



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:57 am BST

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 : 2001-12-30
Resolution : 2.00 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

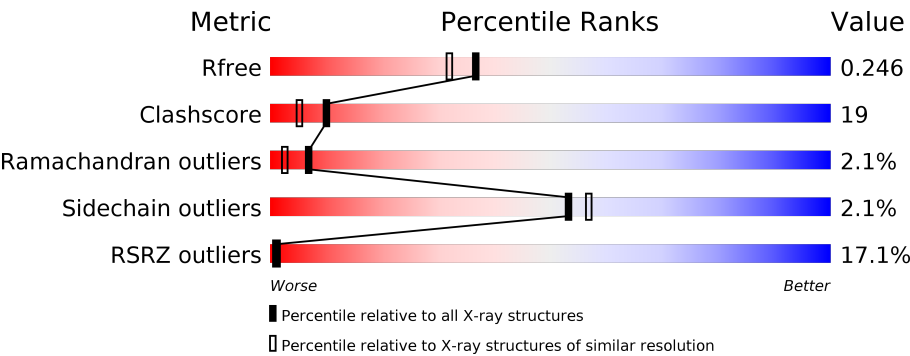
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 respectively. 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>.</div></div>
1	B	547	<div><div>23%</div><div>64%</div><div>29%</div><div>.</div><div>.</div></div>
1	C	547	<div><div>21%</div><div>64%</div><div>29%</div><div>.</div><div>.</div></div>
1	D	547	<div><div>6%</div><div>67%</div><div>27%</div><div>.</div><div>.</div></div>
1	E	547	<div><div>18%</div><div>64%</div><div>29%</div><div>.</div><div>.</div></div>
1	F	547	<div><div>21%</div><div>66%</div><div>27%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
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	J	4020	-	-	-	X
2	SO4	K	4021	-	-	-	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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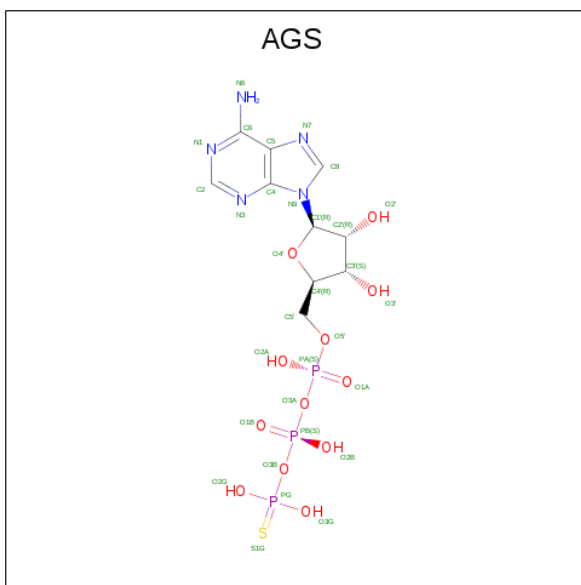
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0

- 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

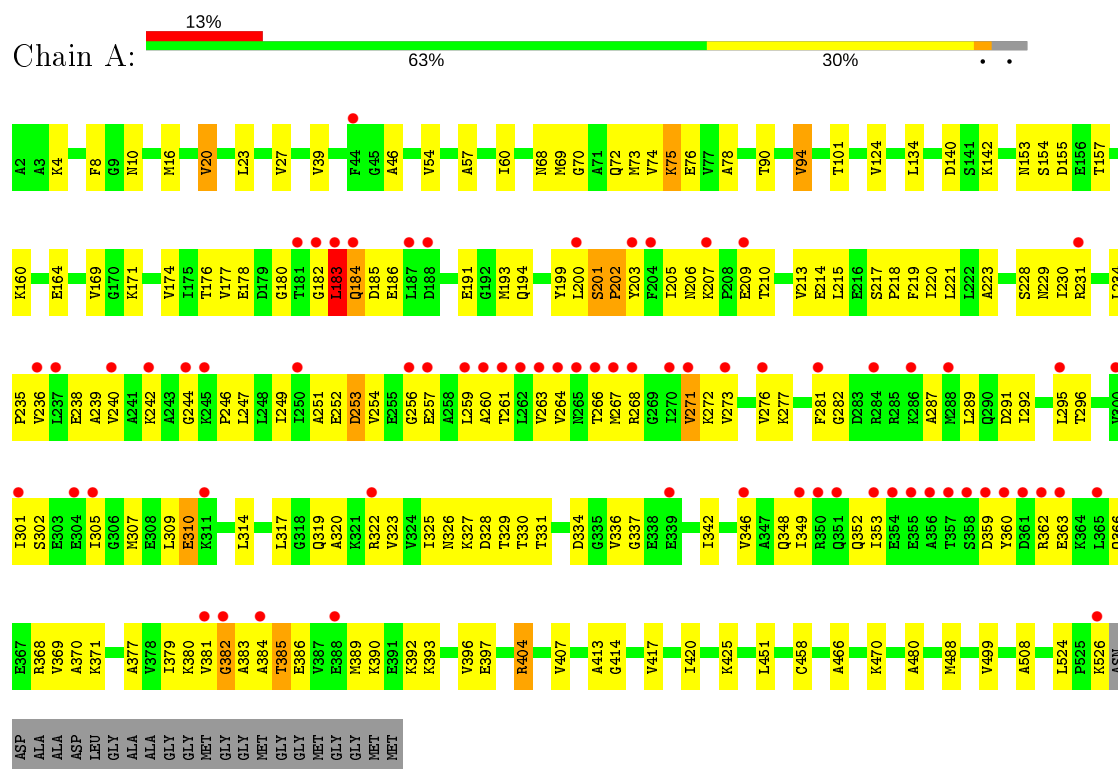
- Molecule 6 is water.

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

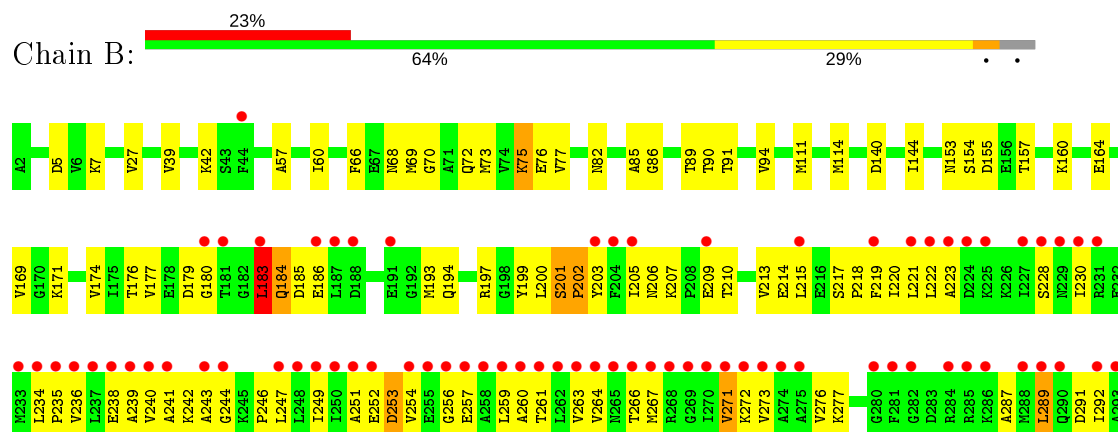
3 Residue-property plots

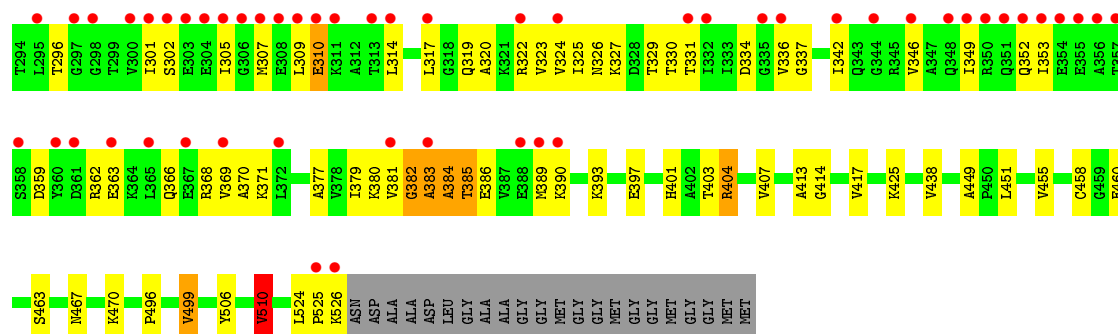
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: groEL protein

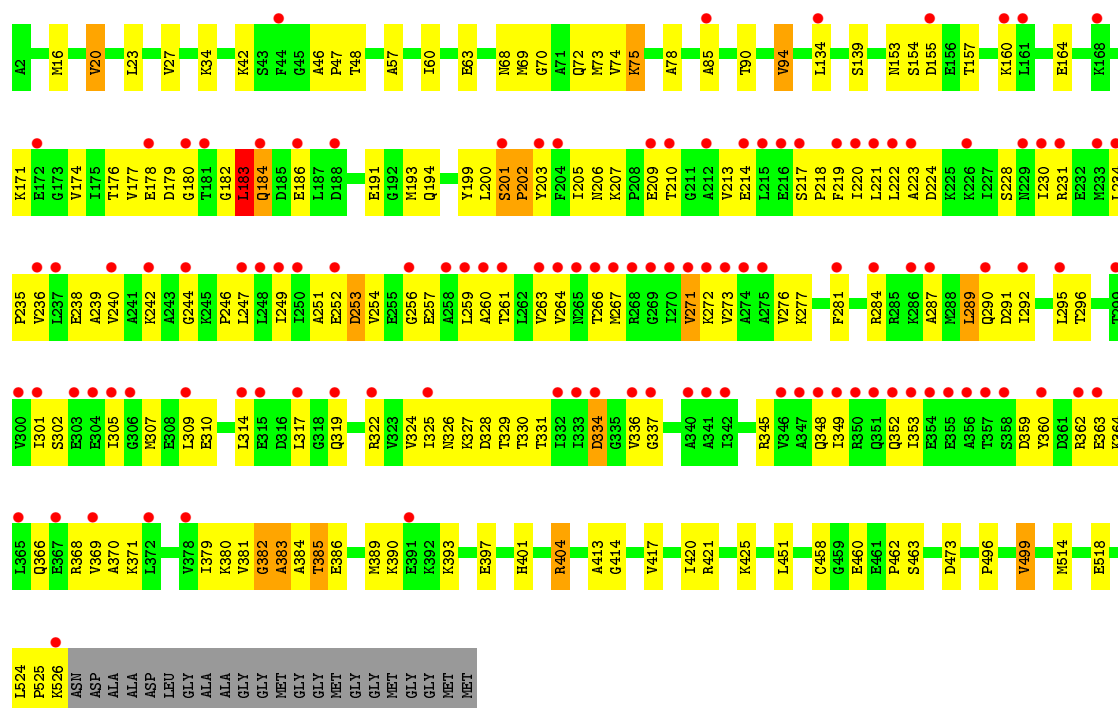


• Molecule 1: groEL protein

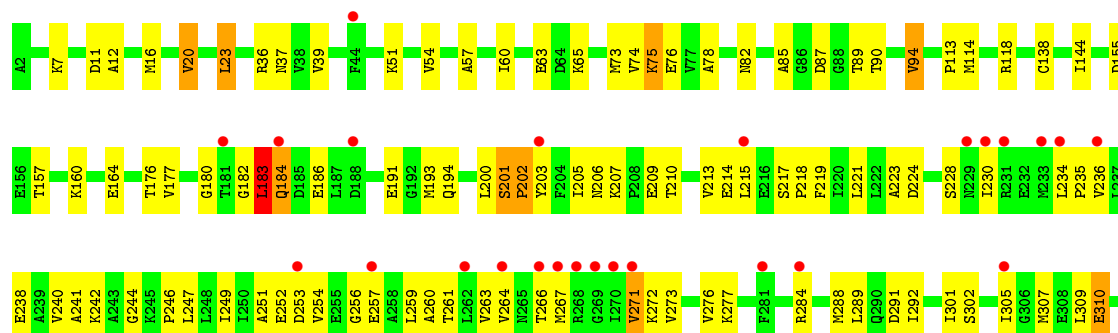


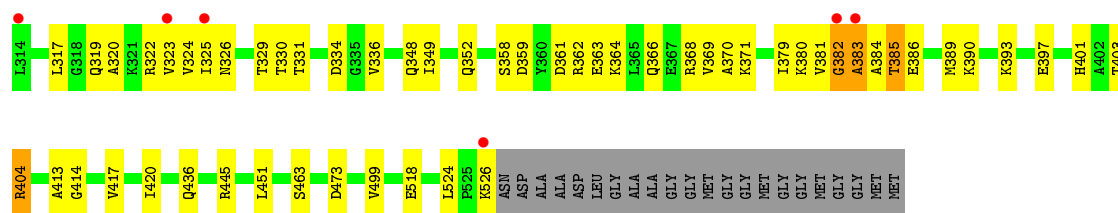


• Molecule 1: groEL protein

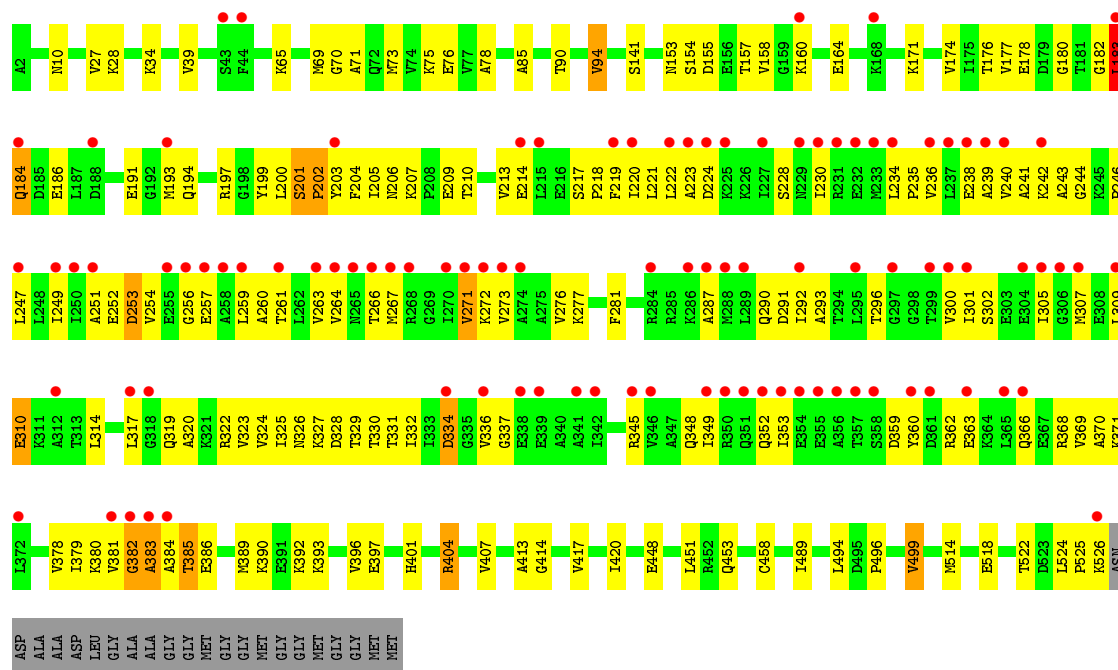


• Molecule 1: groEL protein

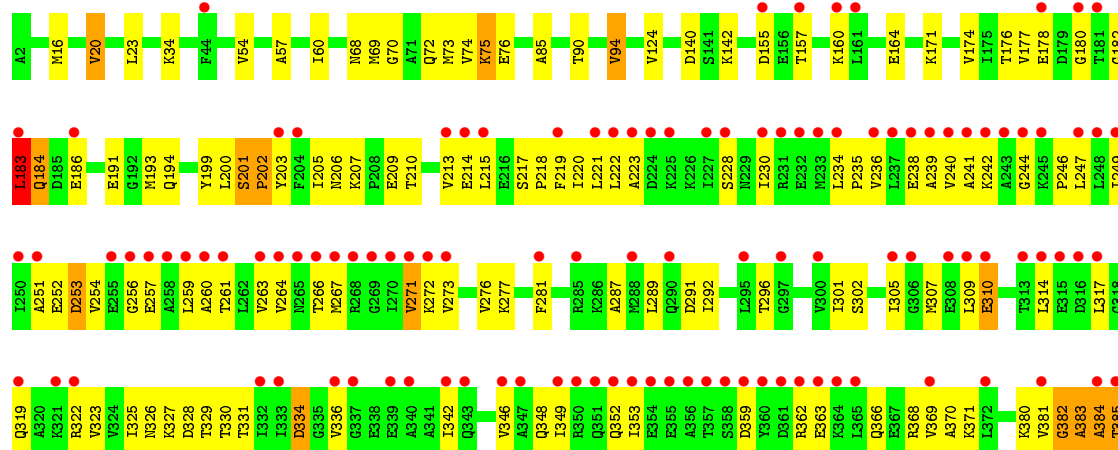


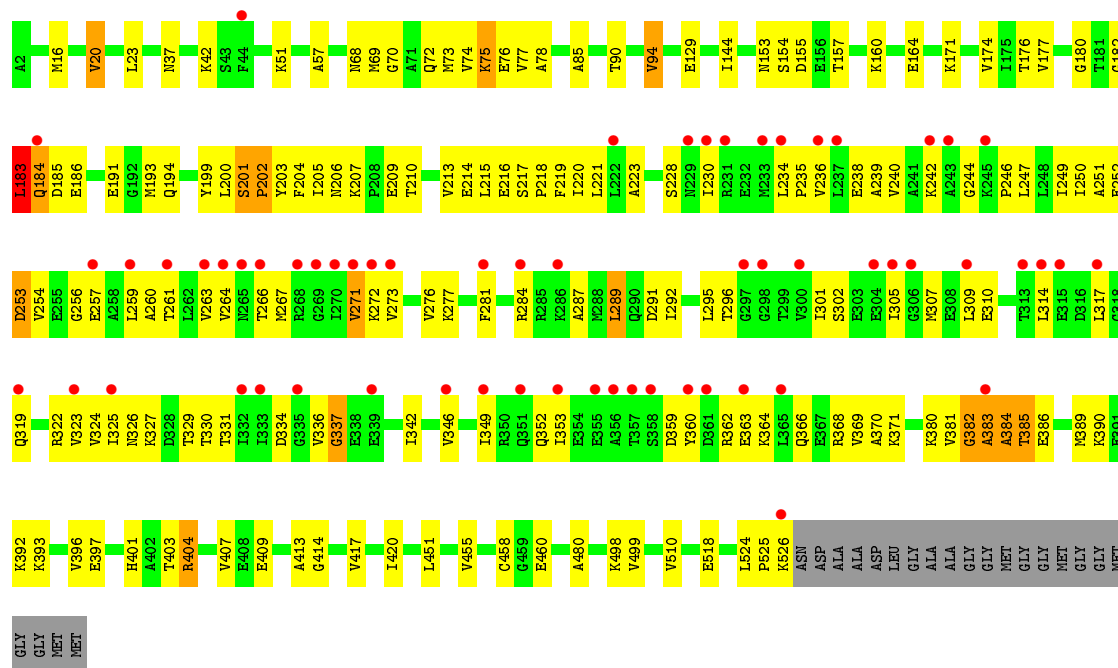
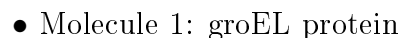
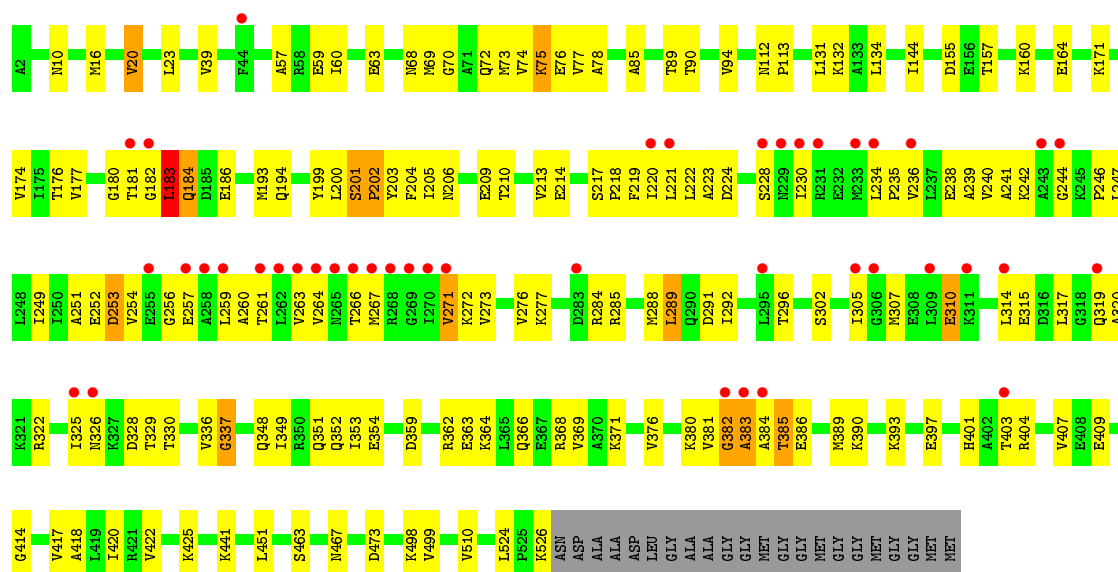
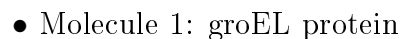


