 (98%)	116 (2%)	59	62

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 ⓘ

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	26,33,33	4.25	1 (3%)	22,52,52	1.20	2 (9%)
2	SO4	A	4001	-	4,4,4	1.57	1 (25%)	6,6,6	1.11	0
2	SO4	A	4007	-	4,4,4	1.55	1 (25%)	6,6,6	1.10	0
2	SO4	A	4008	-	4,4,4	1.57	1 (25%)	6,6,6	1.08	0
5	AGS	B	1	3,4	26,33,33	4.30	1 (3%)	22,52,52	1.18	1 (4%)
2	SO4	B	4009	-	4,4,4	1.57	1 (25%)	6,6,6	1.06	0
2	SO4	B	4010	-	4,4,4	1.59	1 (25%)	6,6,6	1.08	0
5	AGS	C	1	3,4	26,33,33	4.36	1 (3%)	22,52,52	1.14	1 (4%)
2	SO4	C	4011	-	4,4,4	1.57	1 (25%)	6,6,6	1.08	0
2	SO4	C	4012	-	4,4,4	1.61	1 (25%)	6,6,6	1.10	0
5	AGS	D	551	3,4	26,33,33	4.46	4 (15%)	22,52,52	1.16	0
5	AGS	E	1	3,4	26,33,33	4.47	1 (3%)	22,52,52	1.18	1 (4%)
2	SO4	E	4005	-	4,4,4	1.48	1 (25%)	6,6,6	1.11	0
2	SO4	E	4006	-	4,4,4	1.58	1 (25%)	6,6,6	1.07	0
5	AGS	F	1	3,4	26,33,33	4.35	3 (11%)	22,52,52	1.03	0
2	SO4	F	4004	-	4,4,4	1.51	1 (25%)	6,6,6	1.13	0
5	AGS	G	1	3,4	26,33,33	4.49	1 (3%)	22,52,52	1.18	2 (9%)
2	SO4	G	4002	-	4,4,4	1.58	1 (25%)	6,6,6	1.11	0
5	AGS	H	1	3,4	26,33,33	4.35	1 (3%)	22,52,52	1.21	1 (4%)
2	SO4	H	4017	-	4,4,4	1.58	1 (25%)	6,6,6	1.09	0
2	SO4	H	4018	-	4,4,4	1.58	1 (25%)	6,6,6	1.06	0
5	AGS	I	1	3,4	26,33,33	4.39	1 (3%)	22,52,52	1.16	1 (4%)
5	AGS	J	1	3,4	26,33,33	4.37	3 (11%)	22,52,52	1.07	0
2	SO4	J	4019	-	4,4,4	1.57	1 (25%)	6,6,6	1.07	0
2	SO4	J	4020	-	4,4,4	1.59	1 (25%)	6,6,6	1.08	0
5	AGS	K	1	3,4	26,33,33	4.37	2 (7%)	22,52,52	1.02	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	K	4021	-	4,4,4	1.61	1 (25%)	6,6,6	1.09	0
2	SO4	K	4022	-	4,4,4	1.56	1 (25%)	6,6,6	1.09	0
5	AGS	L	1	3,4	26,33,33	4.34	1 (3%)	22,52,52	1.12	1 (4%)
2	SO4	L	4003	-	4,4,4	1.57	1 (25%)	6,6,6	1.10	0
5	AGS	M	1	3,4	26,33,33	4.35	1 (3%)	22,52,52	1.12	2 (9%)
2	SO4	M	4013	-	4,4,4	1.63	1 (25%)	6,6,6	1.09	0
2	SO4	M	4014	-	4,4,4	1.60	1 (25%)	6,6,6	1.08	0
5	AGS	N	1	3,4	26,33,33	4.39	1 (3%)	22,52,52	1.11	1 (4%)
2	SO4	N	4015	-	4,4,4	1.59	1 (25%)	6,6,6	1.10	0
2	SO4	N	4016	-	4,4,4	1.58	1 (25%)	6,6,6	1.09	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	-	0/17/38/38	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	-	0/17/38/38	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	-	0/17/38/38	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	-	0/17/38/38	0/3/3/3
5	AGS	E	1	3,4	-	0/17/38/38	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	-	0/17/38/38	0/3/3/3
2	SO4	F	4004	-	-	0/0/0/0	0/0/0/0
5	AGS	G	1	3,4	-	0/17/38/38	0/3/3/3
2	SO4	G	4002	-	-	0/0/0/0	0/0/0/0
5	AGS	H	1	3,4	-	0/17/38/38	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	-	0/17/38/38	0/3/3/3
5	AGS	J	1	3,4	-	0/17/38/38	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	-	0/17/38/38	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	-	0/17/38/38	0/3/3/3
2	SO4	L	4003	-	-	0/0/0/0	0/0/0/0
5	AGS	M	1	3,4	-	0/17/38/38	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	-	0/17/38/38	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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-22.32	1.48	1.90
5	E	1	AGS	PG-S1G	-22.23	1.48	1.90
5	D	551	AGS	PG-S1G	-22.12	1.48	1.90
5	N	1	AGS	PG-S1G	-21.78	1.49	1.90
5	I	1	AGS	PG-S1G	-21.78	1.49	1.90
5	H	1	AGS	PG-S1G	-21.67	1.49	1.90
5	C	1	AGS	PG-S1G	-21.65	1.49	1.90
5	J	1	AGS	PG-S1G	-21.64	1.49	1.90
5	K	1	AGS	PG-S1G	-21.62	1.49	1.90
5	M	1	AGS	PG-S1G	-21.58	1.49	1.90
5	F	1	AGS	PG-S1G	-21.48	1.49	1.90
5	L	1	AGS	PG-S1G	-21.47	1.49	1.90
5	B	1	AGS	PG-S1G	-21.29	1.50	1.90
5	A	1	AGS	PG-S1G	-21.16	1.50	1.90
5	F	1	AGS	PG-O3G	-2.13	1.47	1.55
5	D	551	AGS	C2'-C1'	-2.11	1.50	1.53