• Molecule 1: groEL protein

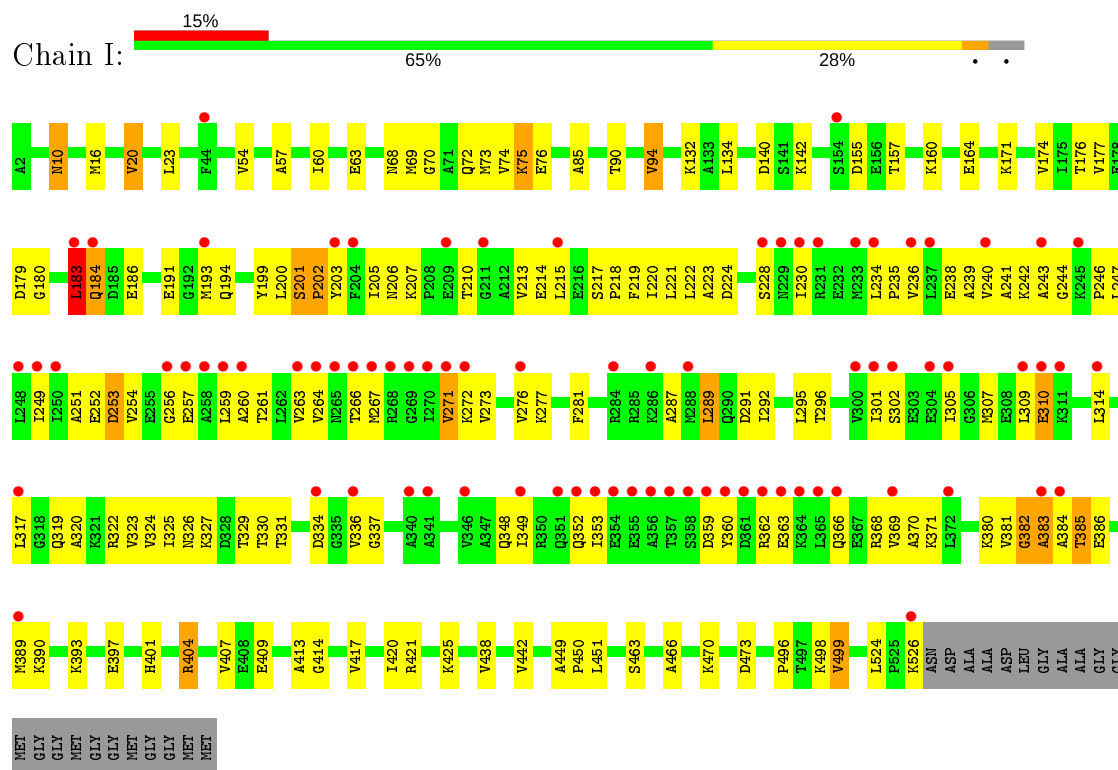


• Molecule 1: groEL protein

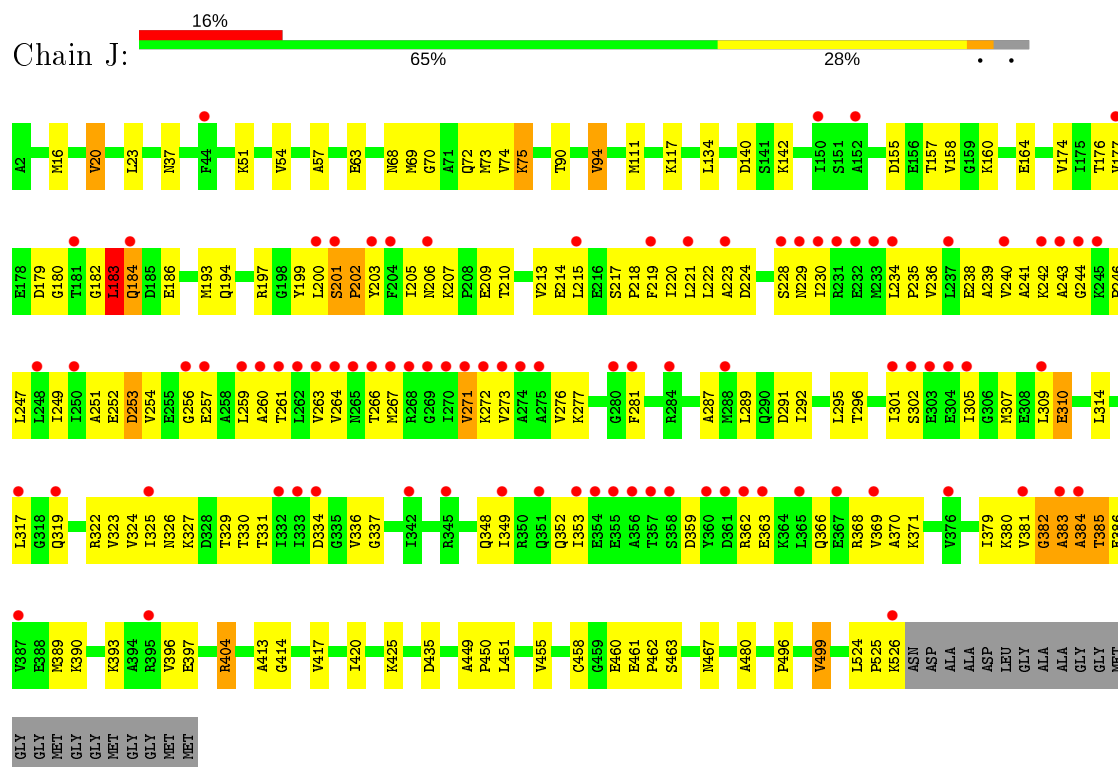




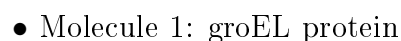
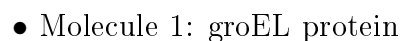
- Molecule 1: groEL protein

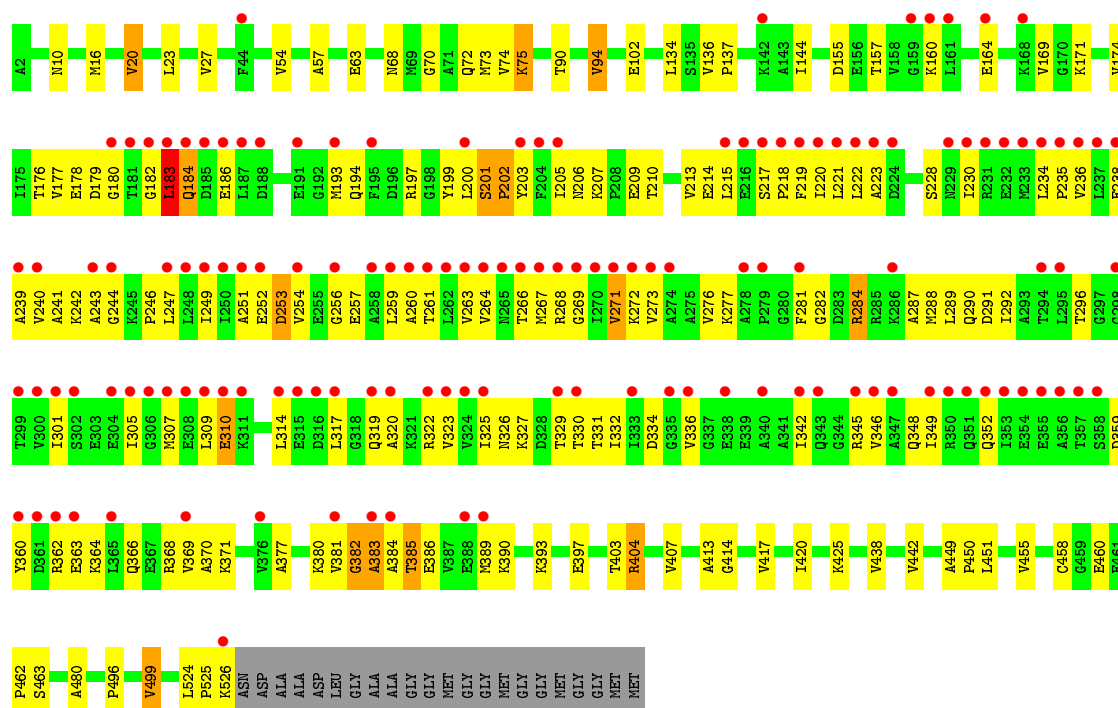


- Molecule 1: groEL protein

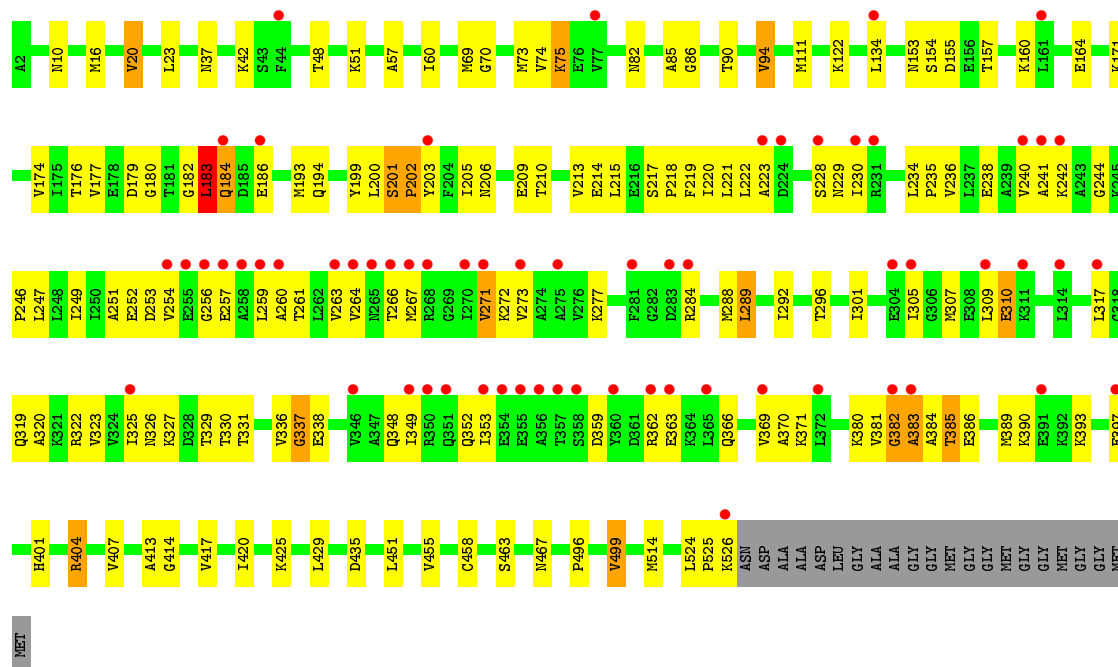


- Molecule 1: groEL protein





• 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 0.229 , 0.246	Depositor DCC
R_{free} test set	12780 reflections (1.98%)	wwPDB-VP
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:414:GLY:O	1:D:417:VAL:HG13	1.96	0.66
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.78	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:268:ARG:O	1:B:257:GLU:HG3	1.97	0.64
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.28	0.64
1: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:177:VAL:HG21	1:I:397:GLU:HG3	1.80	0.63
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.79	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:213:VAL:HB	1:J:325:ILE:CG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.81	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:186:GLU:HB2	1:E:380:LYS:HB2	1.82	0.62
1:E:228:SER:O	1:E:257:GLU:HB3	1.99	0.62
1: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:176:THR:HG21	1:M:322:ARG:HH12	1.63	0.62
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.27	0.62
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.81	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:A:360:TYR:OH	1:G:384:ALA:HA	2.00	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:291:ASP:OD2	1:G:368:ARG:HD2	2.01	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.81	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:177:VAL:HG21	1:C:397:GLU:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.84	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:219:PHE:HB3	1:M:317:LEU:HD23	1.81	0.60
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.82	0.60
1:M:362:ARG:O	1:M:366:GLN:HG3	2.02	0.60
1: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: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:H:360:TYR:OH	1:N:384:ALA:HA	2.04	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:E:34:LYS:HG3	1:E:458:CYS:SG	2.46	0.56
1:A:282:GLY:HA3	1:G:181:THR:O	2.05	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:386:GLU:O	1:H:390:LYS:HG2	2.07	0.55
1:H:23:LEU:CD2	1:H:74:VAL:HG13	2.37	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:L:200:LEU:O	1:L:201:SER:HB3	2.07	0.55
1:K:272:LYS:NZ	1:L:229:ASN:HD21	2.04	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:386:GLU:O	1:G:390:LYS:HG2	2.07	0.55
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.89	0.55
1: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:229:ASN:ND2	1:G:244:GLY:CA	2.71	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: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:177:VAL:HG21	1:B:397:GLU:HG3	1.90	0.53
1:B:219:PHE:O	1:B:247:LEU:HD12	2.08	0.53
1: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:326:ASN:HD22	1:N:329:THR:HB	1.74	0.53
1:N:23:LEU:CD2	1:N:74:VAL:HG13	2.38	0.53
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.91	0.53
1:B:239:ALA:O	1:B:314:LEU:HD11	2.09	0.53
1: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:252:GLU:O	1:E:253:ASP:HB2	2.10	0.52
1:E:193:MET:HE2	1:E:292:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:GLN:O	1:E:336:VAL:HG23	2.10	0.52
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.92	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:305:ILE:O	1:M:305:ILE:HG22	2.09	0.51
1:M:284:ARG:NH1	1:M:364:LYS:NZ	2.58	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:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:C:134:LEU:HD21	1:C:425:LYS:NZ	2.25	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:E:183:LEU:CD1	1:E:184:GLN:HG3	2.40	0.51
1:D:384:ALA:HA	1:E:360:TYR:OH	2.11	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:231:ARG:NH2	1:G:241:ALA:HB1	2.26	0.50
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: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:215:LEU:HB2	1:N:323:VAL:HG22	1.93	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: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:176:THR:HG21	1:E:322:ARG:HH12	1.75	0.49
1:E:239:ALA:O	1:E:314:LEU:HD11	2.12	0.49
1:G:23:LEU:CD2	1:G:74:VAL:HG13	2.42	0.49
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.94	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:236:VAL:O	1:E:240:VAL:HG23	2.12	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.92	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:A:229:ASN:ND2	1:G:244:GLY:HA3	2.28	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: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: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:L:23:LEU:CD2	1:L:74:VAL:HG13	2.42	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:193:MET:CE	1:M:292:ILE:HG12	2.43	0.48
1:M:281:PHE:H	1:M:284:ARG:HD2	1.76	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:E:153:ASN:O	1:E:154:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLU:OE2	1:E:526:LYS:HE2	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:B:200:LEU:HG	1:B:276:VAL:HA	1.96	0.48
1:A:46:ALA:HB2	1:B:76:GLU:HG2	1.93	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:252:GLU:O	1:F:253:ASP:HB2	2.14	0.48
1:F:180:GLY:HA3	1:F:381:VAL:O	2.13	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:193:MET:HE2	1:A:292:ILE:HG12	1.96	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.95	0.47
1: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:219:PHE:O	1:K:247:LEU:HD12	2.13	0.47
1:K:234:LEU:O	1:K:238:GLU:HG3	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: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:A:231:ARG:NH1	1:G:242:LYS:HG2	2.28	0.47
1:H:239:ALA:O	1:H:314:LEU:HD11	2.15	0.47
1:H:271:VAL:HG12	1:H:273:VAL:HG23	1.96	0.47
1:L:78:ALA:HB1	1:L:89:THR:HB	1.97	0.47
1: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:199:TYR:CZ	1:M:327:LYS:HA	2.50	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: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:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:C:23:LEU:CD2	1:C:74:VAL:HG13	2.45	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:215:LEU:HB2	1:A:323:VAL:HG22	1.98	0.46
1:A:169:VAL:HG13	1:A:377:ALA:HB2	1.97	0.46
1: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:N:155:ASP:OD1	1:N:157:THR:HB	2.14	0.46
1:M:63:GLU:OE2	1:N:526:LYS:HE2	2.15	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:169:VAL:CG1	1:B:377:ALA:HB2	2.45	0.46
1:B:325:ILE:HG22	1:B:330:THR:HA	1.96	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:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.46
1:K:325:ILE:HA	1:K:329:THR:O	2.15	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:200:LEU:HG	1:F:276:VAL:HA	1.98	0.46
1:F:234:LEU:N	1:F:235:PRO:HD2	2.30	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:158:VAL:HG13	1:J:396:VAL:HG22	1.98	0.46
1:J:219:PHE:O	1:J:247:LEU:HD12	2.15	0.46
1:J:223:ALA:O	1:J:251:ALA:HA	2.15	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.16	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:171:LYS:HB2	1:F:407:VAL:HG11	1.98	0.45
1:F:219:PHE:O	1:F:247:LEU:HD12	2.16	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: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:F:124:VAL:HG21	1:F:508:ALA:CB	2.47	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:K:174:VAL:HG22	1:K:194:GLN:NE2	2.32	0.45
1:K:217:SER:N	1:K:218:PRO:HD3	2.31	0.45
1:J:272:LYS:NZ	1:K:229:ASN:OD1	2.50	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:K:88:GLY:HA2	5:K:1:AGS:PB	2.57	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:266:THR:HG22	1:K:271:VAL:O	2.17	0.44
1:K:222:LEU:HB3	1:K:289:LEU:CD2	2.48	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
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:K:134:LEU:HD21	1:K:425:LYS:NZ	2.32	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:M:210:THR:HG22	1:M:210:THR:O	2.18	0.43
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.17	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:183:LEU:CD2	1:C:384:ALA:HB2	2.47	0.43
1:C:348:GLN:O	1:C:352:GLN:HG2	2.18	0.43
1: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:266:THR:HG22	1:B:271:VAL:O	2.19	0.43
1:B:218:PRO:HD2	1:B:320:ALA:O	2.18	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:180:GLY:HA3	1:N:381:VAL:O	2.18	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: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:240:VAL:HG11	1:F:247:LEU:HB2	2.00	0.43
1:F:178:GLU:OE2	1:F:322:ARG:NH1	2.51	0.43
1: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:234:LEU:O	1:B:238:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.52	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:191:GLU:O	1:F:334:ASP:HA	2.18	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	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:284:ARG:HH11	1:M:364:LYS:CE	2.32	0.42
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.00	0.42
5:N:1:AGS:O2G	5:N:1:AGS:S1G	2.54	0.42
1: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:D:36:ARG:HG3	1:E:518:GLU:HG2	2.00	0.42
1:E:348:GLN:O	1:E:352:GLN:HG2	2.19	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:524:LEU:O	1:G:526:LYS:N	2.52	0.42
1:G:85:ALA:O	1:G:401:HIS:HE1	2.02	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:131:LEU:HD13	1:G:422:VAL:HG21	2.02	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: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:179:ASP:HB3	1:I:389:MET:CE	2.49	0.42
1:I:336:VAL:O	1:I:337:GLY:C	2.58	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:A:4:LYS:HG3	1:G:59:GLU:O	2.19	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: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:242:LYS:C	1:B:244:GLY:N	2.73	0.41
1:B:240:VAL:HG11	1:B:247:LEU:HB2	2.01	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:295:LEU:HD13	1:J:295:LEU:O	2.20	0.41
1:J:177:VAL:HA	1:J:379:ILE:O	2.20	0.41
1:K:171:LYS:HB2	1:K:407:VAL:HG11	2.02	0.41
1:K:366:GLN:HA	1:K:369:VAL:HG22	2.01	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:28:LYS:HD2	1:E:453:GLN:NE2	2.36	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: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: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:C:272:LYS:HZ3	1:D:228:SER:HB2	1.85	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: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:199:TYR:CZ	1:K:327:LYS:HA	2.56	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:J:381:VAL:O	1:J:382:GLY:O	2.39	0.41
1:J:182:GLY:HA2	1:J:383:ALA:CB	2.50	0.41
1:I:63:GLU:HB2	1:J:524:LEU:CD2	2.50	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:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:E:224:ASP:HB3	1:E:302:SER:HB3	2.01	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:200:LEU:HG	1:K:276:VAL:HA	2.03	0.40
1:K:240:VAL:HG11	1:K:247:LEU:HB2	2.02	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%)	9	4
1	B	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	6	2
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	7	2
1	D	523/547 (96%)	492 (94%)	22 (4%)	9 (2%)	9	4
1	E	523/547 (96%)	485 (93%)	27 (5%)	11 (2%)	7	2
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	6	2
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	7	2

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

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%)	47	49
1	B	404/413 (98%)	397 (98%)	7 (2%)	60	65
1	C	404/413 (98%)	396 (98%)	8 (2%)	55	58
1	D	404/413 (98%)	394 (98%)	10 (2%)	47	49
1	E	404/413 (98%)	397 (98%)	7 (2%)	60	65
1	F	404/413 (98%)	396 (98%)	8 (2%)	55	58
1	G	404/413 (98%)	395 (98%)	9 (2%)	52	55
1	H	404/413 (98%)	397 (98%)	7 (2%)	60	65
1	I	404/413 (98%)	395 (98%)	9 (2%)	52	55
1	J	404/413 (98%)	397 (98%)	7 (2%)	60	65
1	K	404/413 (98%)	396 (98%)	8 (2%)	55	58
1	L	404/413 (98%)	394 (98%)	10 (2%)	47	49
1	M	404/413 (98%)	396 (98%)	8 (2%)	55	58
1	N	404/413 (98%)	396 (98%)	8 (2%)	55	58
All	All	5656/5782 (98%)	5540 (98%)	116 (2%)	53	57

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
2	SO4	K	4021	-	4,4,4	1.56	1 (25%)	6,6,6	1.14	0
2	SO4	E	4006	-	4,4,4	1.53	1 (25%)	6,6,6	1.12	0
5	AGS	C	1	3,4	26,33,33	3.87	2 (7%)	26,52,52	1.12	2 (7%)
2	SO4	K	4022	-	4,4,4	1.51	1 (25%)	6,6,6	1.14	0
2	SO4	A	4007	-	4,4,4	1.50	1 (25%)	6,6,6	1.16	0
2	SO4	M	4013	-	4,4,4	1.58	1 (25%)	6,6,6	1.15	0
5	AGS	I	1	3,4	26,33,33	3.89	2 (7%)	26,52,52	1.09	2 (7%)
2	SO4	C	4011	-	4,4,4	1.53	1 (25%)	6,6,6	1.13	0
5	AGS	N	1	3,4	26,33,33	3.90	3 (11%)	26,52,52	1.11	2 (7%)
2	SO4	E	4005	-	4,4,4	1.43	1 (25%)	6,6,6	1.16	0
2	SO4	C	4012	-	4,4,4	1.56	1 (25%)	6,6,6	1.16	0
2	SO4	H	4017	-	4,4,4	1.53	1 (25%)	6,6,6	1.14	0
5	AGS	A	1	3,4	26,33,33	3.76	1 (3%)	26,52,52	1.20	2 (7%)
5	AGS	B	1	3,4	26,33,33	3.81	2 (7%)	26,52,52	1.12	2 (7%)
5	AGS	K	1	3,4	26,33,33	3.88	4 (15%)	26,52,52	1.08	2 (7%)
2	SO4	J	4019	-	4,4,4	1.52	1 (25%)	6,6,6	1.12	0
5	AGS	H	1	3,4	26,33,33	3.85	1 (3%)	26,52,52	1.18	2 (7%)
2	SO4	F	4004	-	4,4,4	1.45	1 (25%)	6,6,6	1.18	0
2	SO4	B	4009	-	4,4,4	1.52	1 (25%)	6,6,6	1.11	0
2	SO4	J	4020	-	4,4,4	1.54	1 (25%)	6,6,6	1.13	0
2	SO4	A	4008	-	4,4,4	1.52	1 (25%)	6,6,6	1.13	0
2	SO4	N	4016	-	4,4,4	1.53	1 (25%)	6,6,6	1.14	0
5	AGS	E	1	3,4	26,33,33	3.96	3 (11%)	26,52,52	1.13	2 (7%)
2	SO4	L	4003	-	4,4,4	1.52	1 (25%)	6,6,6	1.16	0
2	SO4	M	4014	-	4,4,4	1.55	1 (25%)	6,6,6	1.13	0
2	SO4	H	4018	-	4,4,4	1.53	1 (25%)	6,6,6	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	N	4015	-	4,4,4	1.54	1 (25%)	6,6,6	1.16	0
5	AGS	G	1	3,4	26,33,33	3.99	2 (7%)	26,52,52	1.18	2 (7%)
2	SO4	B	4010	-	4,4,4	1.54	1 (25%)	6,6,6	1.13	0
5	AGS	F	1	3,4	26,33,33	3.86	3 (11%)	26,52,52	1.04	1 (3%)
5	AGS	D	551	3,4	26,33,33	3.96	5 (19%)	26,52,52	1.07	1 (3%)
5	AGS	J	1	3,4	26,33,33	3.88	4 (15%)	26,52,52	1.11	2 (7%)
5	AGS	L	1	3,4	26,33,33	3.85	2 (7%)	26,52,52	1.11	2 (7%)
5	AGS	M	1	3,4	26,33,33	3.86	1 (3%)	26,52,52	1.11	2 (7%)
2	SO4	G	4002	-	4,4,4	1.53	1 (25%)	6,6,6	1.17	0
2	SO4	A	4001	-	4,4,4	1.52	1 (25%)	6,6,6	1.16	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	C	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	H	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	G	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	A	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	B	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	K	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	E	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	F	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	D	551	3,4	-	3/17/38/38	0/3/3/3
5	AGS	I	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	J	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	L	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	M	1	3,4	-	3/17/38/38	0/3/3/3
5	AGS	N	1	3,4	-	3/17/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-19.57	1.48	1.90
5	E	1	AGS	PG-S1G	-19.49	1.48	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	551	AGS	PG-S1G	-19.39	1.48	1.90
5	N	1	AGS	PG-S1G	-19.10	1.49	1.90
5	I	1	AGS	PG-S1G	-19.09	1.49	1.90
5	H	1	AGS	PG-S1G	-18.99	1.49	1.90
5	C	1	AGS	PG-S1G	-18.98	1.49	1.90
5	J	1	AGS	PG-S1G	-18.97	1.49	1.90
5	K	1	AGS	PG-S1G	-18.95	1.49	1.90
5	M	1	AGS	PG-S1G	-18.92	1.49	1.90
5	F	1	AGS	PG-S1G	-18.83	1.49	1.90
5	L	1	AGS	PG-S1G	-18.82	1.49	1.90
5	B	1	AGS	PG-S1G	-18.66	1.50	1.90
5	A	1	AGS	PG-S1G	-18.55	1.50	1.90
5	K	1	AGS	O4'-C1'	3.14	1.45	1.41
2	M	4013	SO4	O1-S	3.08	1.62	1.46
2	K	4021	SO4	O1-S	3.02	1.62	1.46
2	C	4012	SO4	O1-S	3.01	1.62	1.46
2	B	4010	SO4	O1-S	3.00	1.62	1.46
2	M	4014	SO4	O1-S	2.99	1.62	1.46
2	N	4015	SO4	O1-S	2.98	1.62	1.46
2	C	4011	SO4	O1-S	2.98	1.62	1.46
2	H	4018	SO4	O1-S	2.98	1.62	1.46
2	J	4019	SO4	O1-S	2.97	1.62	1.46
2	J	4020	SO4	O1-S	2.97	1.62	1.46
2	E	4006	SO4	O1-S	2.97	1.62	1.46
2	H	4017	SO4	O1-S	2.97	1.62	1.46
2	B	4009	SO4	O1-S	2.96	1.62	1.46
2	N	4016	SO4	O1-S	2.96	1.62	1.46
2	A	4008	SO4	O1-S	2.96	1.62	1.46
2	A	4001	SO4	O1-S	2.95	1.62	1.46
2	G	4002	SO4	O1-S	2.95	1.62	1.46
2	L	4003	SO4	O1-S	2.93	1.61	1.46
2	K	4022	SO4	O1-S	2.93	1.61	1.46
2	A	4007	SO4	O1-S	2.89	1.61	1.46
2	F	4004	SO4	O1-S	2.81	1.61	1.46
2	E	4005	SO4	O1-S	2.77	1.61	1.46
5	F	1	AGS	C2-N3	2.29	1.35	1.32
5	D	551	AGS	C2'-C1'	-2.29	1.50	1.53
5	D	551	AGS	C2-N3	2.22	1.35	1.32
5	F	1	AGS	PG-O3G	-2.22	1.47	1.54
5	J	1	AGS	C2-N3	2.17	1.35	1.32
5	J	1	AGS	O4'-C1'	2.16	1.44	1.41
5	L	1	AGS	C2'-C1'	-2.13	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	C2-N3	2.12	1.35	1.32
5	N	1	AGS	C2-N3	2.12	1.35	1.32
5	D	551	AGS	PG-O3G	-2.10	1.48	1.54
5	E	1	AGS	PG-O3G	-2.08	1.48	1.54
5	K	1	AGS	C2-N3	2.07	1.35	1.32
5	I	1	AGS	C2'-C1'	-2.07	1.50	1.53
5	J	1	AGS	PG-O3G	-2.05	1.48	1.54
5	C	1	AGS	PG-O3G	-2.04	1.48	1.54
5	B	1	AGS	PG-O3G	-2.04	1.48	1.54
5	N	1	AGS	PG-O3G	-2.04	1.48	1.54
5	K	1	AGS	PG-O3G	-2.03	1.48	1.54
5	D	551	AGS	C4-N3	2.02	1.38	1.35
5	E	1	AGS	C2-N3	2.01	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	AGS	C5-C6-N6	3.11	125.08	120.35
5	M	1	AGS	C5-C6-N6	3.10	125.06	120.35
5	G	1	AGS	C5-C6-N6	3.06	125.00	120.35
5	A	1	AGS	C5-C6-N6	2.95	124.83	120.35
5	L	1	AGS	C5-C6-N6	2.85	124.69	120.35
5	C	1	AGS	C5-C6-N6	2.85	124.68	120.35
5	K	1	AGS	C5-C6-N6	2.81	124.63	120.35
5	K	1	AGS	O4'-C1'-C2'	-2.79	102.84	106.93
5	B	1	AGS	C5-C6-N6	2.79	124.59	120.35
5	E	1	AGS	C5-C6-N6	2.77	124.57	120.35
5	N	1	AGS	C5-C6-N6	2.70	124.46	120.35
5	J	1	AGS	C5-C6-N6	2.69	124.44	120.35
5	J	1	AGS	O4'-C1'-C2'	-2.66	103.04	106.93
5	F	1	AGS	C5-C6-N6	2.64	124.36	120.35
5	G	1	AGS	O4'-C1'-C2'	-2.60	103.13	106.93
5	I	1	AGS	C5-C6-N6	2.56	124.24	120.35
5	A	1	AGS	O4'-C1'-C2'	-2.53	103.23	106.93
5	D	551	AGS	C5-C6-N6	2.36	123.94	120.35
5	N	1	AGS	O4'-C1'-C2'	-2.36	103.48	106.93
5	B	1	AGS	O4'-C1'-C2'	-2.20	103.71	106.93
5	M	1	AGS	O4'-C1'-C2'	-2.18	103.73	106.93
5	C	1	AGS	O4'-C1'-C2'	-2.16	103.77	106.93
5	E	1	AGS	O4'-C1'-C2'	-2.12	103.82	106.93
5	L	1	AGS	O4'-C1'-C2'	-2.10	103.86	106.93
5	H	1	AGS	O4'-C1'-C2'	-2.06	103.91	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	AGS	O4'-C1'-C2'	-2.03	103.95	106.93

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	AGS	PB-O3B-PG-O2G
5	C	1	AGS	PB-O3B-PG-O3G
5	I	1	AGS	PB-O3B-PG-O2G
5	I	1	AGS	PB-O3B-PG-O3G
5	N	1	AGS	PB-O3B-PG-O2G
5	N	1	AGS	PB-O3B-PG-O3G
5	G	1	AGS	PB-O3B-PG-O2G
5	G	1	AGS	PB-O3B-PG-O3G
5	A	1	AGS	PB-O3B-PG-O2G
5	A	1	AGS	PB-O3B-PG-O3G
5	B	1	AGS	PB-O3B-PG-O2G
5	B	1	AGS	PB-O3B-PG-O3G
5	K	1	AGS	PB-O3B-PG-O2G
5	K	1	AGS	PB-O3B-PG-O3G
5	H	1	AGS	PB-O3B-PG-O2G
5	H	1	AGS	PB-O3B-PG-O3G
5	F	1	AGS	PB-O3B-PG-O2G
5	F	1	AGS	PB-O3B-PG-O3G
5	J	1	AGS	PB-O3B-PG-O2G
5	J	1	AGS	PB-O3B-PG-O3G
5	D	551	AGS	PB-O3B-PG-O2G
5	D	551	AGS	PB-O3B-PG-O3G
5	E	1	AGS	PB-O3B-PG-O2G
5	E	1	AGS	PB-O3B-PG-O3G
5	L	1	AGS	PB-O3B-PG-O2G
5	L	1	AGS	PB-O3B-PG-O3G
5	M	1	AGS	PB-O3B-PG-O2G
5	M	1	AGS	PB-O3B-PG-O3G
5	C	1	AGS	PA-O3A-PB-O1B
5	I	1	AGS	PA-O3A-PB-O1B
5	N	1	AGS	PA-O3A-PB-O1B
5	G	1	AGS	PA-O3A-PB-O1B
5	A	1	AGS	PA-O3A-PB-O1B
5	B	1	AGS	PA-O3A-PB-O1B
5	K	1	AGS	PA-O3A-PB-O1B
5	H	1	AGS	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	F	1	AGS	PA-O3A-PB-O1B
5	J	1	AGS	PA-O3A-PB-O1B
5	D	551	AGS	PA-O3A-PB-O1B
5	E	1	AGS	PA-O3A-PB-O1B
5	L	1	AGS	PA-O3A-PB-O1B
5	M	1	AGS	PA-O3A-PB-O1B

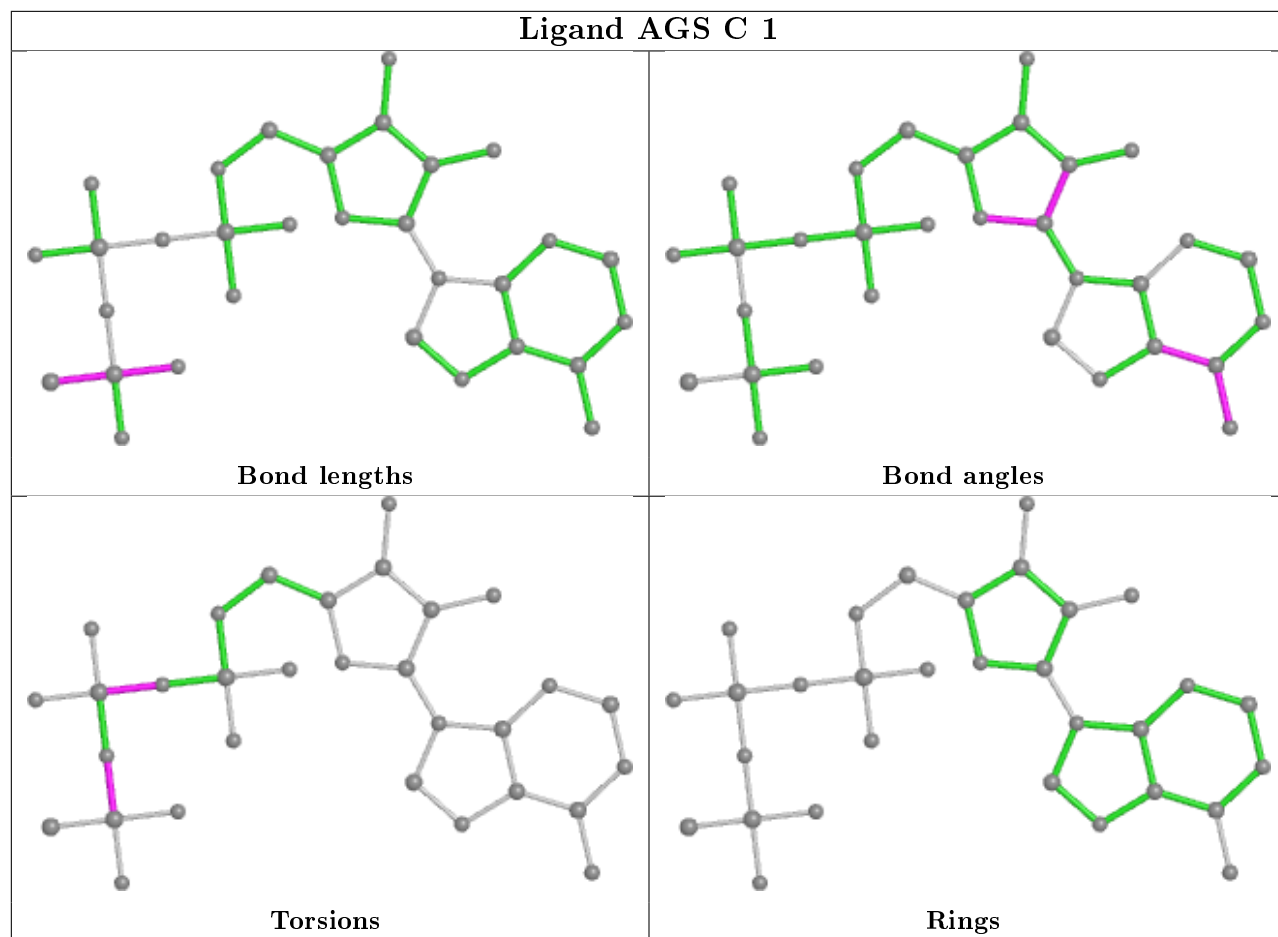
There are no ring outliers.