5	D	551	AGS	PG-O3G	-2.02	1.48	1.55
5	J	1	AGS	C2-N3	2.04	1.35	1.32
5	J	1	AGS	O4'-C1'	2.04	1.44	1.41
5	D	551	AGS	C2-N3	2.09	1.35	1.32
5	F	1	AGS	C2-N3	2.16	1.35	1.32
2	E	4005	SO4	O1-S	2.84	1.61	1.45
2	F	4004	SO4	O1-S	2.89	1.61	1.45
2	A	4007	SO4	O1-S	2.96	1.61	1.45
2	K	4022	SO4	O1-S	3.00	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4003	SO4	O1-S	3.00	1.61	1.45
2	G	4002	SO4	O1-S	3.02	1.62	1.45
2	A	4001	SO4	O1-S	3.02	1.62	1.45
2	A	4008	SO4	O1-S	3.03	1.62	1.45
2	N	4016	SO4	O1-S	3.03	1.62	1.45
2	B	4009	SO4	O1-S	3.03	1.62	1.45
5	K	1	AGS	O4'-C1'	3.03	1.45	1.41
2	H	4017	SO4	O1-S	3.04	1.62	1.45
2	E	4006	SO4	O1-S	3.04	1.62	1.45
2	J	4020	SO4	O1-S	3.04	1.62	1.45
2	J	4019	SO4	O1-S	3.04	1.62	1.45
2	H	4018	SO4	O1-S	3.05	1.62	1.45
2	C	4011	SO4	O1-S	3.05	1.62	1.45
2	N	4015	SO4	O1-S	3.05	1.62	1.45
2	M	4014	SO4	O1-S	3.06	1.62	1.45
2	B	4010	SO4	O1-S	3.07	1.62	1.45
2	C	4012	SO4	O1-S	3.08	1.62	1.45
2	K	4021	SO4	O1-S	3.09	1.62	1.45
2	M	4013	SO4	O1-S	3.15	1.62	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	AGS	PB-O3B-PG	-2.16	125.38	132.35
5	N	1	AGS	PB-O3B-PG	-2.08	125.63	132.35
5	K	1	AGS	PB-O3B-PG	-2.04	125.76	132.35
5	A	1	AGS	N3-C2-N1	-2.02	127.10	128.86
5	M	1	AGS	PB-O3B-PG	-2.01	125.84	132.35
5	G	1	AGS	PB-O3B-PG	-2.01	125.86	132.35
5	E	1	AGS	C5-C6-N6	2.01	124.57	120.47
5	B	1	AGS	C5-C6-N6	2.02	124.59	120.47
5	K	1	AGS	C5-C6-N6	2.04	124.63	120.47
5	C	1	AGS	C5-C6-N6	2.06	124.68	120.47
5	L	1	AGS	C5-C6-N6	2.07	124.69	120.47
5	A	1	AGS	C5-C6-N6	2.14	124.83	120.47
5	G	1	AGS	C5-C6-N6	2.22	125.00	120.47
5	M	1	AGS	C5-C6-N6	2.25	125.06	120.47
5	H	1	AGS	C5-C6-N6	2.26	125.08	120.47

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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%)	0.72	69 (13%) 4 4	28, 64, 121, 132	0
1	B	525/547 (95%)	1.33	125 (23%) 1 1	24, 59, 149, 159	0
1	C	525/547 (95%)	1.15	116 (22%) 1 1	29, 71, 141, 152	0
1	D	525/547 (95%)	0.47	31 (5%) 23 23	25, 48, 99, 115	0
1	E	525/547 (95%)	0.99	98 (18%) 1 1	23, 55, 134, 145	0
1	F	525/547 (95%)	1.27	116 (22%) 1 1	27, 66, 150, 159	0
1	G	525/547 (95%)	0.58	43 (8%) 12 12	26, 50, 113, 126	0
1	H	525/547 (95%)	0.64	61 (11%) 5 5	26, 56, 118, 130	0
1	I	525/547 (95%)	0.96	81 (15%) 2 2	31, 69, 132, 143	0
1	J	525/547 (95%)	1.02	89 (16%) 2 2	31, 73, 138, 146	0
1	K	525/547 (95%)	1.43	141 (26%) 1 1	31, 78, 151, 159	0
1	L	525/547 (95%)	0.89	91 (17%) 2 2	29, 66, 136, 149	0
1	M	525/547 (95%)	1.35	136 (25%) 1 1	30, 77, 152, 160	0
1	N	525/547 (95%)	0.71	63 (12%) 5 5	28, 65, 118, 129	0
All	All	7350/7658 (95%)	0.96	1260 (17%) 2 2	23, 60, 140, 160	0

All (1260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ILE	13.5
1	F	309	LEU	12.8
1	K	270	ILE	12.2
1	K	271	VAL	12.1
1	K	305	ILE	11.8
1	B	349	ILE	11.6
1	M	270	ILE	11.4
1	K	349	ILE	11.3

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Mol	Chain	Res	Type	RSRZ
1	F	240	VAL	10.8
1	J	356	ALA	10.6
1	F	233	MET	10.6
1	B	233	MET	10.5
1	E	353	ILE	10.5
1	E	356	ALA	10.4
1	J	271	VAL	10.2
1	F	353	ILE	10.2
1	B	356	ALA	10.1
1	M	353	ILE	10.1
1	I	270	ILE	10.1
1	J	270	ILE	10.0
1	C	356	ALA	10.0
1	K	309	LEU	9.9
1	L	266	THR	9.9
1	M	259	LEU	9.8
1	F	314	LEU	9.7
1	M	233	MET	9.6
1	B	230	ILE	9.5
1	B	353	ILE	9.5
1	K	259	LEU	9.4
1	E	309	LEU	9.4
1	K	260	ALA	9.4
1	N	349	ILE	9.4
1	M	237	LEU	9.3
1	E	271	VAL	9.3
1	F	259	LEU	9.2
1	C	270	ILE	9.2
1	J	269	GLY	9.1
1	M	221	LEU	9.1
1	K	236	VAL	9.1
1	K	237	LEU	8.9
1	K	233	MET	8.8
1	M	271	VAL	8.8
1	C	353	ILE	8.8
1	F	349	ILE	8.7
1	J	349	ILE	8.6
1	B	264	VAL	8.5
1	M	223	ALA	8.5
1	M	314	LEU	8.3
1	D	271	VAL	8.3
1	M	240	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
1	K	231	ARG	8.1
1	K	360	TYR	8.1
1	F	270	ILE	8.1
1	K	267	MET	8.1
1	J	268	ARG	8.0
1	I	305	ILE	8.0
1	B	301	ILE	7.9
1	M	309	LEU	7.9
1	J	357	THR	7.9
1	M	267	MET	7.9
1	I	271	VAL	7.8
1	B	227	ILE	7.8
1	B	258	ALA	7.8
1	B	365	LEU	7.8
1	J	233	MET	7.8
1	B	281	PHE	7.7
1	A	270	ILE	7.7
1	F	360	TYR	7.7
1	M	272	LYS	7.7
1	K	356	ALA	7.7
1	K	264	VAL	7.6
1	M	357	THR	7.6
1	M	268	ARG	7.6
1	M	349	ILE	7.5
1	B	268	ARG	7.5
1	L	271	VAL	7.4
1	K	265	ASN	7.3
1	H	309	LEU	7.3
1	K	203	TYR	7.3
1	K	268	ARG	7.3
1	M	266	THR	7.3
1	J	309	LEU	7.2
1	M	356	ALA	7.2
1	I	264	VAL	7.2
1	A	356	ALA	7.2
1	L	270	ILE	7.1
1	K	353	ILE	7.1
1	C	271	VAL	7.0
1	A	353	ILE	7.0
1	I	265	ASN	6.9
1	I	356	ALA	6.9
1	M	239	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	E	230	ILE	6.8
1	K	340	ALA	6.8
1	B	259	LEU	6.8
1	M	251	ALA	6.7
1	F	227	ILE	6.7
1	E	234	LEU	6.7
1	E	349	ILE	6.7
1	N	263	VAL	6.7
1	E	233	MET	6.7
1	I	268	ARG	6.7
1	L	231	ARG	6.7
1	M	264	VAL	6.7
1	F	219	PHE	6.7
1	M	244	GLY	6.7
1	J	44	PHE	6.6
1	C	268	ARG	6.6
1	L	264	VAL	6.6
1	J	353	ILE	6.6
1	M	273	VAL	6.6
1	F	230	ILE	6.6
1	M	358	SER	6.6
1	F	268	ARG	6.6
1	F	357	THR	6.6
1	J	317	LEU	6.5
1	F	203	TYR	6.5
1	F	272	LYS	6.5
1	F	267	MET	6.5
1	F	255	GLU	6.5
1	E	223	ALA	6.5
1	B	271	VAL	6.5
1	J	526	LYS	6.4
1	B	257	GLU	6.4
1	B	229	ASN	6.4
1	K	240	VAL	6.4
1	K	227	ILE	6.4
1	B	355	GLU	6.4
1	I	349	ILE	6.4
1	N	270	ILE	6.4
1	B	265	ASN	6.3
1	M	204	PHE	6.3
1	B	309	LEU	6.3
1	E	268	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	J	237	LEU	6.3
1	J	264	VAL	6.3
1	E	266	THR	6.3
1	I	230	ILE	6.3
1	G	230	ILE	6.2
1	M	263	VAL	6.2
1	B	307	MET	6.2
1	E	305	ILE	6.2
1	K	204	PHE	6.2
1	K	232	GLU	6.2
1	C	342	ILE	6.1
1	J	266	THR	6.1
1	H	233	MET	6.1
1	L	305	ILE	6.1
1	L	383	ALA	6.1
1	E	270	ILE	6.1
1	F	222	LEU	6.1
1	K	230	ILE	6.1
1	B	357	THR	6.1
1	I	353	ILE	6.0
1	M	305	ILE	6.0
1	F	342	ILE	6.0
1	N	230	ILE	5.9
1	C	263	VAL	5.9
1	B	286	LYS	5.9
1	F	305	ILE	5.9
1	B	270	ILE	5.9
1	N	264	VAL	5.9
1	F	237	LEU	5.9
1	F	317	LEU	5.9
1	K	256	GLY	5.8
1	E	300	VAL	5.8
1	M	336	VAL	5.8
1	F	231	ARG	5.8
1	C	249	ILE	5.8
1	F	271	VAL	5.8
1	L	269	GLY	5.8
1	J	305	ILE	5.8
1	C	266	THR	5.8
1	E	357	THR	5.8
1	F	234	LEU	5.8
1	L	230	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	K	223	ALA	5.7
1	I	266	THR	5.7
1	K	219	PHE	5.7
1	B	240	VAL	5.7
1	I	352	GLN	5.7
1	B	269	GLY	5.6
1	B	203	TYR	5.6
1	G	383	ALA	5.6
1	L	309	LEU	5.6
1	C	369	VAL	5.6
1	M	265	ASN	5.6
1	K	306	GLY	5.6
1	L	268	ARG	5.6
1	K	228	SER	5.5
1	C	237	LEU	5.5
1	I	526	LYS	5.5
1	L	234	LEU	5.5
1	H	270	ILE	5.5
1	E	312	ALA	5.5
1	J	351	GLN	5.5
1	K	269	GLY	5.5
1	B	342	ILE	5.4
1	G	44	PHE	5.4
1	F	389	MET	5.4
1	C	203	TYR	5.4
1	J	358	SER	5.4
1	C	259	LEU	5.4
1	M	249	ILE	5.4
1	E	272	LYS	5.4
1	F	245	LYS	5.4
1	K	188	ASP	5.4
1	I	360	TYR	5.4
1	B	251	ALA	5.4
1	J	263	VAL	5.4
1	B	236	VAL	5.3
1	I	203	TYR	5.3
1	J	229	ASN	5.3
1	M	365	LEU	5.3
1	I	272	LYS	5.3
1	B	305	ILE	5.3
1	K	241	ALA	5.3
1	M	203	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	231	ARG	5.3
1	M	335	GLY	5.3
1	M	342	ILE	5.3
1	E	351	GLN	5.3
1	F	44	PHE	5.3
1	C	261	THR	5.3
1	K	234	LEU	5.3
1	I	234	LEU	5.2
1	C	365	LEU	5.2
1	H	234	LEU	5.2
1	E	203	TYR	5.2
1	C	256	GLY	5.2
1	G	271	VAL	5.2
1	F	355	GLU	5.2
1	I	355	GLU	5.2
1	B	237	LEU	5.2
1	C	357	THR	5.2
1	L	259	LEU	5.2
1	B	351	GLN	5.1
1	K	273	VAL	5.1
1	K	383	ALA	5.1
1	J	219	PHE	5.1
1	K	272	LYS	5.1
1	C	44	PHE	5.1
1	K	281	PHE	5.1
1	F	273	VAL	5.1
1	C	295	LEU	5.1
1	H	526	LYS	5.1
1	M	219	PHE	5.1
1	H	243	ALA	5.1
1	A	263	VAL	5.1
1	B	273	VAL	5.1
1	I	231	ARG	5.1
1	J	231	ARG	5.1
1	K	44	PHE	5.1
1	B	234	LEU	5.1