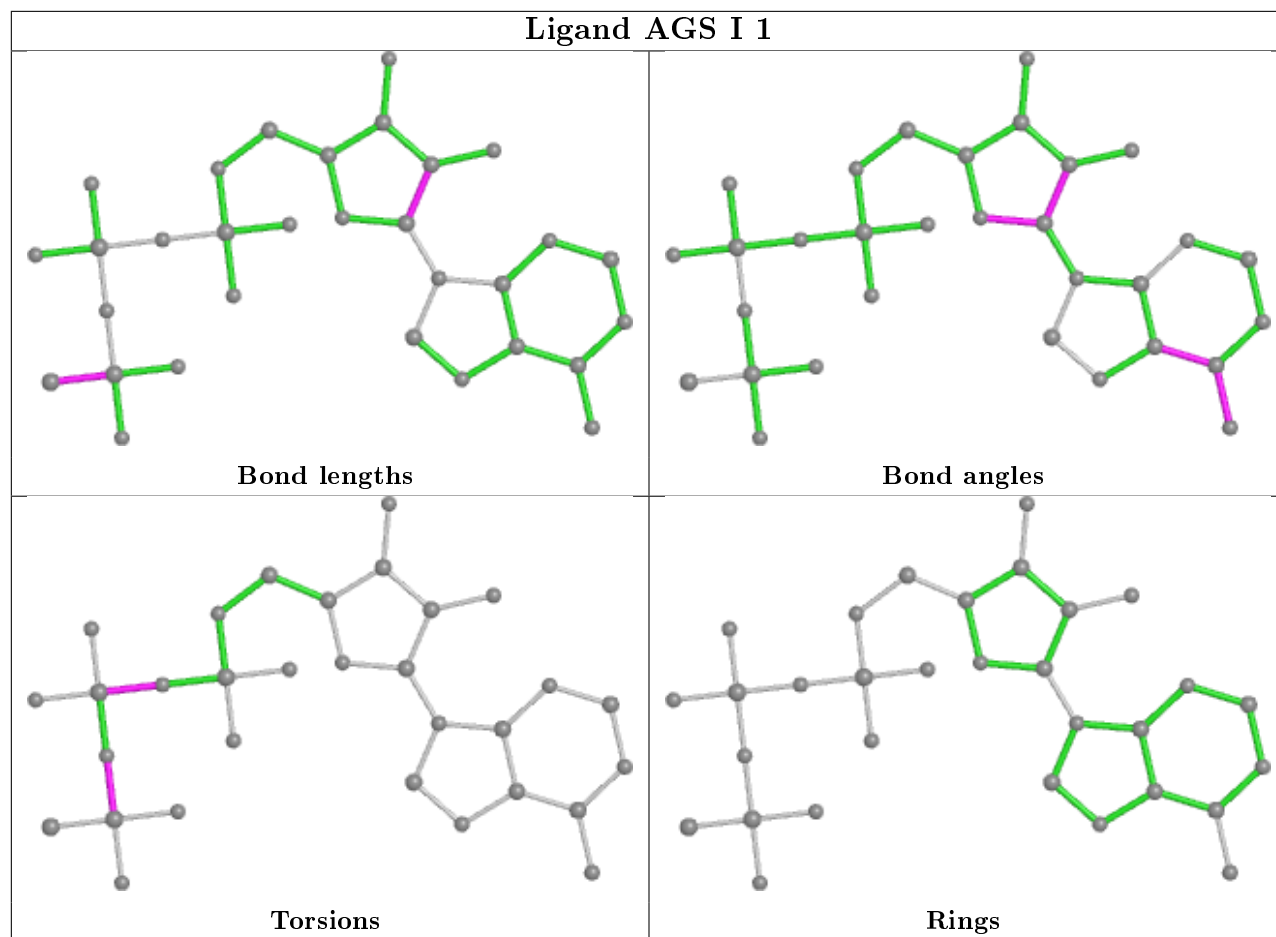
15 monomers are involved in 56 short contacts:

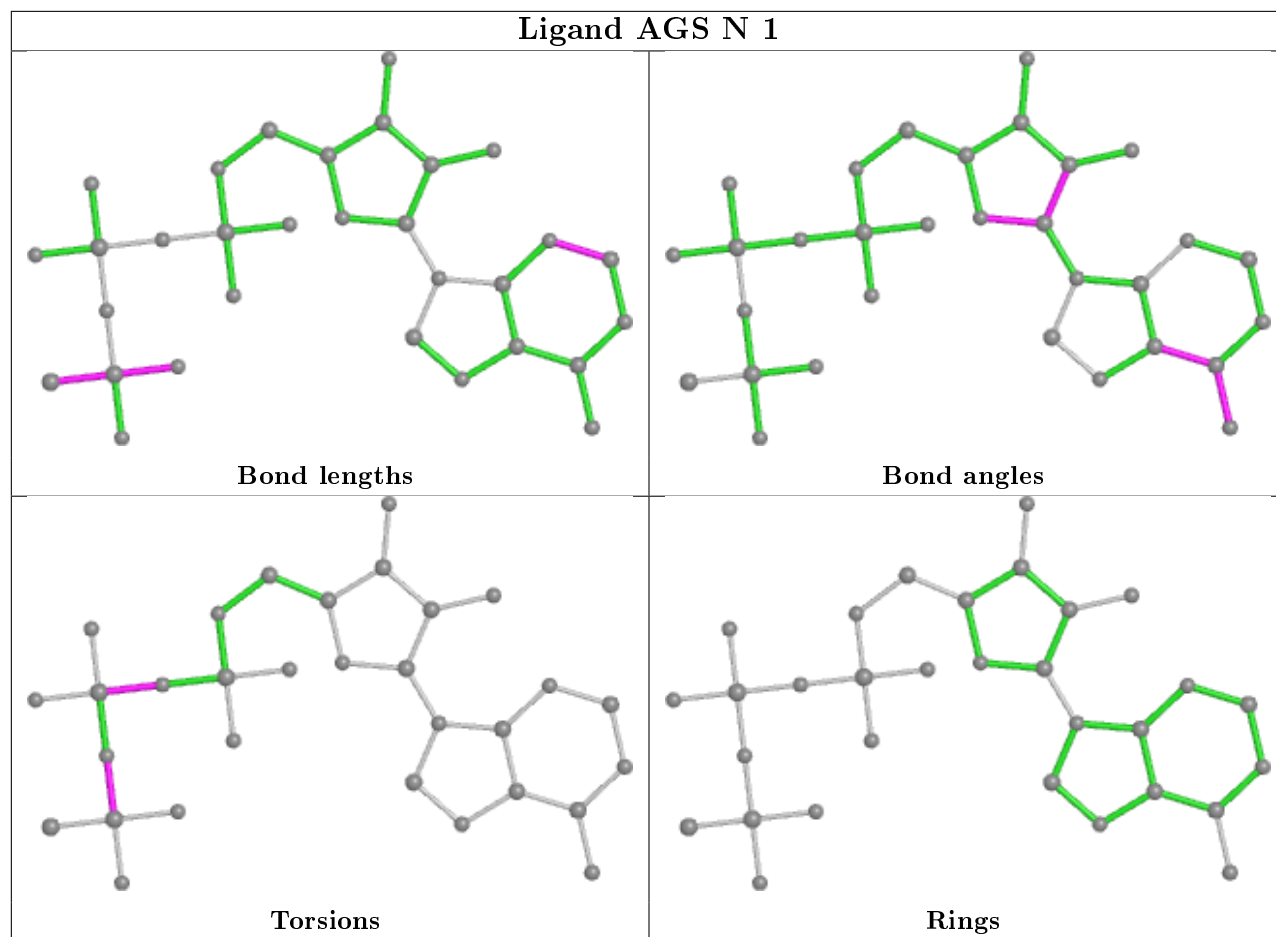
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	AGS	3	0
5	I	1	AGS	4	0
5	N	1	AGS	4	0
2	E	4005	SO4	1	0
5	A	1	AGS	3	0
5	B	1	AGS	4	0
5	K	1	AGS	5	0
5	H	1	AGS	4	0
5	E	1	AGS	4	0
5	G	1	AGS	4	0
5	F	1	AGS	3	0
5	D	551	AGS	4	0
5	J	1	AGS	3	0
5	L	1	AGS	5	0
5	M	1	AGS	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