1	F	264	VAL	5.0
1	I	267	MET	5.0
1	M	317	LEU	5.0
1	F	263	VAL	5.0
1	M	186	GLU	5.0
1	B	306	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	230	ILE	5.0
1	F	241	ALA	5.0
1	L	258	ALA	5.0
1	C	244	GLY	5.0
1	C	304	GLU	5.0
1	C	264	VAL	5.0
1	M	260	ALA	5.0
1	A	44	PHE	5.0
1	L	227	ILE	5.0
1	B	262	LEU	4.9
1	C	372	LEU	4.9
1	A	349	ILE	4.9
1	K	335	GLY	4.9
1	K	275	ALA	4.9
1	H	229	ASN	4.9
1	J	265	ASN	4.9
1	G	270	ILE	4.9
1	B	44	PHE	4.9
1	B	526	LYS	4.9
1	M	195	PHE	4.9
1	D	270	ILE	4.9
1	E	301	ILE	4.9
1	H	353	ILE	4.9
1	C	360	TYR	4.9
1	H	268	ARG	4.9
1	H	356	ALA	4.8
1	D	230	ILE	4.8
1	F	365	LEU	4.8
1	I	309	LEU	4.8
1	J	281	PHE	4.8
1	M	340	ALA	4.8
1	D	44	PHE	4.8
1	K	263	VAL	4.8
1	B	266	THR	4.8
1	C	333	ILE	4.8
1	L	317	LEU	4.8
1	I	243	ALA	4.8
1	L	233	MET	4.8
1	C	362	ARG	4.8
1	G	267	MET	4.7
1	E	355	GLU	4.7
1	I	363	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	256	GLY	4.7
1	M	250	ILE	4.7
1	I	233	MET	4.7
1	J	204	PHE	4.7
1	G	265	ASN	4.7
1	C	233	MET	4.7
1	M	355	GLU	4.7
1	K	358	SER	4.7
1	B	317	LEU	4.7
1	F	243	ALA	4.7
1	C	274	ALA	4.6
1	K	160	LYS	4.6
1	F	269	GLY	4.6
1	H	357	THR	4.6
1	F	336	VAL	4.6
1	M	351	GLN	4.6
1	K	247	LEU	4.6
1	L	356	ALA	4.6
1	F	306	GLY	4.6
1	L	203	TYR	4.6
1	F	315	GLU	4.6
1	B	250	ILE	4.6
1	G	259	LEU	4.6
1	E	358	SER	4.6
1	K	302	SER	4.6
1	B	243	ALA	4.6
1	A	182	GLY	4.5
1	B	372	LEU	4.5
1	M	222	LEU	4.5
1	H	44	PHE	4.5
1	K	357	THR	4.5
1	A	361	ASP	4.5
1	B	295	LEU	4.5
1	E	247	LEU	4.5
1	A	357	THR	4.5
1	E	44	PHE	4.5
1	A	268	ARG	4.5
1	F	258	ALA	4.5
1	F	356	ALA	4.5
1	M	218	PRO	4.5
1	E	231	ARG	4.5
1	E	264	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	358	SER	4.5
1	I	351	GLN	4.5
1	I	357	THR	4.5
1	C	346	VAL	4.5
1	E	263	VAL	4.5
1	L	255	GLU	4.5
1	E	273	VAL	4.4
1	D	526	LYS	4.4
1	F	242	LYS	4.4
1	J	262	LEU	4.4
1	K	362	ARG	4.4
1	B	223	ALA	4.4
1	M	238	GLU	4.4
1	K	283	ASP	4.4
1	E	384	ALA	4.4
1	G	258	ALA	4.4
1	C	350	ARG	4.4
1	B	383	ALA	4.4
1	M	230	ILE	4.4
1	G	306	GLY	4.4
1	L	267	MET	4.4
1	B	358	SER	4.4
1	N	281	PHE	4.4
1	B	363	GLU	4.4
1	H	383	ALA	4.4
1	B	221	LEU	4.4
1	C	265	ASN	4.4
1	E	265	ASN	4.4
1	D	305	ILE	4.4
1	B	300	VAL	4.4
1	K	334	ASP	4.4
1	A	257	GLU	4.3
1	A	271	VAL	4.3
1	C	267	MET	4.3
1	L	244	GLY	4.3
1	C	355	GLU	4.3
1	F	244	GLY	4.3
1	J	260	ALA	4.3
1	C	284	ARG	4.3
1	M	231	ARG	4.3
1	C	292	ILE	4.3
1	F	236	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	365	LEU	4.3
1	B	261	THR	4.3
1	B	209	GLU	4.3
1	E	237	LEU	4.2
1	F	266	THR	4.2
1	B	260	ALA	4.2
1	B	180	GLY	4.2
1	K	351	GLN	4.2
1	B	304	GLU	4.2
1	F	249	ILE	4.2
1	G	264	VAL	4.2
1	M	526	LYS	4.2
1	H	305	ILE	4.2
1	L	526	LYS	4.2
1	J	362	ARG	4.2
1	E	383	ALA	4.2
1	J	257	GLU	4.2
1	F	224	ASP	4.2
1	M	295	LEU	4.2
1	F	260	ALA	4.2
1	B	302	SER	4.2
1	C	340	ALA	4.2
1	J	383	ALA	4.2
1	F	346	VAL	4.2
1	K	346	VAL	4.2
1	F	351	GLN	4.2
1	L	314	LEU	4.1
1	M	262	LEU	4.1
1	B	354	GLU	4.1
1	C	351	GLN	4.1
1	B	225	LYS	4.1
1	L	229	ASN	4.1
1	M	44	PHE	4.1
1	E	354	GLU	4.1
1	C	273	VAL	4.1
1	E	346	VAL	4.1
1	J	360	TYR	4.1
1	M	258	ALA	4.1
1	F	225	LYS	4.1
1	F	358	SER	4.1
1	E	240	VAL	4.1
1	B	311	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	228	SER	4.1
1	K	299	THR	4.1
1	C	231	ARG	4.0
1	D	268	ARG	4.0
1	F	261	THR	4.0
1	F	369	VAL	4.0
1	K	331	THR	4.0
1	H	265	ASN	4.0
1	I	184	GLN	4.0
1	E	360	TYR	4.0
1	J	203	TYR	4.0
1	I	384	ALA	4.0
1	K	332	ILE	4.0
1	A	187	LEU	4.0
1	I	44	PHE	4.0
1	D	264	VAL	4.0
1	H	349	ILE	4.0
1	J	333	ILE	4.0
1	G	268	ARG	4.0
1	D	266	THR	4.0
1	K	355	GLU	4.0
1	M	161	LEU	4.0
1	F	256	GLY	4.0
1	C	526	LYS	3.9
1	C	161	LEU	3.9
1	F	221	LEU	3.9
1	H	355	GLU	3.9
1	K	350	ARG	3.9
1	B	244	GLY	3.9
1	L	311	LYS	3.9
1	B	289	LEU	3.9
1	N	356	ALA	3.9
1	I	358	SER	3.9
1	B	293	ALA	3.9
1	K	307	MET	3.9
1	M	307	MET	3.9
1	J	367	GLU	3.9
1	B	224	ASP	3.9
1	J	355	GLU	3.9
1	E	295	LEU	3.8
1	M	269	GLY	3.8
1	B	219	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	258	ALA	3.8
1	I	269	GLY	3.8
1	M	180	GLY	3.8
1	C	219	PHE	3.8
1	L	44	PHE	3.8
1	F	265	ASN	3.8
1	J	267	MET	3.8
1	M	347	ALA	3.8
1	C	286	LYS	3.8
1	E	242	LYS	3.8
1	C	181	THR	3.8
1	J	365	LEU	3.8
1	G	229	ASN	3.8
1	K	301	ILE	3.8
1	M	160	LYS	3.8
1	J	361	ASP	3.8
1	E	255	GLU	3.8
1	E	257	GLU	3.8
1	B	282	GLY	3.8
1	G	182	GLY	3.7
1	L	224	ASP	3.7
1	G	233	MET	3.7
1	J	342	ILE	3.7
1	K	181	THR	3.7
1	K	372	LEU	3.7
1	F	381	VAL	3.7
1	K	274	ALA	3.7
1	M	350	ARG	3.7
1	G	266	THR	3.7
1	G	325	ILE	3.7
1	C	309	LEU	3.7
1	K	369	VAL	3.7
1	I	211	GLY	3.7
1	C	347	ALA	3.7
1	H	346	VAL	3.7
1	E	345	ARG	3.7
1	F	181	THR	3.7
1	F	214	GLU	3.7
1	J	381	VAL	3.7
1	K	266	THR	3.7
1	M	333	ILE	3.6
1	K	250	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	256	GLY	3.6
1	A	183	LEU	3.6
1	F	248	LEU	3.6
1	H	264	VAL	3.6
1	A	261	THR	3.6
1	M	261	THR	3.6
1	B	191	GLU	3.6
1	K	304	GLU	3.6
1	B	241	ALA	3.6
1	L	239	ALA	3.6
1	M	301	ILE	3.6
1	B	314	LEU	3.6
1	F	396	VAL	3.6
1	K	311	LYS	3.6
1	J	319	GLN	3.6
1	L	186	GLU	3.6
1	I	237	LEU	3.6
1	J	272	LYS	3.6
1	A	265	ASN	3.6
1	I	204	PHE	3.6
1	L	353	ILE	3.6
1	B	238	GLU	3.6
1	J	280	GLY	3.6
1	L	219	PHE	3.5
1	N	258	ALA	3.5
1	E	220	ILE	3.5
1	F	232	GLU	3.5
1	G	262	LEU	3.5
1	K	222	LEU	3.5
1	K	276	VAL	3.5
1	M	254	VAL	3.5
1	H	266	THR	3.5
1	F	178	GLU	3.5
1	J	273	VAL	3.5
1	F	340	ALA	3.5
1	C	229	ASN	3.5
1	C	204	PHE	3.5
1	C	281	PHE	3.5
1	I	369	VAL	3.5
1	L	185	ASP	3.5
1	M	236	VAL	3.5
1	J	243	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	215	LEU	3.5
1	M	188	ASP	3.5
1	A	203	TYR	3.5
1	B	275	ALA	3.5
1	L	228	SER	3.5
1	A	237	LEU	3.5
1	A	231	ARG	3.5
1	H	242	LYS	3.4
1	F	251	ALA	3.4
1	H	259	LEU	3.4
1	L	222	LEU	3.4
1	K	352	GLN	3.4
1	F	215	LEU	3.4
1	F	372	LEU	3.4
1	B	360	TYR	3.4
1	K	345	ARG	3.4
1	M	286	LYS	3.4
1	M	384	ALA	3.4
1	L	247	LEU	3.4
1	I	240	VAL	3.4
1	K	213	VAL	3.4
1	N	44	PHE	3.4
1	L	275	ALA	3.4
1	K	221	LEU	3.4
1	N	266	THR	3.4
1	N	526	LYS	3.4
1	F	180	GLY	3.4
1	C	212	ALA	3.4
1	E	284	ARG	3.4
1	I	258	ALA	3.4
1	K	243	ALA	3.4
1	M	383	ALA	3.4
1	L	349	ILE	3.4
1	M	168	LYS	3.4
1	J	261	THR	3.4
1	B	263	VAL	3.4
1	K	191	GLU	3.4
1	F	337	GLY	3.4
1	K	310	GLU	3.3
1	N	363	GLU	3.3
1	N	365	LEU	3.3
1	B	298	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	263	VAL	3.3
1	M	346	VAL	3.3
1	E	267	MET	3.3
1	L	307	MET	3.3
1	M	389	MET	3.3
1	K	152	ALA	3.3
1	A	284	ARG	3.3
1	B	249	ILE	3.3
1	C	332	ILE	3.3
1	G	181	THR	3.3
1	M	229	ASN	3.3
1	C	358	SER	3.3
1	A	276	VAL	3.3
1	K	202	PRO	3.3
1	M	235	PRO	3.3
1	H	360	TYR	3.3
1	A	266	THR	3.3
1	C	186	GLU	3.3
1	B	222	LEU	3.3
1	D	325	ILE	3.3
1	M	217	SER	3.3
1	E	215	LEU	3.3
1	A	381	VAL	3.3
1	C	300	VAL	3.3
1	F	300	VAL	3.3
1	E	229	ASN	3.3
1	L	310	GLU	3.3
1	M	354	GLU	3.3
1	C	240	VAL	3.3
1	C	223	ALA	3.3
1	C	306	GLY	3.3
1	A	204	PHE	3.3
1	C	322	ARG	3.3
1	E	219	PHE	3.3
1	M	322	ARG	3.3
1	N	231	ARG	3.3
1	K	342	ILE	3.3
1	M	300	VAL	3.3
1	H	361	ASP	3.2
1	K	224	ASP	3.2
1	I	245	LYS	3.2
1	M	343	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	358	SER	3.2
1	D	281	PHE	3.2
1	A	365	LEU	3.2
1	B	525	PRO	3.2
1	A	188	ASP	3.2
1	J	242	LYS	3.2
1	C	319	GLN	3.2
1	H	263	VAL	3.2
1	K	376	VAL	3.2
1	F	361	ASP	3.2
1	M	360	TYR	3.2
1	J	354	GLU	3.2
1	J	363	GLU	3.2
1	I	259	LEU	3.2
1	K	297	GLY	3.2
1	K	214	GLU	3.2
1	E	342	ILE	3.2
1	J	248	LEU	3.2
1	K	242	LYS	3.2
1	K	245	LYS	3.2
1	E	304	GLU	3.2
1	I	340	ALA	3.2
1	K	255	GLU	3.2
1	M	320	ALA	3.2
1	I	215	LEU	3.2