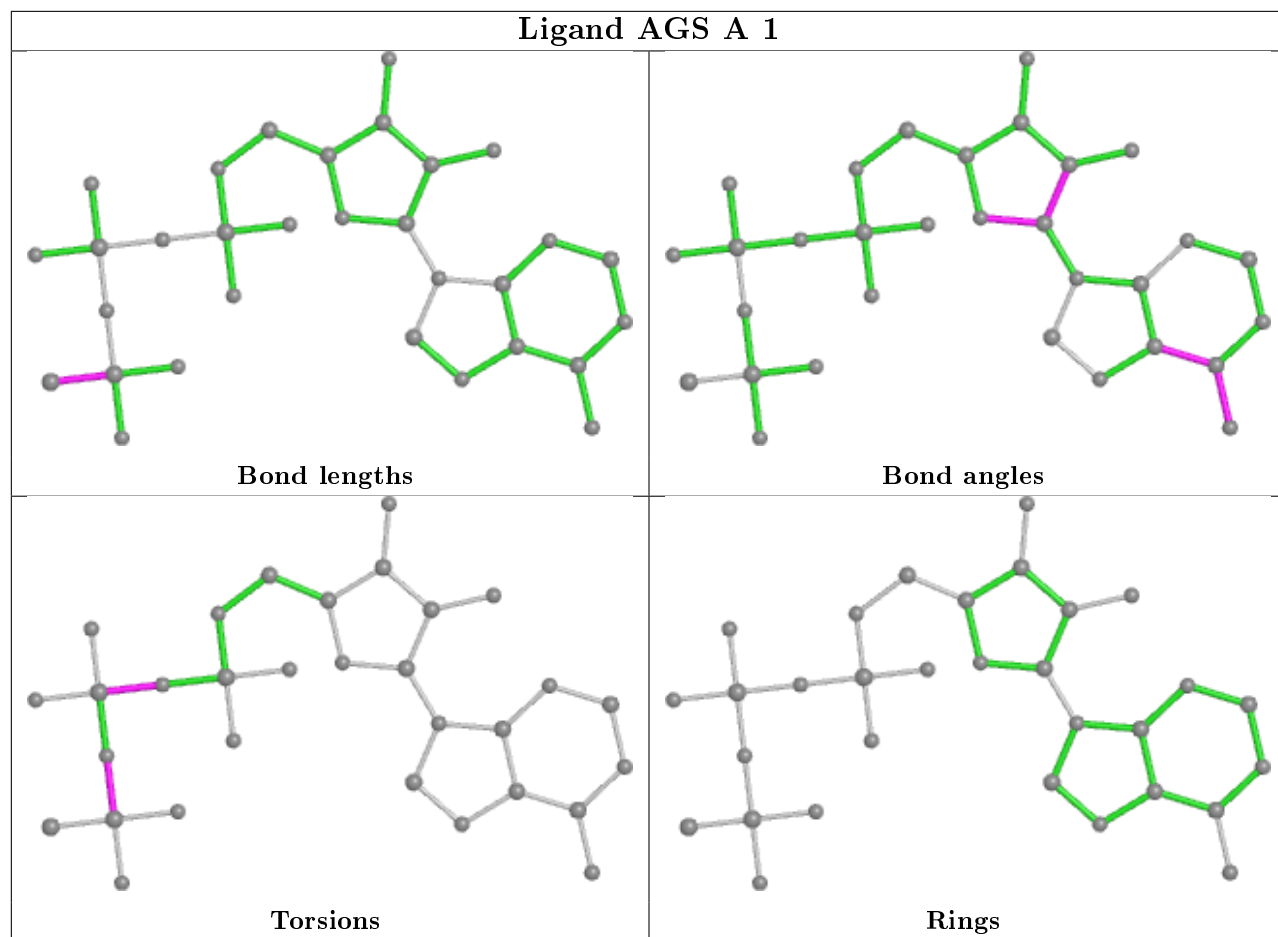
Ligand AGS C 1



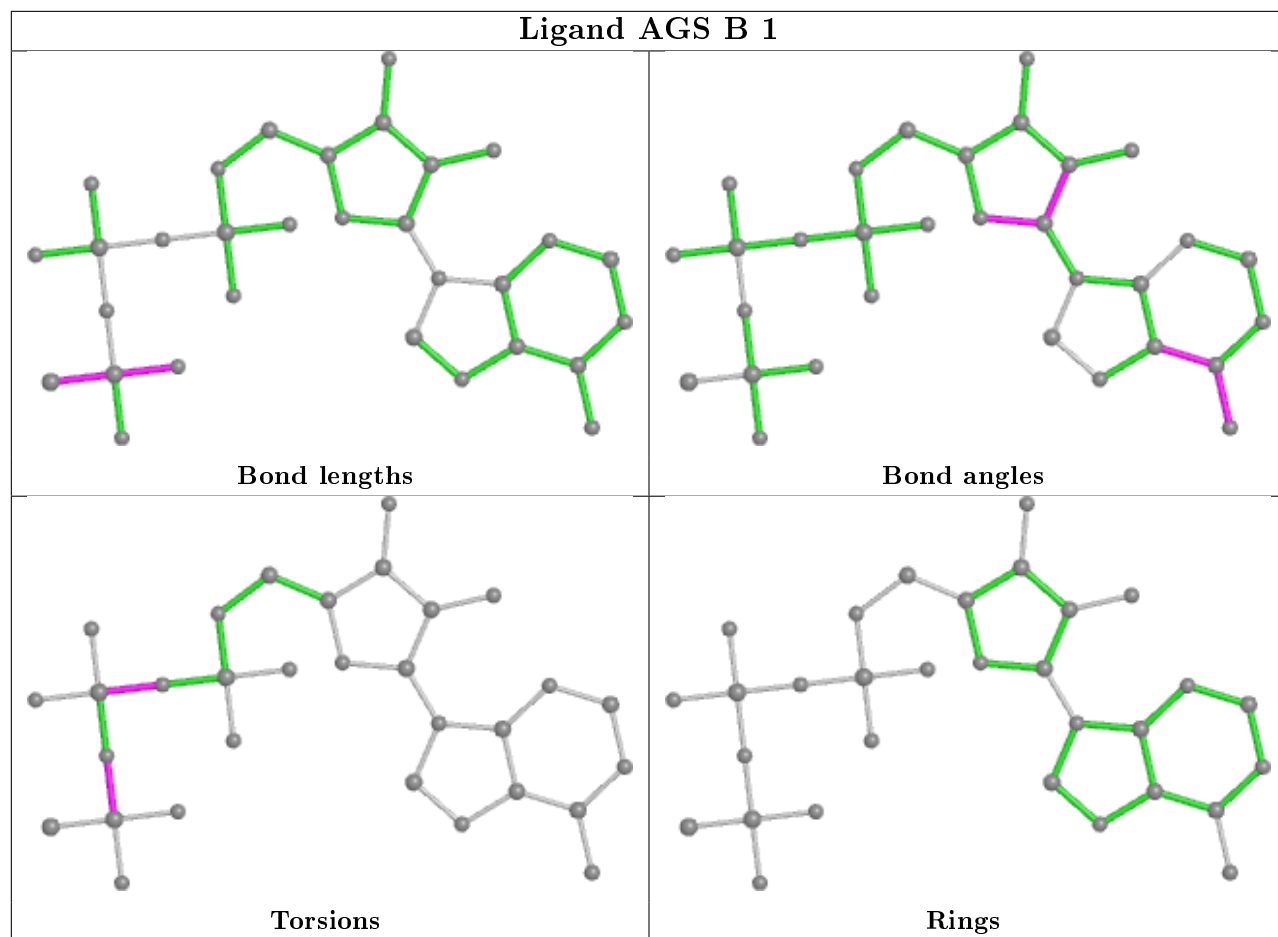




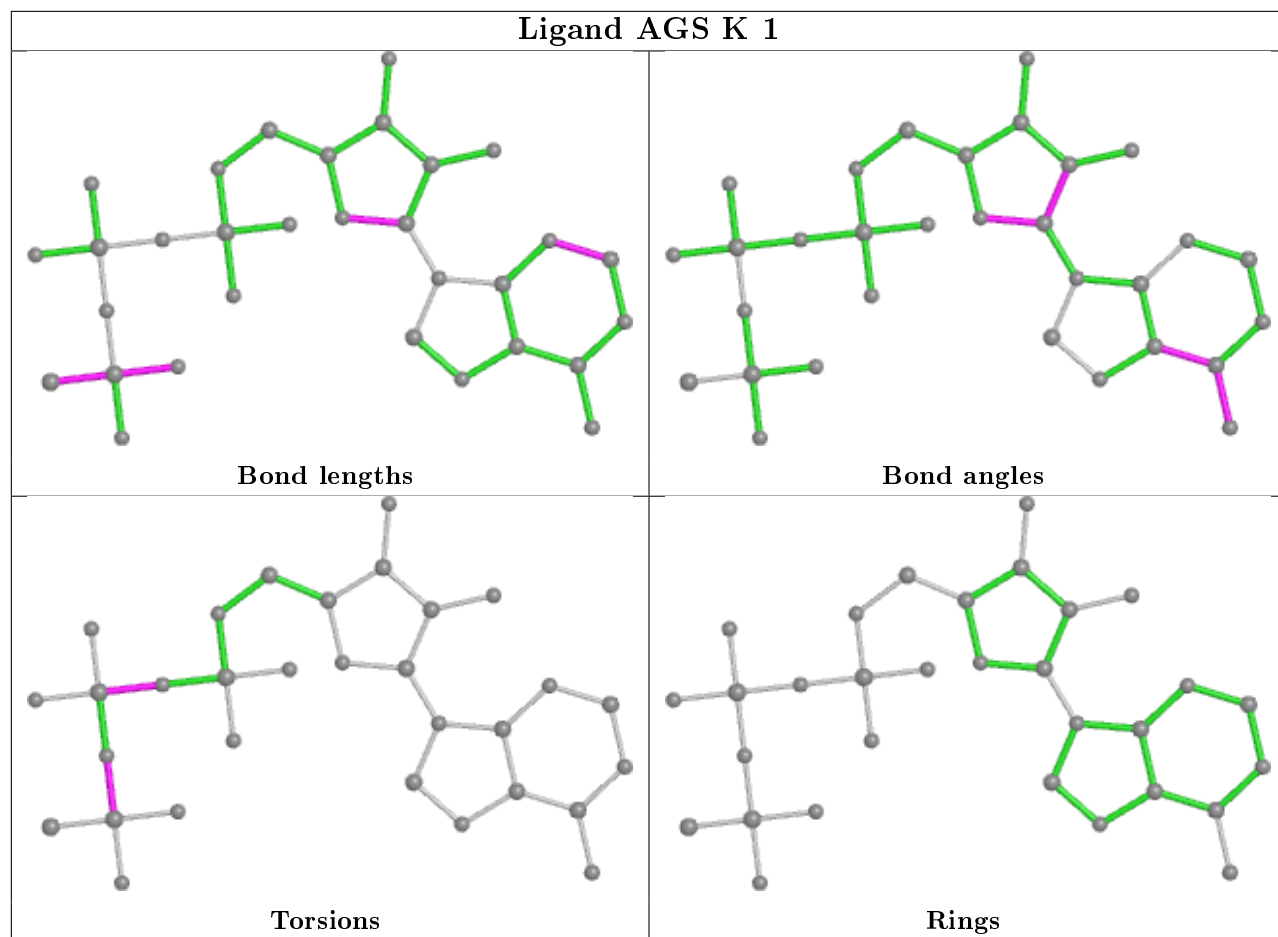
Ligand AGS A 1



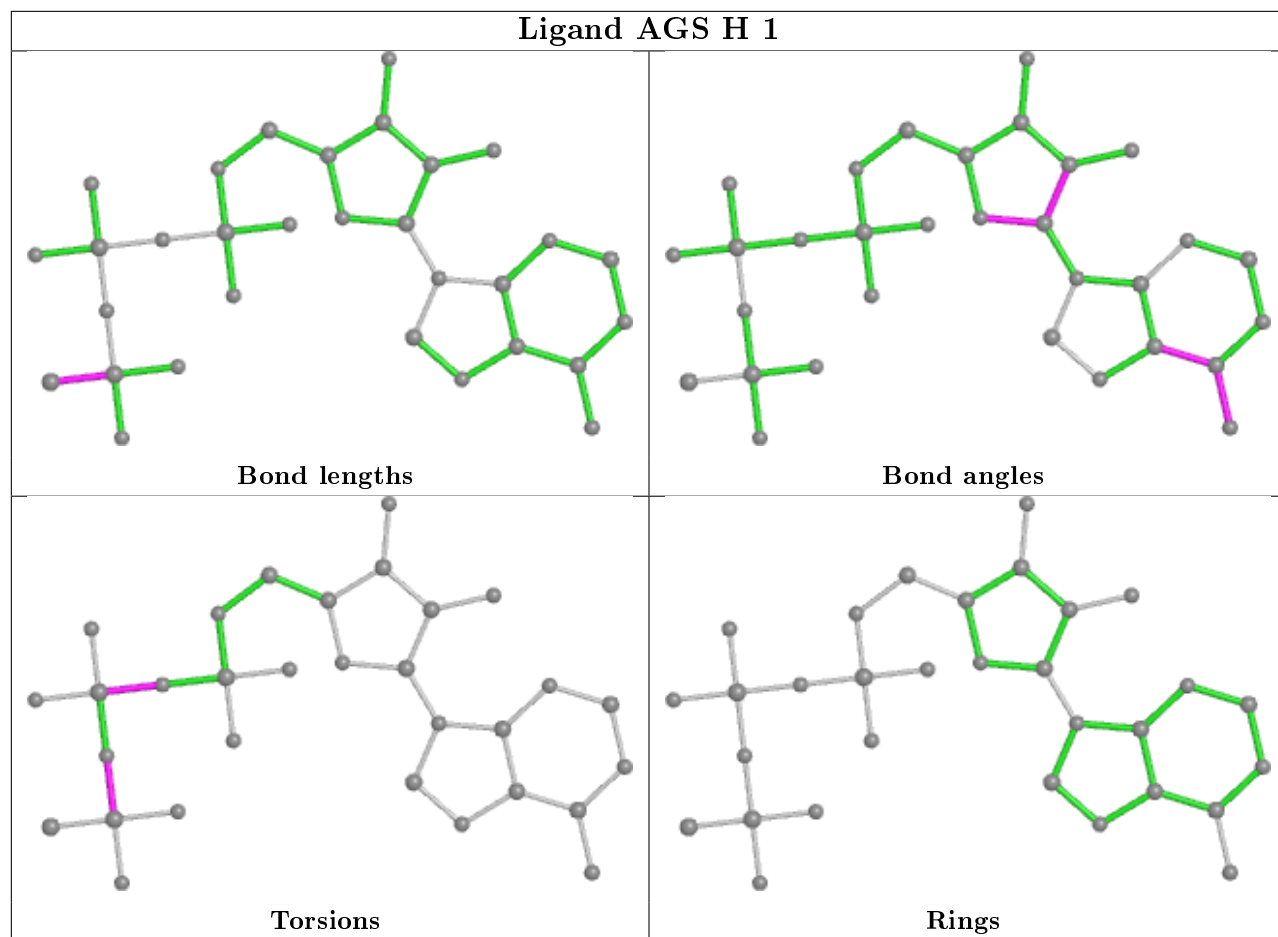
Ligand AGS B 1

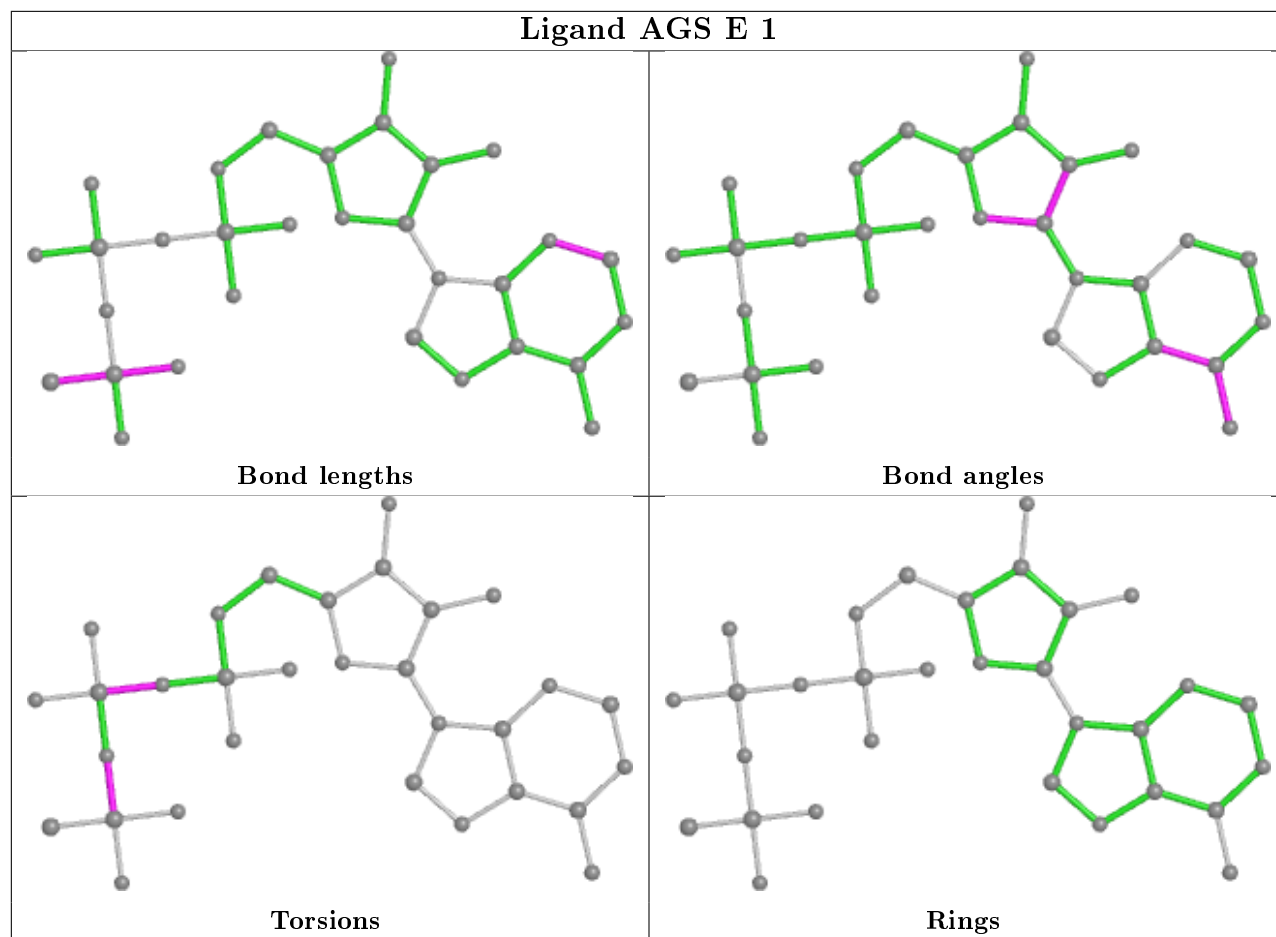


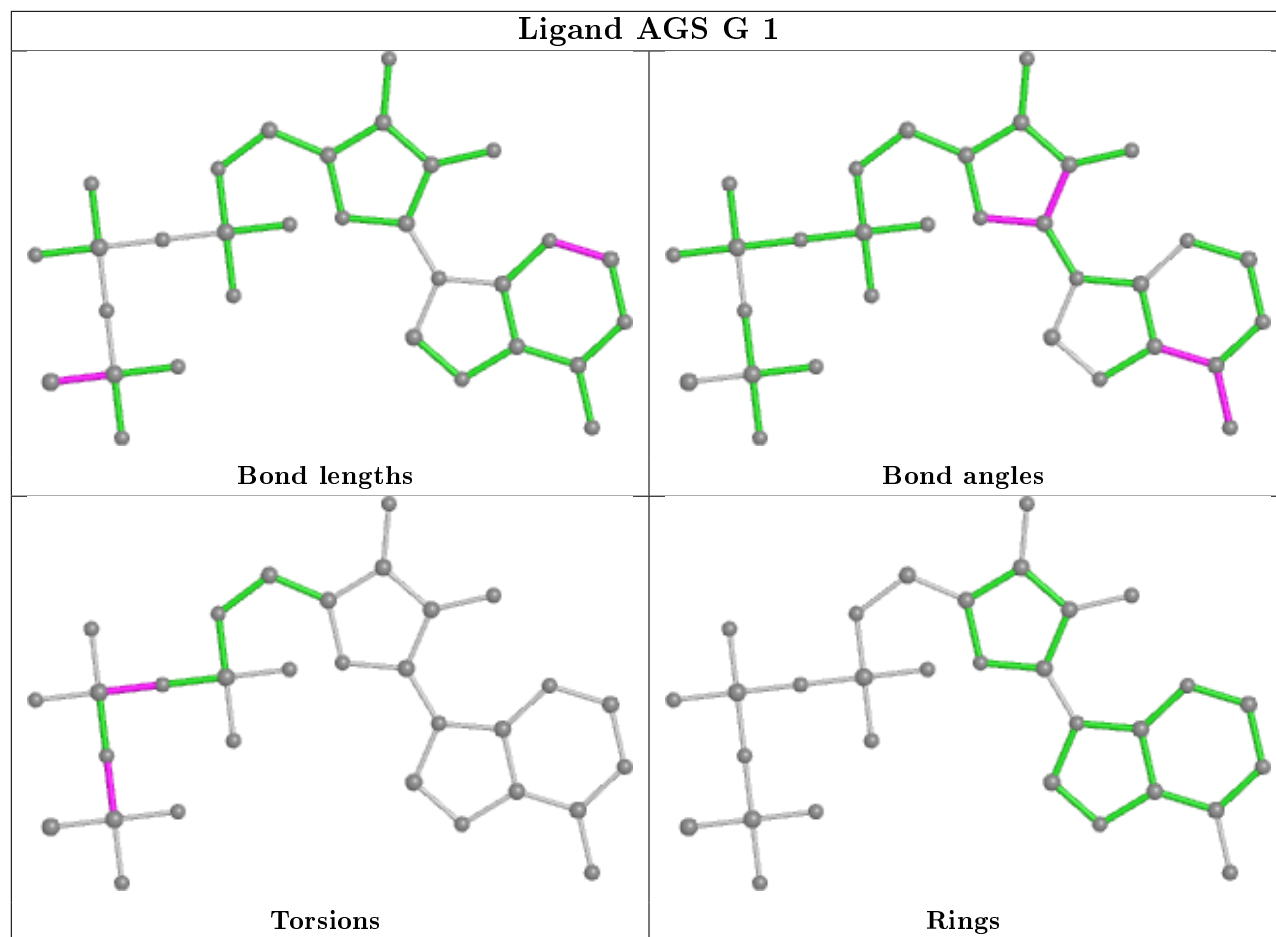
Ligand AGS K 1

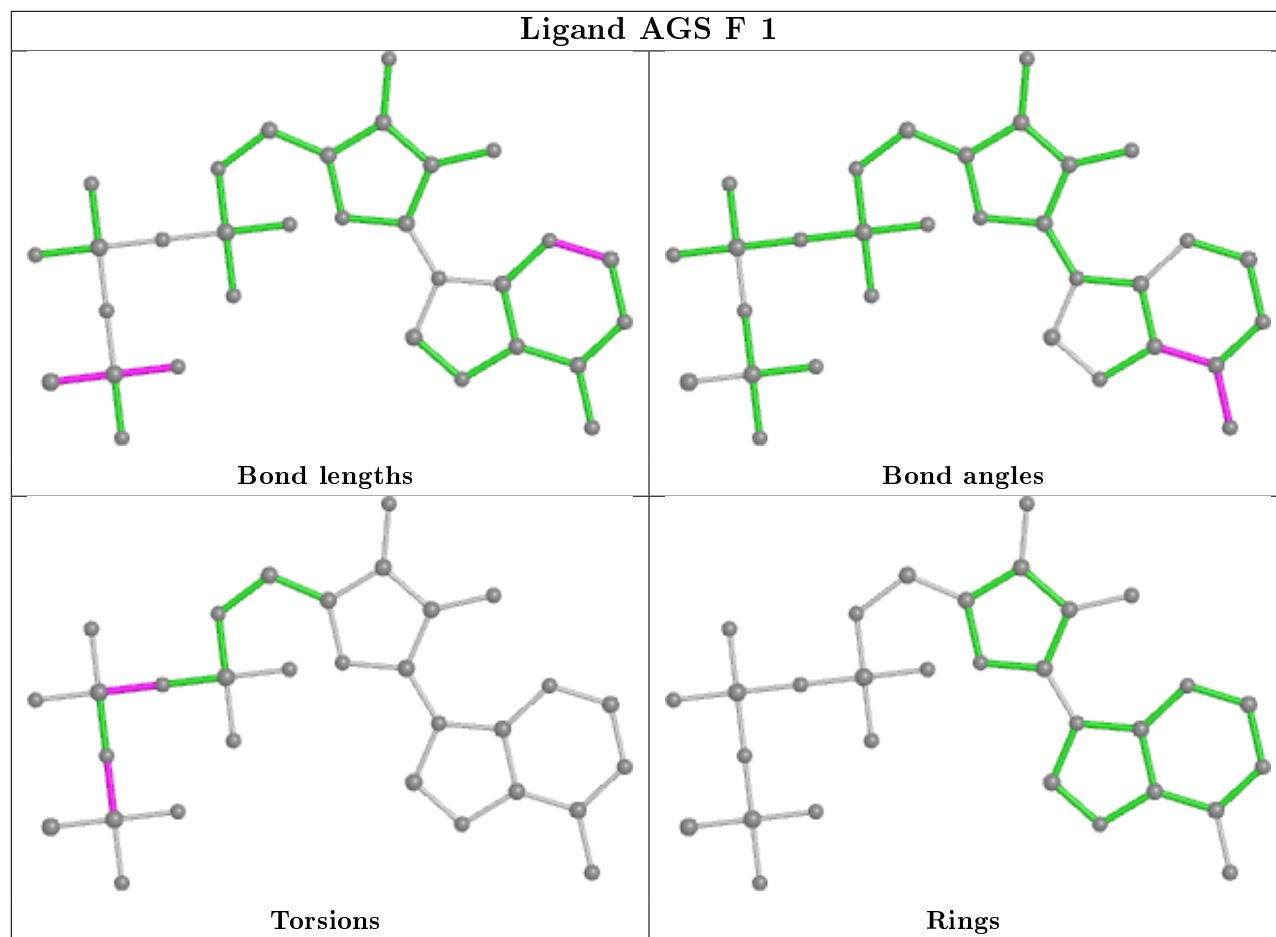


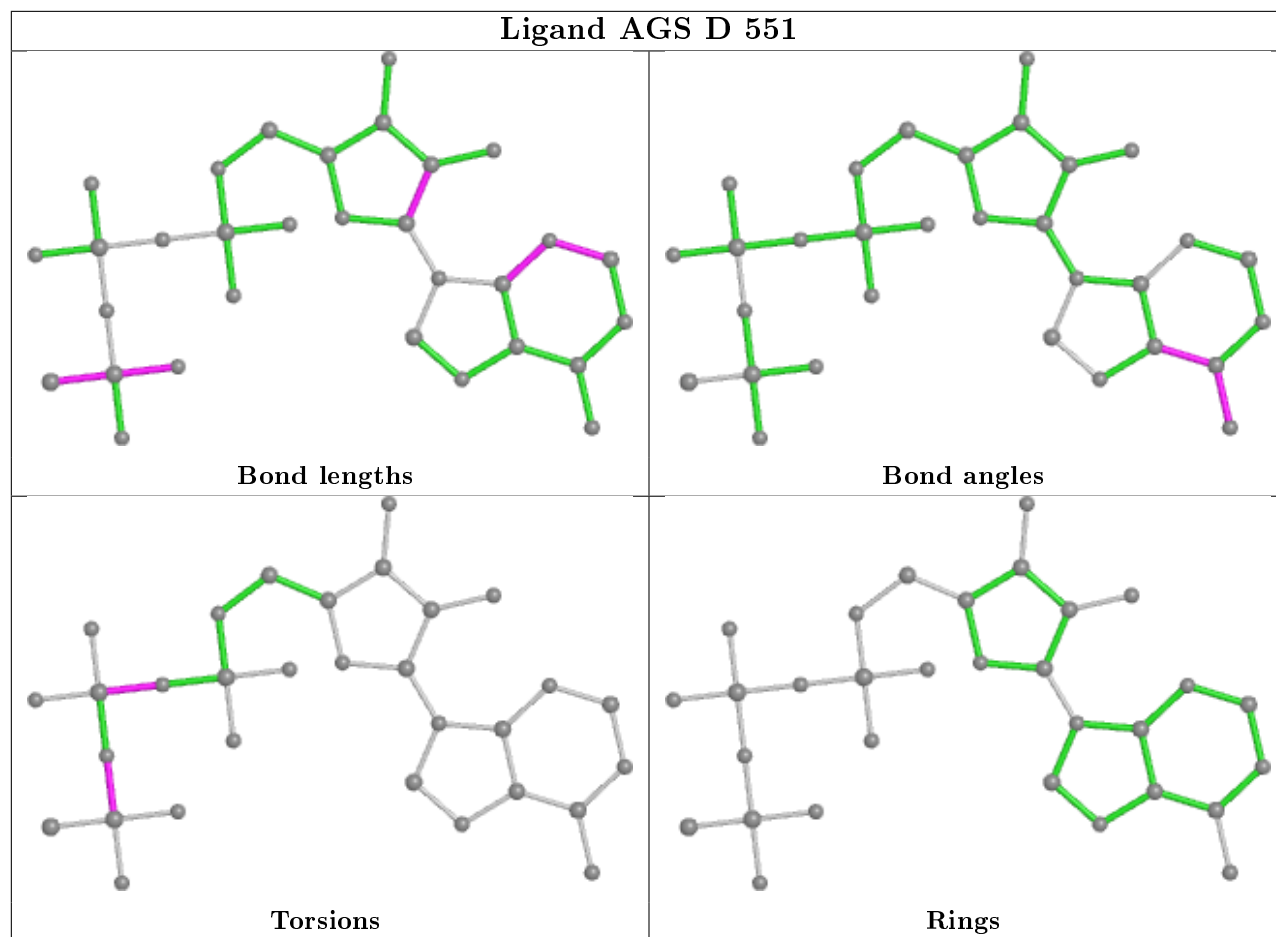
Ligand AGS H 1

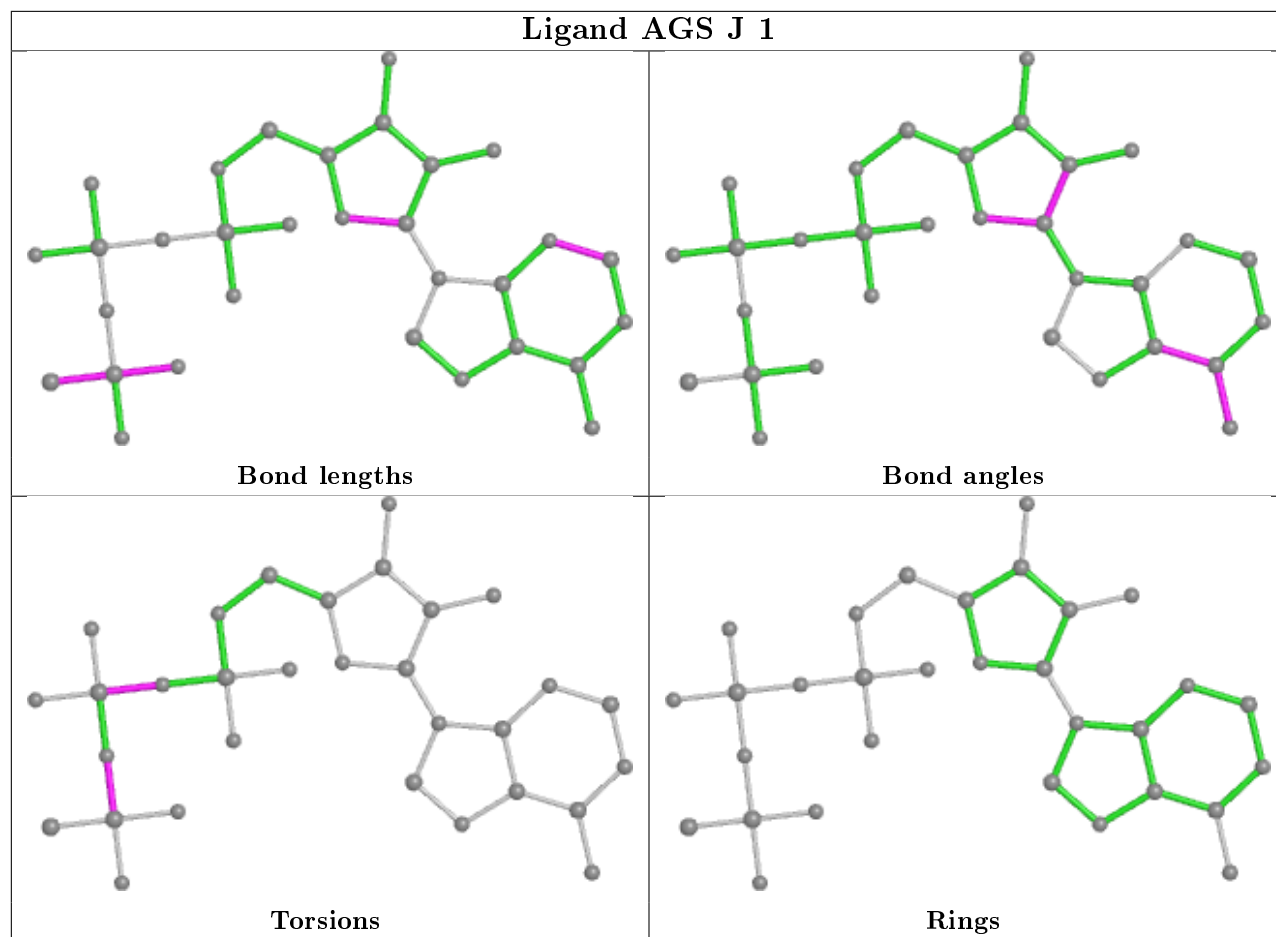




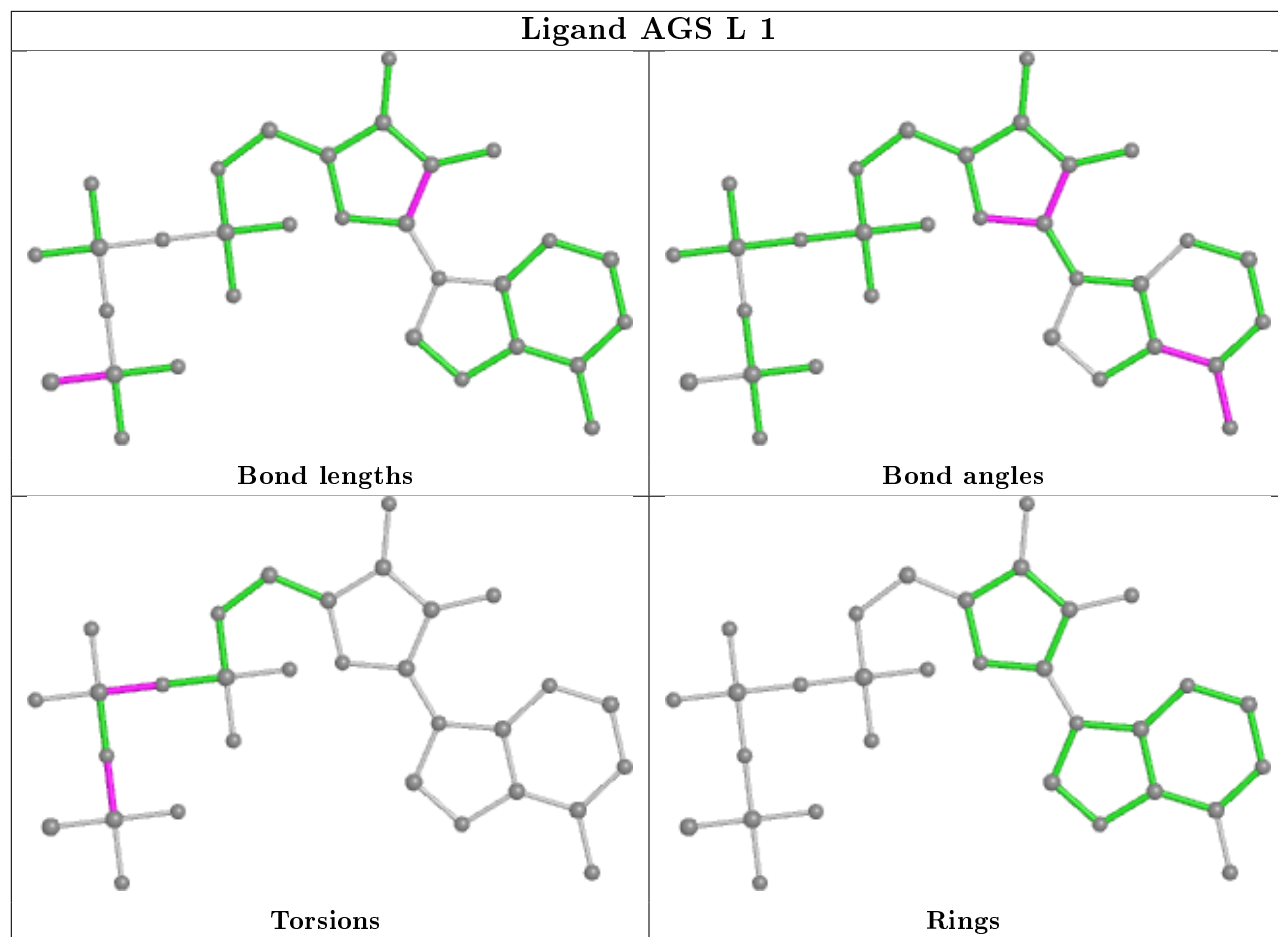


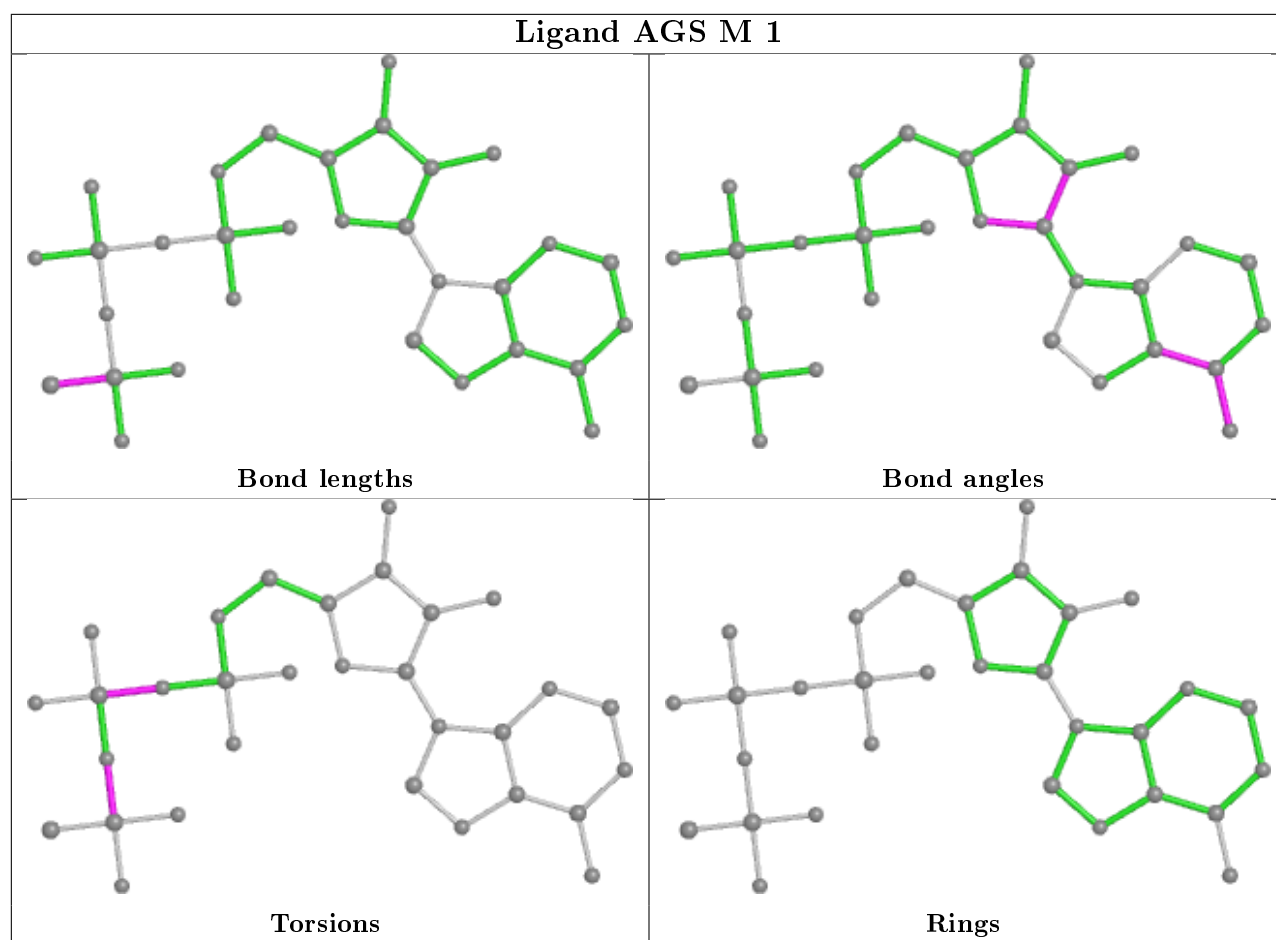






Ligand AGS L 1





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%)	3 3	28, 64, 121, 132	0
1	B	525/547 (95%)	1.34	126 (24%)	0 0	24, 59, 149, 159	0
1	C	525/547 (95%)	1.15	115 (21%)	0 0	29, 71, 141, 152	0
1	D	525/547 (95%)	0.47	31 (5%)	22 21	25, 48, 99, 115	0
1	E	525/547 (95%)	0.99	99 (18%)	1 1	23, 55, 134, 145	0
1	F	525/547 (95%)	1.27	115 (21%)	0 0	27, 66, 150, 159	0
1	G	525/547 (95%)	0.58	43 (8%)	11 11	26, 50, 113, 126	0
1	H	525/547 (95%)	0.64	61 (11%)	4 4	26, 56, 118, 130	0
1	I	525/547 (95%)	0.96	81 (15%)	2 1	31, 69, 132, 143	0
1	J	525/547 (95%)	1.02	89 (16%)	1 1	31, 73, 138, 146	0
1	K	525/547 (95%)	1.43	139 (26%)	0 0	31, 78, 151, 159	0
1	L	525/547 (95%)	0.90	90 (17%)	1 1	29, 66, 136, 149	0
1	M	525/547 (95%)	1.35	136 (25%)	0 0	30, 77, 152, 160	0
1	N	525/547 (95%)	0.71	63 (12%)	4 3	28, 65, 118, 129	0
All	All	7350/7658 (95%)	0.97	1257 (17%)	1 1	23, 60, 140, 160	0

All (1257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ILE	13.6
1	F	309	LEU	12.7
1	K	270	ILE	12.2
1	K	271	VAL	12.0
1	K	305	ILE	11.7
1	B	349	ILE	11.6
1	M	270	ILE	11.5
1	K	349	ILE	11.3

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Mol	Chain	Res	Type	RSRZ
1	F	240	VAL	10.9
1	F	233	MET	10.7
1	J	356	ALA	10.6
1	B	233	MET	10.5
1	E	353	ILE	10.5
1	E	356	ALA	10.4
1	F	353	ILE	10.2
1	M	353	ILE	10.2
1	J	271	VAL	10.2
1	B	356	ALA	10.2
1	I	270	ILE	10.1
1	J	270	ILE	10.0
1	C	356	ALA	10.0
1	L	266	THR	10.0
1	M	259	LEU	9.9
1	K	309	LEU	9.8
1	F	314	LEU	9.7
1	B	230	ILE	9.5
1	M	233	MET	9.5
1	N	349	ILE	9.4
1	K	259	LEU	9.3
1	B	353	ILE	9.3
1	K	260	ALA	9.3
1	E	309	LEU	9.2
1	E	271	VAL	9.2
1	M	237	LEU	9.2
1	J	269	GLY	9.2
1	F	259	LEU	9.1
1	C	270	ILE	9.1
1	K	236	VAL	9.1
1	M	221	LEU	9.0
1	K	237	LEU	8.9
1	C	353	ILE	8.8
1	K	233	MET	8.8
1	M	271	VAL	8.8
1	F	349	ILE	8.7
1	M	223	ALA	8.6
1	J	349	ILE	8.6
1	B	264	VAL	8.5
1	D	271	VAL	8.3
1	M	314	LEU	8.3
1	M	240	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
1	F	270	ILE	8.2
1	K	231	ARG	8.2
1	K	360	TYR	8.1
1	B	301	ILE	8.1
1	I	305	ILE	8.0
1	K	267	MET	8.0
1	J	357	THR	8.0
1	J	268	ARG	8.0
1	B	227	ILE	7.9
1	M	267	MET	7.9
1	I	271	VAL	7.8
1	J	233	MET	7.8
1	B	365	LEU	7.8
1	B	258	ALA	7.7
1	M	309	LEU	7.7
1	K	356	ALA	7.7
1	A	270	ILE	7.7
1	B	281	PHE	7.7
1	F	360	TYR	7.7
1	M	272	LYS	7.7
1	K	264	VAL	7.7
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	K	265	ASN	7.4
1	L	271	VAL	7.4
1	K	203	TYR	7.4
1	M	266	THR	7.3
1	H	309	LEU	7.3
1	M	356	ALA	7.3
1	J	309	LEU	7.3
1	K	268	ARG	7.2
1	A	356	ALA	7.2
1	I	264	VAL	7.2
1	L	270	ILE	7.1
1	K	353	ILE	7.0
1	C	271	VAL	7.0
1	M	239	ALA	6.9
1	A	353	ILE	6.9
1	I	265	ASN	6.9
1	I	356	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	K	340	ALA	6.9
1	E	234	LEU	6.8
1	E	230	ILE	6.8
1	I	268	ARG	6.7
1	E	233	MET	6.7
1	F	227	ILE	6.7
1	N	263	VAL	6.7
1	B	259	LEU	6.7
1	E	349	ILE	6.7
1	M	244	GLY	6.7
1	L	231	ARG	6.7