1	B	346	VAL	3.2
1	F	322	ARG	3.2
1	C	242	LYS	3.2
1	A	355	GLU	3.2
1	A	363	GLU	3.2
1	A	260	ALA	3.2
1	L	324	VAL	3.2
1	M	181	THR	3.2
1	A	304	GLU	3.1
1	F	186	GLU	3.1
1	K	139	SER	3.1
1	D	231	ARG	3.1
1	L	272	LYS	3.1
1	F	354	GLU	3.1
1	D	236	VAL	3.1
1	J	240	VAL	3.1
1	D	383	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	187	LEU	3.1
1	H	351	GLN	3.1
1	G	305	ILE	3.1
1	H	230	ILE	3.1
1	M	224	ASP	3.1
1	A	264	VAL	3.1
1	K	300	VAL	3.1
1	L	206	ASN	3.1
1	I	383	ALA	3.1
1	E	184	GLN	3.1
1	L	382	GLY	3.1
1	N	203	TYR	3.1
1	D	323	VAL	3.1
1	I	336	VAL	3.1
1	L	381	VAL	3.1
1	C	272	LYS	3.1
1	B	361	ASP	3.1
1	C	363	GLU	3.1
1	G	257	GLU	3.1
1	N	362	ARG	3.1
1	K	288	MET	3.1
1	C	180	GLY	3.1
1	F	384	ALA	3.1
1	N	357	THR	3.1
1	B	352	GLN	3.1
1	C	317	LEU	3.1
1	F	161	LEU	3.1
1	F	352	GLN	3.1
1	B	284	ARG	3.1
1	F	332	ILE	3.1
1	A	384	ALA	3.0
1	B	256	GLY	3.0
1	C	260	ALA	3.0
1	E	382	GLY	3.0
1	A	181	THR	3.0
1	B	215	LEU	3.0
1	M	323	VAL	3.0
1	N	325	ILE	3.0
1	C	341	ALA	3.0
1	K	308	GLU	3.0
1	K	320	ALA	3.0
1	N	351	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	302	SER	3.0
1	G	231	ARG	3.0
1	B	267	MET	3.0
1	G	311	LYS	3.0
1	M	247	LEU	3.0
1	E	292	ILE	3.0
1	I	302	SER	3.0
1	E	526	LYS	3.0
1	A	388	GLU	3.0
1	K	257	GLU	3.0
1	L	265	ASN	3.0
1	F	347	ALA	3.0
1	K	361	ASP	3.0
1	M	304	GLU	3.0
1	F	155	ASP	3.0
1	J	234	LEU	3.0
1	N	257	GLU	3.0
1	M	369	VAL	3.0
1	A	382	GLY	3.0
1	F	362	ARG	3.0
1	F	295	LEU	3.0
1	A	273	VAL	2.9
1	E	236	VAL	2.9
1	A	281	PHE	2.9
1	F	204	PHE	2.9
1	H	286	LYS	2.9
1	N	354	GLU	2.9
1	A	245	LYS	2.9
1	C	222	LEU	2.9
1	C	247	LEU	2.9
1	N	284	ARG	2.9
1	C	315	GLU	2.9
1	H	304	GLU	2.9
1	B	254	VAL	2.9
1	K	381	VAL	2.9
1	L	249	ILE	2.9
1	F	319	GLN	2.9
1	I	310	GLU	2.9
1	K	380	LYS	2.9
1	D	269	GLY	2.9
1	B	313	THR	2.9
1	D	267	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	325	ILE	2.9
1	D	229	ASN	2.9
1	H	363	GLU	2.9
1	K	312	ALA	2.9
1	K	341	ALA	2.9
1	M	243	ALA	2.9
1	B	248	LEU	2.9
1	L	161	LEU	2.9
1	H	300	VAL	2.9
1	C	305	ILE	2.9
1	B	188	ASP	2.9
1	E	258	ALA	2.9
1	E	274	ALA	2.9
1	I	257	GLU	2.9
1	M	216	GLU	2.9
1	E	224	ASP	2.9
1	C	301	ILE	2.9
1	B	255	GLU	2.9
1	B	390	LYS	2.9
1	M	308	GLU	2.9
1	G	269	GLY	2.9
1	H	269	GLY	2.9
1	G	243	ALA	2.9
1	H	314	LEU	2.9
1	I	314	LEU	2.9
1	M	363	GLU	2.9
1	C	220	ILE	2.8
1	L	325	ILE	2.8
1	M	299	THR	2.8
1	G	234	LEU	2.8
1	K	323	VAL	2.8
1	L	240	VAL	2.8
1	N	346	VAL	2.8
1	B	332	ILE	2.8
1	J	250	ILE	2.8
1	F	238	GLU	2.8
1	C	352	GLN	2.8
1	J	184	GLN	2.8
1	C	221	LEU	2.8
1	B	280	GLY	2.8
1	M	182	GLY	2.8
1	C	172	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	226	LYS	2.8
1	L	308	GLU	2.8
1	H	271	VAL	2.8
1	F	385	THR	2.8
1	N	304	GLU	2.8
1	N	360	TYR	2.8
1	K	526	LYS	2.8
1	H	365	LEU	2.8
1	N	369	VAL	2.8
1	A	362	ARG	2.8
1	E	251	ALA	2.8
1	F	223	ALA	2.8
1	K	205	ILE	2.8
1	M	362	ARG	2.8
1	B	252	GLU	2.8
1	E	307	MET	2.8
1	K	317	LEU	2.8
1	B	228	SER	2.8
1	G	384	ALA	2.8
1	N	265	ASN	2.8
1	K	164	GLU	2.8
1	I	365	LEU	2.8
1	E	188	ASP	2.7
1	I	361	ASP	2.7
1	A	184	GLN	2.7
1	E	250	ILE	2.7
1	D	203	TYR	2.7
1	N	283	ASP	2.7
1	B	274	ALA	2.7
1	I	229	ASN	2.7
1	I	260	ALA	2.7
1	C	336	VAL	2.7
1	L	336	VAL	2.7
1	A	301	ILE	2.7
1	C	250	ILE	2.7
1	M	220	ILE	2.7
1	B	348	GLN	2.7
1	L	184	GLN	2.7
1	B	183	LEU	2.7
1	K	220	ILE	2.7
1	C	334	ASP	2.7
1	J	303	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	304	GLU	2.7
1	I	284	ARG	2.7
1	A	295	LEU	2.7
1	H	237	LEU	2.7
1	M	248	LEU	2.7
1	N	309	LEU	2.7
1	A	209	GLU	2.7
1	A	346	VAL	2.7
1	B	336	VAL	2.7
1	E	232	GLU	2.7
1	M	279	PRO	2.7
1	H	315	GLU	2.7
1	G	314	LEU	2.7
1	K	295	LEU	2.7
1	M	193	MET	2.7
1	M	319	GLN	2.7
1	L	273	VAL	2.7
1	K	325	ILE	2.7
1	L	333	ILE	2.7
1	N	353	ILE	2.7
1	C	367	GLU	2.7
1	B	272	LYS	2.7
1	B	350	ARG	2.7
1	C	299	THR	2.7
1	L	284	ARG	2.7
1	L	313	THR	2.7
1	D	262	LEU	2.7
1	I	209	GLU	2.6
1	I	304	GLU	2.6
1	A	256	GLY	2.6
1	C	269	GLY	2.6
1	N	382	GLY	2.6
1	A	250	ILE	2.6
1	B	205	ILE	2.6
1	J	301	ILE	2.6
1	N	241	ALA	2.6
1	I	389	MET	2.6
1	M	234	LEU	2.6
1	K	253	ASP	2.6
1	A	305	ILE	2.6
1	E	249	ILE	2.6
1	I	250	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	315	GLU	2.6
1	N	311	LYS	2.6
1	C	248	LEU	2.6
1	F	343	GLN	2.6
1	F	250	ILE	2.6
1	F	350	ARG	2.6
1	B	186	GLU	2.6
1	E	339	GLU	2.6
1	L	315	GLU	2.6
1	G	309	LEU	2.6
1	M	183	LEU	2.6
1	L	462	PRO	2.6
1	J	177	VAL	2.6
1	L	232	GLU	2.6
1	I	256	GLY	2.6
1	H	317	LEU	2.6
1	A	300	VAL	2.6
1	E	381	VAL	2.6
1	C	209	GLU	2.6
1	D	257	GLU	2.6
1	E	361	ASP	2.6
1	I	154	SER	2.6
1	I	286	LYS	2.6
1	M	205	ILE	2.6
1	N	267	MET	2.6
1	H	297	GLY	2.6
1	H	335	GLY	2.6
1	F	281	PHE	2.6
1	A	259	LEU	2.6
1	B	322	ARG	2.5
1	D	234	LEU	2.6
1	M	215	LEU	2.6
1	M	376	VAL	2.5
1	N	254	VAL	2.5
1	B	335	GLY	2.5
1	H	261	THR	2.5
1	A	242	LYS	2.5
1	C	215	LEU	2.5
1	B	381	VAL	2.5
1	C	354	GLU	2.5
1	E	318	GLY	2.5
1	J	232	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	256	GLY	2.5
1	G	261	THR	2.5
1	J	288	MET	2.5
1	E	352	GLN	2.5
1	M	184	GLN	2.5
1	I	301	ILE	2.5
1	E	317	LEU	2.5
1	F	339	GLU	2.5
1	L	200	LEU	2.5
1	C	85	ALA	2.5
1	D	382	GLY	2.5
1	K	180	GLY	2.5
1	J	387	VAL	2.5
1	C	391	GLU	2.5
1	E	214	GLU	2.5
1	L	262	LEU	2.5
1	B	239	ALA	2.5
1	J	304	GLU	2.5
1	C	160	LYS	2.5
1	H	245	LYS	2.5
1	C	217	SER	2.5
1	F	359	ASP	2.5
1	M	298	GLY	2.5
1	I	183	LEU	2.5
1	I	372	LEU	2.5
1	J	275	ALA	2.5
1	H	284	ARG	2.5
1	N	268	ARG	2.5
1	J	334	ASP	2.5
1	B	303	GLU	2.5
1	B	367	GLU	2.5
1	C	337	GLY	2.5
1	F	363	GLU	2.5
1	N	305	ILE	2.5
1	K	321	LYS	2.5
1	L	281	PHE	2.5
1	E	261	THR	2.4
1	K	261	THR	2.4
1	M	330	THR	2.4
1	M	361	ASP	2.4
1	F	333	ILE	2.4
1	F	239	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	351	GLN	2.4
1	J	181	THR	2.4
1	A	354	GLU	2.4
1	L	283	ASP	2.4
1	J	228	SER	2.4
1	L	306	GLY	2.4
1	B	308	GLU	2.4
1	K	284	ARG	2.4
1	J	152	ALA	2.4
1	E	299	THR	2.4
1	G	283	ASP	2.4
1	H	313	THR	2.4
1	M	316	ASP	2.4
1	E	365	LEU	2.4
1	G	221	LEU	2.4
1	J	302	SER	2.4
1	K	248	LEU	2.4
1	L	215	LEU	2.4
1	M	200	LEU	2.4
1	G	236	VAL	2.4
1	I	276	VAL	2.4
1	D	184	GLN	2.4
1	F	285	ARG	2.4
1	M	232	GLU	2.4
1	M	311	LYS	2.4
1	J	332	ILE	2.4
1	J	384	ALA	2.4
1	K	175	ILE	2.4
1	N	260	ALA	2.4
1	M	302	SER	2.4
1	C	214	GLU	2.4
1	E	338	GLU	2.4
1	M	159	GLY	2.4
1	N	259	LEU	2.4
1	A	286	LYS	2.4
1	H	236	VAL	2.4
1	M	185	ASP	2.4
1	I	288	MET	2.4
1	K	333	ILE	2.4
1	I	362	ARG	2.4
1	K	326	ASN	2.4
1	M	164	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	384	ALA	2.4
1	B	285	ARG	2.4
1	C	184	GLN	2.4
1	D	284	ARG	2.4
1	H	272	LYS	2.4
1	K	290	GLN	2.4
1	K	364	LYS	2.4
1	G	382	GLY	2.4
1	H	306	GLY	2.4
1	M	329	THR	2.4
1	C	155	ASP	2.4
1	J	215	LEU	2.3
1	K	161	LEU	2.3
1	L	204	PHE	2.3
1	M	310	GLU	2.3
1	C	236	VAL	2.3
1	E	225	LYS	2.3
1	E	286	LYS	2.3
1	M	324	VAL	2.3
1	C	287	ALA	2.3
1	B	344	GLY	2.3
1	F	157	THR	2.3
1	L	256	GLY	2.3
1	I	334	ASP	2.3
1	L	361	ASP	2.3
1	B	310	GLU	2.3
1	L	332	ILE	2.3
1	C	168	LYS	2.3
1	J	245	LYS	2.3
1	J	200	LEU	2.3
1	N	317	LEU	2.3
1	N	77	VAL	2.3
1	I	354	GLU	2.3
1	N	350	ARG	2.3
1	A	360	TYR	2.3
1	M	187	LEU	2.3
1	N	161	LEU	2.3
1	I	300	VAL	2.3
1	M	381	VAL	2.3
1	I	364	LYS	2.3
1	K	239	ALA	2.3
1	A	322	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	292	ILE	2.3
1	H	333	ILE	2.3
1	E	168	LYS	2.3
1	E	289	LEU	2.3
1	N	314	LEU	2.3
1	B	204	PHE	2.3
1	H	273	VAL	2.3
1	I	346	VAL	2.3
1	L	347	ALA	2.3
1	K	184	GLN	2.3
1	M	191	GLU	2.3
1	C	325	ILE	2.3
1	J	150	ILE	2.3
1	K	249	ILE	2.3