1	M	264	VAL	6.7
1	J	353	ILE	6.7
1	C	268	ARG	6.7
1	M	358	SER	6.6
1	F	219	PHE	6.6
1	J	44	PHE	6.6
1	F	203	TYR	6.6
1	L	264	VAL	6.6
1	M	273	VAL	6.6
1	M	251	ALA	6.6
1	F	268	ARG	6.6
1	J	317	LEU	6.6
1	F	230	ILE	6.6
1	F	272	LYS	6.5
1	F	357	THR	6.5
1	F	267	MET	6.5
1	B	271	VAL	6.5
1	K	227	ILE	6.5
1	E	223	ALA	6.4
1	J	526	LYS	6.4
1	B	229	ASN	6.4
1	B	257	GLU	6.4
1	F	255	GLU	6.4
1	B	265	ASN	6.4
1	I	349	ILE	6.4
1	B	355	GLU	6.3
1	K	240	VAL	6.3
1	E	268	ARG	6.3
1	N	270	ILE	6.3
1	B	309	LEU	6.3
1	M	204	PHE	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	B	307	MET	6.3
1	G	230	ILE	6.2
1	I	230	ILE	6.2
1	J	266	THR	6.2
1	M	263	VAL	6.2
1	K	204	PHE	6.2
1	L	383	ALA	6.2
1	F	222	LEU	6.2
1	E	270	ILE	6.1
1	K	232	GLU	6.1
1	C	342	ILE	6.1
1	E	305	ILE	6.1
1	L	305	ILE	6.1
1	H	233	MET	6.1
1	I	353	ILE	6.1
1	B	357	THR	6.1
1	K	230	ILE	6.0
1	F	342	ILE	6.0
1	M	305	ILE	6.0
1	F	305	ILE	5.9
1	N	230	ILE	5.9
1	C	263	VAL	5.9
1	B	286	LYS	5.9
1	B	270	ILE	5.9
1	F	237	LEU	5.9
1	N	264	VAL	5.9
1	F	317	LEU	5.8
1	E	300	VAL	5.8
1	F	271	VAL	5.8
1	C	266	THR	5.8
1	F	231	ARG	5.8
1	L	269	GLY	5.8
1	C	249	ILE	5.8
1	J	305	ILE	5.8
1	K	256	GLY	5.8
1	E	357	THR	5.8
1	F	234	LEU	5.7
1	L	230	ILE	5.7
1	K	223	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	M	336	VAL	5.7
1	I	266	THR	5.7
1	G	383	ALA	5.7
1	B	240	VAL	5.7
1	I	352	GLN	5.6
1	M	265	ASN	5.6
1	B	203	TYR	5.6
1	K	219	PHE	5.6
1	L	309	LEU	5.6
1	L	268	ARG	5.6
1	I	526	LYS	5.6
1	B	269	GLY	5.6
1	K	306	GLY	5.6
1	C	369	VAL	5.5
1	L	234	LEU	5.5
1	B	342	ILE	5.5
1	F	389	MET	5.5
1	G	44	PHE	5.5
1	H	270	ILE	5.5
1	C	203	TYR	5.5
1	C	237	LEU	5.5
1	C	259	LEU	5.5
1	K	228	SER	5.5
1	E	312	ALA	5.4
1	J	351	GLN	5.4
1	K	269	GLY	5.4
1	F	245	LYS	5.4
1	I	360	TYR	5.4
1	J	263	VAL	5.4
1	J	358	SER	5.4
1	B	236	VAL	5.4
1	M	249	ILE	5.4
1	E	272	LYS	5.4
1	B	305	ILE	5.4
1	K	188	ASP	5.4
1	M	203	TYR	5.4
1	I	203	TYR	5.3
1	B	251	ALA	5.3
1	B	231	ARG	5.3
1	J	229	ASN	5.3
1	M	365	LEU	5.3
1	M	342	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	K	241	ALA	5.3
1	M	335	GLY	5.3
1	I	272	LYS	5.3
1	E	351	GLN	5.3
1	F	44	PHE	5.2
1	C	365	LEU	5.2
1	E	203	TYR	5.2
1	C	261	THR	5.2
1	C	357	THR	5.2
1	K	234	LEU	5.2
1	G	271	VAL	5.2
1	H	234	LEU	5.2
1	I	234	LEU	5.2
1	F	273	VAL	5.2
1	K	383	ALA	5.2
1	B	351	GLN	5.2
1	F	355	GLU	5.2
1	B	237	LEU	5.2
1	K	272	LYS	5.2
1	C	256	GLY	5.1
1	I	355	GLU	5.1
1	C	295	LEU	5.1
1	L	259	LEU	5.1
1	K	273	VAL	5.1
1	J	219	PHE	5.1
1	I	267	MET	5.1
1	C	230	ILE	5.1
1	H	526	LYS	5.1
1	C	44	PHE	5.1
1	I	231	ARG	5.1
1	M	317	LEU	5.1
1	B	273	VAL	5.1
1	K	44	PHE	5.1
1	B	306	GLY	5.1
1	C	244	GLY	5.1
1	H	243	ALA	5.1
1	F	263	VAL	5.0
1	F	264	VAL	5.0
1	C	304	GLU	5.0
1	K	281	PHE	5.0
1	M	219	PHE	5.0
1	B	234	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	231	ARG	5.0
1	M	260	ALA	5.0
1	M	186	GLU	5.0
1	F	241	ALA	5.0
1	A	44	PHE	5.0
1	A	263	VAL	5.0
1	E	301	ILE	5.0
1	G	270	ILE	5.0
1	C	372	LEU	4.9
1	C	264	VAL	4.9
1	L	258	ALA	4.9
1	H	229	ASN	4.9
1	L	227	ILE	4.9
1	B	262	LEU	4.9
1	A	349	ILE	4.9
1	B	44	PHE	4.9
1	C	333	ILE	4.9
1	B	526	LYS	4.9
1	M	195	PHE	4.9
1	J	265	ASN	4.9
1	D	270	ILE	4.9
1	H	353	ILE	4.9
1	H	356	ALA	4.8
1	K	275	ALA	4.8
1	M	340	ALA	4.8
1	C	360	TYR	4.8
1	D	44	PHE	4.8
1	F	365	LEU	4.8
1	J	281	PHE	4.8
1	H	268	ARG	4.8
1	G	267	MET	4.8
1	I	363	GLU	4.8
1	I	309	LEU	4.8
1	L	317	LEU	4.8
1	K	335	GLY	4.8
1	L	233	MET	4.8
1	B	266	THR	4.8
1	C	362	ARG	4.8
1	D	230	ILE	4.8
1	M	250	ILE	4.8
1	J	256	GLY	4.8
1	K	263	VAL	4.7