1	M	325	ILE	2.3
1	N	358	SER	2.3
1	A	351	GLN	2.3
1	B	247	LEU	2.3
1	G	295	LEU	2.3
1	L	237	LEU	2.3
1	J	274	ALA	2.3
1	L	257	GLU	2.3
1	M	388	GLU	2.3
1	B	369	VAL	2.3
1	G	244	GLY	2.3
1	K	322	ARG	2.3
1	A	262	LEU	2.2
1	C	234	LEU	2.2
1	E	287	ALA	2.2
1	E	341	ALA	2.2
1	F	288	MET	2.2
1	J	221	LEU	2.2
1	K	183	LEU	2.2
1	K	371	LYS	2.2
1	N	240	VAL	2.2
1	C	290	GLN	2.2
1	H	339	GLU	2.2
1	J	345	ARG	2.2
1	C	201	SER	2.2
1	A	311	LYS	2.2
1	A	288	MET	2.2
1	D	233	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	359	ASP	2.2
1	A	200	LEU	2.2
1	M	274	ALA	2.2
1	N	275	ALA	2.2
1	K	367	GLU	2.2
1	C	378	VAL	2.2
1	E	350	ARG	2.2
1	H	231	ARG	2.2
1	N	273	VAL	2.2
1	E	256	GLY	2.2
1	G	228	SER	2.2
1	I	311	LYS	2.2
1	A	359	ASP	2.2
1	N	224	ASP	2.2
1	B	288	MET	2.2
1	B	389	MET	2.2
1	C	258	ALA	2.2
1	E	193	MET	2.2
1	E	288	MET	2.2
1	J	325	ILE	2.2
1	K	386	GLU	2.2
1	N	186	GLU	2.2
1	K	278	ALA	2.2
1	N	383	ALA	2.2
1	D	181	THR	2.2
1	E	222	LEU	2.2
1	K	229	ASN	2.2
1	A	244	GLY	2.2
1	E	334	ASP	2.2
1	E	238	GLU	2.2
1	F	257	GLU	2.2
1	K	366	GLN	2.2
1	F	321	LYS	2.2
1	L	225	LYS	2.2
1	C	275	ALA	2.2
1	L	201	SER	2.2
1	E	363	GLU	2.2
1	N	255	GLU	2.2
1	A	240	VAL	2.2
1	F	213	VAL	2.2
1	G	263	VAL	2.2
1	J	369	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	395	ARG	2.2
1	K	319	GLN	2.2
1	N	242	LYS	2.2
1	I	193	MET	2.2
1	C	216	GLU	2.2
1	F	297	GLY	2.2
1	K	363	GLU	2.2
1	H	332	ILE	2.2
1	C	188	ASP	2.2
1	D	314	LEU	2.2
1	I	317	LEU	2.2
1	A	526	LYS	2.2
1	H	319	GLN	2.2
1	N	184	GLN	2.2
1	J	376	VAL	2.2
1	L	190	VAL	2.2
1	G	326	ASN	2.2
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	B	297	GLY	2.2
1	B	331	THR	2.2
1	M	306	GLY	2.2
1	F	160	LYS	2.2
1	I	228	SER	2.2
1	F	183	LEU	2.1
1	C	303	GLU	2.1
1	L	236	VAL	2.1
1	N	391	GLU	2.1
1	A	207	LYS	2.1
1	D	188	ASP	2.1
1	J	223	ALA	2.1
1	J	244	GLY	2.1
1	B	181	THR	2.1
1	C	348	GLN	2.1
1	E	227	ILE	2.1
1	G	220	ILE	2.1
1	K	292	ILE	2.1
1	L	289	LEU	2.1
1	J	284	ARG	2.1
1	M	281	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	239	ALA	2.1
1	M	294	THR	2.1
1	E	160	LYS	2.1
1	K	168	LYS	2.1
1	L	245	LYS	2.1
1	F	316	ASP	2.1
1	A	350	ARG	2.1
1	E	372	LEU	2.1
1	L	372	LEU	2.1
1	A	236	VAL	2.1
1	C	178	GLU	2.1
1	H	257	GLU	2.1
1	L	213	VAL	2.1
1	L	369	VAL	2.1
1	N	271	VAL	2.1
1	A	267	MET	2.1
1	E	43	SER	2.1
1	N	228	SER	2.1
1	F	313	THR	2.1
1	L	212	ALA	2.1
1	F	364	LYS	2.1
1	N	355	GLU	2.1
1	J	259	LEU	2.1
1	B	324	VAL	2.1
1	I	236	VAL	2.1
1	K	254	VAL	2.1
1	J	206	ASN	2.1
1	M	278	ALA	2.1
1	E	366	GLN	2.1
1	M	338	GLU	2.1
1	C	134	LEU	2.1
1	E	259	LEU	2.1
1	F	247	LEU	2.1
1	H	222	LEU	2.1
1	I	248	LEU	2.1
1	N	134	LEU	2.1
1	D	253	ASP	2.1
1	F	308	GLU	2.1
1	G	255	GLU	2.1
1	B	290	GLN	2.1
1	C	210	THR	2.1
1	G	403	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	341	ALA	2.1
1	K	401	HIS	2.1
1	E	297	GLY	2.1
1	E	306	GLY	2.1
1	B	388	GLU	2.0
1	H	302	SER	2.0
1	K	315	GLU	2.0
1	C	314	LEU	2.0
1	D	215	LEU	2.0
1	J	230	ILE	2.0
1	M	345	ARG	2.0
1	N	223	ALA	2.0
1	H	281	PHE	2.0
1	C	252	GLU	2.0
1	J	201	SER	2.0
1	F	290	GLN	2.0
1	I	366	GLN	2.0
1	M	142	LYS	2.0
1	L	243	ALA	2.0
1	E	336	VAL	2.0
1	H	323	VAL	2.0
1	L	323	VAL	2.0
1	M	252	GLU	2.0
1	K	298	GLY	2.0
1	G	319	GLN	2.0
1	H	184	GLN	2.0
1	C	364	LYS	2.0
1	M	257	GLU	2.0
1	N	397	GLU	2.0
1	I	249	ILE	2.0
1	K	524	LEU	2.0
1	N	372	LEU	2.0
1	F	188	ASP	2.0
1	L	321	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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(\AA^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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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 [i](#)

There are no such residues in this entry.