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

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Mol	Chain	Res	Type	RSRZ
1	E	273	VAL	4.5
1	B	223	ALA	4.5
1	F	258	ALA	4.5
1	A	357	THR	4.5
1	I	351	GLN	4.4
1	J	262	LEU	4.4
1	C	346	VAL	4.4
1	E	264	VAL	4.4
1	D	526	LYS	4.4
1	E	384	ALA	4.4
1	F	242	LYS	4.4
1	L	255	GLU	4.4
1	M	238	GLU	4.4
1	K	362	ARG	4.4
1	A	271	VAL	4.4
1	B	383	ALA	4.4
1	G	306	GLY	4.4
1	K	283	ASP	4.4
1	E	263	VAL	4.4
1	C	265	ASN	4.4
1	E	265	ASN	4.4
1	B	358	SER	4.4
1	B	363	GLU	4.4
1	L	267	MET	4.4
1	N	281	PHE	4.4
1	B	221	LEU	4.4
1	B	300	VAL	4.4
1	H	383	ALA	4.3
1	F	244	GLY	4.3
1	D	305	ILE	4.3
1	C	350	ARG	4.3
1	K	334	ASP	4.3
1	L	244	GLY	4.3
1	C	284	ARG	4.3
1	M	230	ILE	4.3
1	F	236	VAL	4.3
1	M	231	ARG	4.3
1	A	257	GLU	4.3
1	B	209	GLU	4.3
1	C	355	GLU	4.3
1	J	260	ALA	4.3
1	K	365	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	260	ALA	4.3
1	C	267	MET	4.3
1	M	526	LYS	4.3
1	B	261	THR	4.2
1	C	292	ILE	4.2
1	K	351	GLN	4.2
1	G	264	VAL	4.2
1	B	180	GLY	4.2
1	L	526	LYS	4.2
1	F	266	THR	4.2
1	E	237	LEU	4.2
1	F	249	ILE	4.2
1	F	260	ALA	4.2
1	H	305	ILE	4.2
1	B	304	GLU	4.2
1	J	257	GLU	4.2
1	J	383	ALA	4.2
1	F	224	ASP	4.2
1	E	383	ALA	4.2
1	B	302	SER	4.2
1	F	351	GLN	4.2
1	J	362	ARG	4.1
1	B	225	LYS	4.1
1	F	346	VAL	4.1
1	K	346	VAL	4.1
1	F	228	SER	4.1
1	C	340	ALA	4.1
1	L	314	LEU	4.1
1	M	295	LEU	4.1
1	E	346	VAL	4.1
1	B	354	GLU	4.1
1	C	351	GLN	4.1
1	M	262	LEU	4.1
1	D	268	ARG	4.1
1	C	273	VAL	4.1
1	E	354	GLU	4.1
1	J	360	TYR	4.1
1	M	258	ALA	4.1
1	K	299	THR	4.1
1	F	225	LYS	4.1
1	F	358	SER	4.1
1	F	261	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	311	LYS	4.0
1	M	44	PHE	4.0
1	H	265	ASN	4.0
1	E	240	VAL	4.0
1	I	184	GLN	4.0
1	K	355	GLU	4.0
1	E	360	TYR	4.0
1	L	229	ASN	4.0
1	D	264	VAL	4.0
1	F	369	VAL	4.0
1	I	384	ALA	4.0
1	K	331	THR	4.0
1	A	187	LEU	4.0
1	C	231	ARG	4.0
1	G	268	ARG	4.0
1	J	203	TYR	4.0
1	H	349	ILE	4.0
1	K	332	ILE	4.0
1	I	44	PHE	4.0
1	J	333	ILE	4.0
1	K	350	ARG	4.0
1	H	355	GLU	4.0
1	D	266	THR	3.9
1	B	289	LEU	3.9
1	F	221	LEU	3.9
1	M	161	LEU	3.9
1	I	358	SER	3.9
1	B	244	GLY	3.9
1	F	256	GLY	3.9
1	C	161	LEU	3.9
1	C	526	LYS	3.9
1	N	356	ALA	3.9
1	J	367	GLU	3.9
1	L	311	LYS	3.9
1	K	307	MET	3.9
1	E	295	LEU	3.9
1	B	224	ASP	3.9
1	M	307	MET	3.9
1	I	269	GLY	3.9
1	J	355	GLU	3.9
1	M	180	GLY	3.9
1	B	293	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	361	ASP	3.8
1	G	229	ASN	3.8
1	F	265	ASN	3.8
1	K	258	ALA	3.8
1	J	267	MET	3.8
1	B	219	PHE	3.8
1	C	286	LYS	3.8
1	L	44	PHE	3.8
1	E	255	GLU	3.8
1	K	301	ILE	3.8
1	M	160	LYS	3.8
1	C	309	LEU	3.8
1	M	347	ALA	3.8
1	C	181	THR	3.8
1	E	257	GLU	3.8
1	J	365	LEU	3.8
1	M	350	ARG	3.8
1	B	282	GLY	3.8
1	C	219	PHE	3.8
1	E	242	LYS	3.8
1	I	211	GLY	3.8
1	M	269	GLY	3.8
1	G	233	MET	3.8
1	L	224	ASP	3.8
1	K	181	THR	3.7
1	G	182	GLY	3.7
1	F	381	VAL	3.7
1	K	274	ALA	3.7
1	G	325	ILE	3.7
1	J	342	ILE	3.7
1	K	372	LEU	3.7
1	H	264	VAL	3.7
1	K	369	VAL	3.7
1	M	301	ILE	3.7
1	H	346	VAL	3.7
1	J	381	VAL	3.7
1	F	214	GLU	3.7
1	A	261	THR	3.7
1	F	181	THR	3.7
1	G	266	THR	3.7
1	K	266	THR	3.7
1	K	250	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	333	ILE	3.6
1	E	345	ARG	3.6
1	C	347	ALA	3.6
1	K	304	GLU	3.6
1	L	239	ALA	3.6
1	N	256	GLY	3.6
1	B	314	LEU	3.6
1	M	261	THR	3.6
1	B	191	GLU	3.6
1	C	229	ASN	3.6
1	J	319	GLN	3.6
1	K	276	VAL	3.6
1	I	204	PHE	3.6
1	B	241	ALA	3.6
1	F	248	LEU	3.6
1	I	237	LEU	3.6
1	J	272	LYS	3.6
1	K	311	LYS	3.6
1	F	396	VAL	3.6
1	A	183	LEU	3.6
1	G	262	LEU	3.6
1	A	265	ASN	3.6
1	J	280	GLY	3.6
1	L	219	PHE	3.5
1	L	186	GLU	3.5
1	K	222	LEU	3.5
1	F	178	GLU	3.5
1	F	232	GLU	3.5
1	J	243	ALA	3.5
1	L	353	ILE	3.5
1	H	266	THR	3.5
1	B	238	GLU	3.5
1	M	236	VAL	3.5
1	N	258	ALA	3.5
1	E	220	ILE	3.5
1	J	273	VAL	3.5
1	L	185	ASP	3.5
1	M	254	VAL	3.5
1	A	231	ARG	3.5
1	A	237	LEU	3.5
1	F	340	ALA	3.5
1	H	242	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	204	PHE	3.5
1	C	281	PHE	3.5
1	H	259	LEU	3.5
1	B	275	ALA	3.5
1	I	369	VAL	3.5
1	A	203	TYR	3.5
1	L	228	SER	3.5
1	M	188	ASP	3.4
1	M	286	LYS	3.4
1	F	251	ALA	3.4
1	K	215	LEU	3.4
1	M	383	ALA	3.4
1	B	298	GLY	3.4
1	K	345	ARG	3.4
1	K	213	VAL	3.4
1	K	352	GLN	3.4
1	N	266	THR	3.4
1	L	349	ILE	3.4
1	M	384	ALA	3.4
1	N	526	LYS	3.4
1	F	372	LEU	3.4
1	L	247	LEU	3.4
1	K	310	GLU	3.4
1	B	360	TYR	3.4
1	F	337	GLY	3.4
1	M	168	LYS	3.4
1	F	215	LEU	3.4
1	J	261	THR	3.4
1	K	191	GLU	3.4
1	E	284	ARG	3.4
1	I	258	ALA	3.4
1	K	152	ALA	3.4
1	M	235	PRO	3.4
1	E	215	LEU	3.4
1	L	222	LEU	3.4
1	C	300	VAL	3.4
1	F	300	VAL	3.4
1	I	240	VAL	3.4
1	I	263	VAL	3.4
1	M	346	VAL	3.4
1	N	363	GLU	3.4
1	M	389	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	223	ALA	3.3
1	M	354	GLU	3.3
1	C	332	ILE	3.3
1	N	365	LEU	3.3
1	F	180	GLY	3.3
1	A	284	ARG	3.3
1	B	263	VAL	3.3
1	N	44	PHE	3.3
1	D	325	ILE	3.3
1	B	222	LEU	3.3
1	M	217	SER	3.3
1	A	276	VAL	3.3
1	A	381	VAL	3.3
1	C	186	GLU	3.3
1	L	307	MET	3.3
1	C	212	ALA	3.3
1	K	243	ALA	3.3
1	L	275	ALA	3.3
1	A	266	THR	3.3
1	G	181	THR	3.3
1	B	249	ILE	3.3
1	K	221	LEU	3.3
1	E	267	MET	3.3
1	N	231	ARG	3.3
1	H	360	TYR	3.3
1	K	224	ASP	3.3
1	D	281	PHE	3.3
1	C	322	ARG	3.3
1	L	310	GLU	3.3
1	M	229	ASN	3.3
1	H	361	ASP	3.3
1	C	319	GLN	3.3
1	C	358	SER	3.3
1	H	358	SER	3.3
1	K	245	LYS	3.3
1	A	204	PHE	3.3
1	E	219	PHE	3.3
1	K	342	ILE	3.3
1	B	525	PRO	3.3
1	E	229	ASN	3.3
1	K	202	PRO	3.3
1	C	240	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	263	VAL	3.3
1	M	320	ALA	3.3
1	A	188	ASP	3.2
1	C	306	GLY	3.2
1	I	245	LYS	3.2
1	M	343	GLN	3.2
1	J	363	GLU	3.2
1	M	322	ARG	3.2
1	A	365	LEU	3.2
1	J	354	GLU	3.2
1	K	376	VAL	3.2
1	C	242	LYS	3.2
1	J	248	LEU	3.2
1	I	340	ALA	3.2
1	M	300	VAL	3.2
1	J	242	LYS	3.2
1	K	297	GLY	3.2
1	M	360	TYR	3.2
1	I	259	LEU	3.2
1	E	304	GLU	3.2
1	F	361	ASP	3.2
1	A	355	GLU	3.2
1	F	186	GLU	3.2
1	K	214	GLU	3.2
1	K	255	GLU	3.2
1	I	215	LEU	3.2
1	B	346	VAL	3.2
1	D	231	ARG	3.2
1	F	322	ARG	3.2
1	K	242	LYS	3.2
1	L	272	LYS	3.2
1	C	272	LYS	3.1
1	A	304	GLU	3.1
1	A	363	GLU	3.1
1	E	342	ILE	3.1
1	H	230	ILE	3.1
1	L	324	VAL	3.1
1	H	351	GLN	3.1
1	L	206	ASN	3.1
1	F	354	GLU	3.1
1	A	260	ALA	3.1
1	N	203	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	361	ASP	3.1
1	D	236	VAL	3.1
1	K	288	MET	3.1
1	K	300	VAL	3.1
1	N	362	ARG	3.1
1	D	383	ALA	3.1
1	I	383	ALA	3.1
1	B	256	GLY	3.1
1	M	224	ASP	3.1
1	M	181	THR	3.1
1	B	187	LEU	3.1
1	G	305	ILE	3.1
1	K	139	SER	3.1
1	A	264	VAL	3.1
1	J	240	VAL	3.1
1	L	381	VAL	3.1
1	C	260	ALA	3.1
1	B	284	ARG	3.1
1	C	363	GLU	3.1
1	G	257	GLU	3.1
1	L	382	GLY	3.1
1	B	215	LEU	3.1
1	F	161	LEU	3.1
1	D	323	VAL	3.1
1	G	311	LYS	3.1
1	F	384	ALA	3.1
1	N	357	THR	3.1
1	B	352	GLN	3.1
1	E	184	GLN	3.1
1	A	384	ALA	3.0
1	E	382	GLY	3.0
1	F	352	GLN	3.0
1	K	257	GLU	3.0
1	K	308	GLU	3.0
1	M	247	LEU	3.0
1	E	292	ILE	3.0
1	F	332	ILE	3.0
1	N	325	ILE	3.0
1	M	304	GLU	3.0
1	L	302	SER	3.0
1	B	267	MET	3.0
1	E	526	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	180	GLY	3.0
1	C	247	LEU	3.0
1	C	317	LEU	3.0
1	I	336	VAL	3.0
1	K	320	ALA	3.0
1	M	323	VAL	3.0
1	G	231	ARG	3.0
1	A	181	THR	3.0
1	A	388	GLU	3.0
1	C	315	GLU	3.0
1	J	234	LEU	3.0
1	K	361	ASP	3.0
1	A	382	GLY	3.0
1	D	269	GLY	3.0
1	N	351	GLN	3.0
1	C	341	ALA	3.0
1	N	257	GLU	3.0
1	A	273	VAL	3.0
1	A	281	PHE	3.0
1	E	236	VAL	3.0
1	L	249	ILE	3.0
1	L	265	ASN	3.0
1	F	155	ASP	3.0
1	K	380	LYS	3.0
1	H	304	GLU	3.0
1	B	248	LEU	3.0
1	F	295	LEU	3.0
1	F	347	ALA	3.0
1	K	312	ALA	3.0
1	K	381	VAL	2.9
1	M	369	VAL	2.9
1	F	204	PHE	2.9
1	F	362	ARG	2.9
1	D	267	MET	2.9
1	N	354	GLU	2.9
1	F	319	GLN	2.9
1	E	258	ALA	2.9
1	K	341	ALA	2.9
1	A	245	LYS	2.9
1	I	310	GLU	2.9
1	M	216	GLU	2.9
1	B	313	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	325	ILE	2.9
1	I	302	SER	2.9
1	H	286	LYS	2.9
1	H	363	GLU	2.9
1	C	222	LEU	2.9
1	B	254	VAL	2.9
1	D	229	ASN	2.9
1	B	188	ASP	2.9
1	L	161	LEU	2.9
1	M	299	THR	2.9
1	B	390	LYS	2.9
1	F	238	GLU	2.9
1	H	300	VAL	2.9
1	N	284	ARG	2.9
1	E	224	ASP	2.9
1	E	274	ALA	2.9
1	M	243	ALA	2.9
1	B	255	GLU	2.9
1	I	257	GLU	2.9
1	C	220	ILE	2.9
1	M	363	GLU	2.9
1	H	269	GLY	2.9
1	G	243	ALA	2.9
1	G	234	LEU	2.9
1	C	172	GLU	2.9
1	L	308	GLU	2.9
1	C	301	ILE	2.8
1	C	305	ILE	2.8
1	J	184	GLN	2.8
1	M	308	GLU	2.8
1	H	314	LEU	2.8
1	I	314	LEU	2.8
1	K	323	VAL	2.8
1	L	240	VAL	2.8
1	M	182	GLY	2.8
1	B	332	ILE	2.8
1	J	250	ILE	2.8
1	F	223	ALA	2.8
1	C	221	LEU	2.8
1	G	269	GLY	2.8
1	C	226	LYS	2.8
1	N	346	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	369	VAL	2.8
1	L	325	ILE	2.8
1	F	385	THR	2.8
1	B	252	GLU	2.8
1	I	365	LEU	2.8
1	K	317	LEU	2.8
1	C	352	GLN	2.8
1	A	362	ARG	2.8
1	G	384	ALA	2.8
1	M	362	ARG	2.8
1	K	526	LYS	2.8
1	E	307	MET	2.8
1	E	188	ASP	2.8
1	I	229	ASN	2.8
1	I	361	ASP	2.8
1	N	265	ASN	2.8
1	N	360	TYR	2.8
1	H	271	VAL	2.8
1	K	164	GLU	2.8
1	N	304	GLU	2.8
1	C	250	ILE	2.8
1	K	205	ILE	2.8
1	D	203	TYR	2.8
1	H	365	LEU	2.8
1	L	336	VAL	2.7
1	L	304	GLU	2.7
1	B	228	SER	2.7
1	B	183	LEU	2.7
1	C	334	ASP	2.7
1	N	309	LEU	2.7
1	B	274	ALA	2.7
1	E	251	ALA	2.7
1	B	348	GLN	2.7
1	C	336	VAL	2.7
1	B	280	GLY	2.7
1	I	284	ARG	2.7
1	M	193	MET	2.7
1	A	301	ILE	2.7
1	E	250	ILE	2.7
1	M	220	ILE	2.7
1	N	283	ASP	2.7
1	A	209	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	184	GLN	2.7
1	B	336	VAL	2.7
1	C	299	THR	2.7
1	K	220	ILE	2.7
1	L	184	GLN	2.7
1	M	319	GLN	2.7
1	B	350	ARG	2.7
1	I	260	ALA	2.7
1	A	295	LEU	2.7
1	A	346	VAL	2.7
1	H	315	GLU	2.7
1	B	272	LYS	2.7
1	K	325	ILE	2.7
1	L	333	ILE	2.7
1	C	269	GLY	2.7
1	C	367	GLU	2.7
1	I	209	GLU	2.7
1	D	262	LEU	2.7
1	H	237	LEU	2.7
1	M	248	LEU	2.7
1	M	205	ILE	2.7
1	J	303	GLU	2.7
1	M	279	PRO	2.7
1	N	241	ALA	2.7
1	L	284	ARG	2.7
1	I	389	MET	2.7
1	K	295	LEU	2.7
1	E	232	GLU	2.6
1	N	311	LYS	2.6
1	B	205	ILE	2.6
1	I	250	ILE	2.6
1	J	301	ILE	2.6
1	N	353	ILE	2.6
1	I	304	GLU	2.6
1	L	315	GLU	2.6
1	G	314	LEU	2.6
1	M	234	LEU	2.6
1	N	382	GLY	2.6
1	A	250	ILE	2.6
1	E	249	ILE	2.6
1	F	250	ILE	2.6
1	B	186	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	313	THR	2.6
1	F	343	GLN	2.6
1	K	253	ASP	2.6
1	E	339	GLU	2.6
1	J	177	VAL	2.6
1	L	273	VAL	2.6
1	L	462	PRO	2.6
1	M	315	GLU	2.6
1	I	286	LYS	2.6
1	A	305	ILE	2.6
1	F	350	ARG	2.6
1	H	297	GLY	2.6
1	H	335	GLY	2.6
1	I	256	GLY	2.6
1	C	248	LEU	2.6
1	G	309	LEU	2.6
1	H	317	LEU	2.6
1	L	232	GLU	2.6
1	A	256	GLY	2.6
1	E	381	VAL	2.6
1	B	322	ARG	2.6
1	D	257	GLU	2.6
1	I	301	ILE	2.6
1	N	267	MET	2.6
1	E	318	GLY	2.6
1	C	354	GLU	2.6
1	J	232	GLU	2.6
1	A	259	LEU	2.6
1	A	242	LYS	2.5
1	E	361	ASP	2.5
1	M	215	LEU	2.6
1	A	300	VAL	2.5
1	M	376	VAL	2.5
1	I	154	SER	2.5
1	C	209	GLU	2.5
1	F	281	PHE	2.5
1	C	215	LEU	2.5
1	L	200	LEU	2.5
1	L	262	LEU	2.5
1	M	183	LEU	2.5
1	B	381	VAL	2.5
1	C	85	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	254	VAL	2.5
1	M	256	GLY	2.5
1	E	352	GLN	2.5
1	M	184	GLN	2.5
1	D	234	LEU	2.5
1	E	317	LEU	2.5
1	M	200	LEU	2.5
1	D	382	GLY	2.5
1	H	261	THR	2.5
1	C	391	GLU	2.5
1	E	214	GLU	2.5
1	J	304	GLU	2.5
1	C	160	LYS	2.5
1	K	180	GLY	2.5
1	E	261	THR	2.5
1	G	261	THR	2.5
1	J	288	MET	2.5
1	J	387	VAL	2.5
1	B	303	GLU	2.5
1	B	335	GLY	2.5
1	F	359	ASP	2.5
1	B	239	ALA	2.5
1	F	239	ALA	2.5
1	F	339	GLU	2.5
1	J	275	ALA	2.5
1	H	245	LYS	2.5
1	H	284	ARG	2.5
1	N	268	ARG	2.5
1	C	217	SER	2.5
1	C	337	GLY	2.5
1	F	363	GLU	2.5
1	M	298	GLY	2.5
1	N	305	ILE	2.5
1	K	321	LYS	2.5
1	J	384	ALA	2.5
1	L	281	PHE	2.5
1	I	183	LEU	2.4
1	K	248	LEU	2.4
1	M	330	THR	2.4
1	B	367	GLU	2.4
1	J	334	ASP	2.4
1	L	283	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	361	ASP	2.4
1	J	152	ALA	2.4
1	N	260	ALA	2.4
1	J	181	THR	2.4
1	K	284	ARG	2.4
1	I	372	LEU	2.4
1	M	232	GLU	2.4
1	G	283	ASP	2.4
1	G	236	VAL	2.4
1	F	285	ARG	2.4
1	J	332	ILE	2.4
1	K	333	ILE	2.4
1	L	351	GLN	2.4
1	E	299	THR	2.4
1	H	313	THR	2.4
1	K	261	THR	2.4
1	M	311	LYS	2.4
1	E	365	LEU	2.4
1	G	221	LEU	2.4
1	H	306	GLY	2.4
1	L	306	GLY	2.4
1	M	159	GLY	2.4
1	H	236	VAL	2.4
1	I	276	VAL	2.4
1	B	308	GLU	2.4
1	C	214	GLU	2.4
1	A	286	LYS	2.4
1	M	316	ASP	2.4
1	K	175	ILE	2.4
1	J	228	SER	2.4
1	A	354	GLU	2.4
1	B	344	GLY	2.4
1	E	338	GLU	2.4
1	L	215	LEU	2.4
1	K	364	LYS	2.4
1	C	155	ASP	2.4
1	M	185	ASP	2.4
1	F	333	ILE	2.4
1	J	302	SER	2.4
1	M	302	SER	2.4
1	M	310	GLU	2.4
1	M	329	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	184	GLN	2.4
1	D	284	ARG	2.4
1	G	382	GLY	2.4
1	I	362	ARG	2.4
1	L	204	PHE	2.4
1	N	259	LEU	2.4
1	N	317	LEU	2.4
1	M	324	VAL	2.4
1	M	164	GLU	2.4
1	I	288	MET	2.4
1	L	384	ALA	2.4
1	B	285	ARG	2.4
1	C	184	GLN	2.4
1	F	157	THR	2.4
1	H	272	LYS	2.4
1	L	361	ASP	2.4
1	E	289	LEU	2.3
1	J	215	LEU	2.3
1	K	161	LEU	2.3
1	K	326	ASN	2.3
1	C	168	LYS	2.3
1	E	225	LYS	2.3
1	L	256	GLY	2.3
1	I	334	ASP	2.3
1	I	354	GLU	2.3
1	L	332	ILE	2.3
1	J	245	LYS	2.3
1	K	290	GLN	2.3
1	N	350	ARG	2.3
1	C	236	VAL	2.3
1	M	381	VAL	2.3
1	B	310	GLU	2.3
1	K	249	ILE	2.3
1	A	360	TYR	2.3
1	B	204	PHE	2.3
1	B	247	LEU	2.3
1	J	200	LEU	2.3
1	M	187	LEU	2.3
1	N	161	LEU	2.3
1	N	314	LEU	2.3
1	I	346	VAL	2.3
1	N	77	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	287	ALA	2.3
1	E	286	LYS	2.3
1	E	287	ALA	2.3
1	C	325	ILE	2.3
1	H	333	ILE	2.3
1	J	150	ILE	2.3
1	L	257	GLU	2.3
1	M	325	ILE	2.3
1	E	168	LYS	2.3
1	I	364	LYS	2.3
1	L	237	LEU	2.3
1	N	358	SER	2.3
1	E	341	ALA	2.3
1	H	273	VAL	2.3
1	J	274	ALA	2.3
1	N	240	VAL	2.3
1	M	191	GLU	2.3
1	A	322	ARG	2.3
1	B	389	MET	2.3
1	F	288	MET	2.3
1	K	239	ALA	2.3
1	L	347	ALA	2.3
1	I	300	VAL	2.3
1	G	244	GLY	2.3
1	B	292	ILE	2.3
1	H	339	GLU	2.3
1	A	288	MET	2.2
1	A	311	LYS	2.2
1	E	222	LEU	2.2
1	F	321	LYS	2.2
1	G	295	LEU	2.2
1	K	371	LYS	2.2
1	N	275	ALA	2.2
1	N	224	ASP	2.2
1	A	351	GLN	2.2
1	K	184	GLN	2.2
1	K	322	ARG	2.2
1	M	388	GLU	2.2
1	N	255	GLU	2.2
1	E	256	GLY	2.2
1	A	359	ASP	2.2
1	I	359	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	2.2
1	C	275	ALA	2.2
1	M	274	ALA	2.2
1	N	383	ALA	2.2
1	F	257	GLU	2.2
1	K	367	GLU	2.2
1	K	386	GLU	2.2
1	N	186	GLU	2.2
1	B	369	VAL	2.2
1	C	290	GLN	2.2
1	C	378	VAL	2.2
1	E	350	ARG	2.2
1	J	345	ARG	2.2
1	N	273	VAL	2.2
1	K	229	ASN	2.2
1	D	233	MET	2.2
1	E	193	MET	2.2
1	H	231	ARG	2.2
1	K	278	ALA	2.2
1	K	319	GLN	2.2
1	K	366	GLN	2.2
1	A	262	LEU	2.2
1	C	234	LEU	2.2
1	K	183	LEU	2.2
1	C	201	SER	2.2
1	F	213	VAL	2.2
1	E	334	ASP	2.2
1	E	238	GLU	2.2
1	E	363	GLU	2.2
1	B	288	MET	2.2
1	E	288	MET	2.2
1	I	193	MET	2.2
1	L	225	LYS	2.2
1	D	181	THR	2.2
1	J	325	ILE	2.2
1	A	244	GLY	2.2
1	D	314	LEU	2.2
1	F	183	LEU	2.2
1	I	317	LEU	2.2
1	G	228	SER	2.2
1	L	201	SER	2.2
1	F	310	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	184	GLN	2.2
1	G	326	ASN	2.2
1	C	258	ALA	2.2
1	E	227	ILE	2.2
1	F	297	GLY	2.2
1	K	363	GLU	2.2
1	L	355	GLU	2.2
1	H	332	ILE	2.2
1	A	526	LYS	2.2
1	F	160	LYS	2.2
1	I	311	LYS	2.2
1	J	395	ARG	2.2
1	N	242	LYS	2.2
1	H	319	GLN	2.2
1	G	263	VAL	2.2
1	J	376	VAL	2.2
1	L	190	VAL	2.2
1	L	236	VAL	2.2
1	M	281	PHE	2.2
1	A	339	GLU	2.2
1	C	216	GLU	2.2
1	K	186	GLU	2.2
1	N	391	GLU	2.2
1	B	181	THR	2.2
1	B	297	GLY	2.2
1	J	244	GLY	2.2
1	M	294	THR	2.2
1	M	306	GLY	2.2
1	I	228	SER	2.2
1	J	284	ARG	2.2
1	J	221	LEU	2.1
1	A	236	VAL	2.1
1	A	240	VAL	2.1
1	J	369	VAL	2.1
1	C	188	ASP	2.1
1	D	188	ASP	2.1
1	A	350	ARG	2.1
1	C	348	GLN	2.1
1	C	303	GLU	2.1
1	L	289	LEU	2.1
1	L	372	LEU	2.1
1	A	207	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	245	LYS	2.1
1	I	236	VAL	2.1
1	L	213	VAL	2.1
1	A	267	MET	2.1
1	E	43	SER	2.1
1	B	331	THR	2.1
1	C	178	GLU	2.1
1	E	239	ALA	2.1
1	I	341	ALA	2.1
1	J	223	ALA	2.1
1	L	212	ALA	2.1
1	E	160	LYS	2.1
1	K	168	LYS	2.1
1	G	220	ILE	2.1
1	I	248	LEU	2.1
1	J	259	LEU	2.1
1	H	257	GLU	2.1
1	N	228	SER	2.1
1	F	364	LYS	2.1
1	F	316	ASP	2.1
1	E	366	GLN	2.1
1	K	292	ILE	2.1
1	E	372	LEU	2.1
1	N	134	LEU	2.1
1	K	254	VAL	2.1
1	L	369	VAL	2.1
1	C	210	THR	2.1
1	F	313	THR	2.1
1	D	253	ASP	2.1
1	B	290	GLN	2.1
1	G	255	GLU	2.1
1	M	252	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	B	324	VAL	2.1
1	C	252	GLU	2.1
1	F	308	GLU	2.1
1	J	206	ASN	2.1
1	N	355	GLU	2.1
1	M	278	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	142	LYS	2.1
1	E	297	GLY	2.1
1	B	388	GLU	2.0
1	K	315	GLU	2.0
1	M	338	GLU	2.0
1	C	314	LEU	2.0
1	D	215	LEU	2.0
1	G	319	GLN	2.0
1	E	336	VAL	2.0
1	G	403	THR	2.0
1	K	401	HIS	2.0
1	N	223	ALA	2.0
1	N	271	VAL	2.0
1	H	281	PHE	2.0
1	E	306	GLY	2.0
1	J	201	SER	2.0
1	M	345	ARG	2.0
1	F	290	GLN	2.0
1	I	366	GLN	2.0
1	E	183	LEU	2.0
1	L	323	VAL	2.0
1	H	298	GLY	2.0
1	H	184	GLN	2.0
1	B	235	PRO	2.0
1	N	397	GLU	2.0
1	I	249	ILE	2.0
1	J	230	ILE	2.0
1	L	243	ALA	2.0
1	N	372	LEU	2.0
1	H	323	VAL	2.0
1	M	352	GLN	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. 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	B-factors(Å ²)	Q<0.9
2	SO4	K	4021	5/5	0.55	0.44	137,138,139,139	0
2	SO4	H	4017	5/5	0.68	0.33	145,146,146,146	0
2	SO4	C	4012	5/5	0.70	0.27	141,141,141,142	0
2	SO4	M	4014	5/5	0.74	0.24	142,142,143,143	0
2	SO4	J	4020	5/5	0.75	0.47	160,160,160,160	0
2	SO4	L	4003	5/5	0.75	0.25	130,131,132,132	0
2	SO4	E	4006	5/5	0.75	0.33	118,119,119,120	0
2	SO4	H	4018	5/5	0.75	0.33	125,125,126,126	0
2	SO4	A	4008	5/5	0.77	0.36	150,150,150,150	0
2	SO4	M	4013	5/5	0.81	0.23	126,126,127,127	0
2	SO4	G	4002	5/5	0.82	0.27	128,128,129,129	0
2	SO4	C	4011	5/5	0.83	0.29	137,137,137,138	0
2	SO4	N	4016	5/5	0.83	0.26	137,137,137,138	0
2	SO4	A	4007	5/5	0.84	0.27	128,129,129,129	0
2	SO4	F	4004	5/5	0.84	0.31	137,138,138,138	0
2	SO4	B	4010	5/5	0.84	0.29	137,137,137,138	0
2	SO4	K	4022	5/5	0.84	0.27	145,146,146,146	0
2	SO4	N	4015	5/5	0.85	0.27	132,133,133,133	0
2	SO4	B	4009	5/5	0.86	0.28	118,119,119,120	0
2	SO4	A	4001	5/5	0.86	0.24	119,120,120,120	0
2	SO4	E	4005	5/5	0.87	0.35	140,141,141,141	0
2	SO4	J	4019	5/5	0.89	0.23	123,124,124,124	0
3	MG	L	550	1/1	0.92	0.12	31,31,31,31	0
5	AGS	D	551	31/31	0.94	0.16	25,31,39,41	0
5	AGS	K	1	31/31	0.95	0.13	37,40,51,54	0
5	AGS	J	1	31/31	0.95	0.13	39,42,53,54	0
5	AGS	F	1	31/31	0.95	0.14	34,37,44,45	0
5	AGS	L	1	31/31	0.95	0.14	34,37,45,48	0
5	AGS	M	1	31/31	0.95	0.14	38,42,50,52	0
3	MG	B	550	1/1	0.95	0.14	31,31,31,31	0
5	AGS	G	1	31/31	0.95	0.14	25,32,40,41	0
3	MG	A	550	1/1	0.96	0.18	31,31,31,31	0
5	AGS	B	1	31/31	0.96	0.12	31,37,48,50	0
5	AGS	I	1	31/31	0.96	0.14	37,41,48,51	0
5	AGS	C	1	31/31	0.96	0.14	37,41,49,52	0
5	AGS	E	1	31/31	0.96	0.12	27,30,34,37	0
5	AGS	H	1	31/31	0.96	0.13	30,34,38,42	0

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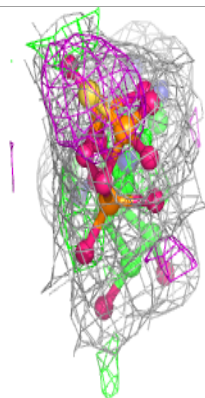
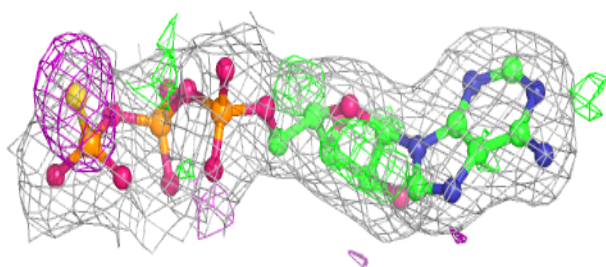
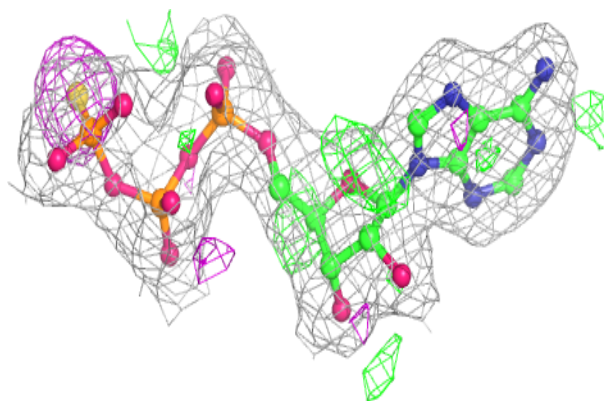
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	K	N	549	1/1	0.96	0.13	41,41,41,41	0
5	AGS	N	1	31/31	0.96	0.14	35,39,47,48	0
5	AGS	A	1	31/31	0.96	0.12	35,38,42,44	0
4	K	K	549	1/1	0.97	0.12	46,46,46,46	0
4	K	C	549	1/1	0.97	0.12	45,45,45,45	0
3	MG	D	550	1/1	0.97	0.14	29,29,29,29	0
3	MG	K	550	1/1	0.97	0.12	35,35,35,35	0
3	MG	F	550	1/1	0.97	0.13	30,30,30,30	0
3	MG	G	550	1/1	0.97	0.19	29,29,29,29	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	I	550	1/1	0.98	0.17	34,34,34,34	0
4	K	G	549	1/1	0.98	0.15	39,39,39,39	0
3	MG	E	550	1/1	0.98	0.10	24,24,24,24	0
3	MG	J	550	1/1	0.98	0.13	37,37,37,37	0
4	K	D	549	1/1	0.98	0.14	34,34,34,34	0
4	K	B	549	1/1	0.98	0.12	38,38,38,38	0
4	K	H	549	1/1	0.98	0.15	41,41,41,41	0
3	MG	M	550	1/1	0.98	0.19	38,38,38,38	0
4	K	L	549	1/1	0.99	0.15	39,39,39,39	0
4	K	A	549	1/1	0.99	0.12	40,40,40,40	0
4	K	E	4007	1/1	0.99	0.11	36,36,36,36	0
3	MG	C	550	1/1	0.99	0.15	36,36,36,36	0
4	K	D	1	1/1	0.99	0.12	30,30,30,30	0
4	K	F	549	1/1	0.99	0.11	41,41,41,41	0
4	K	J	549	1/1	0.99	0.14	47,47,47,47	0
4	K	E	549	1/1	0.99	0.08	31,31,31,31	0
4	K	I	549	1/1	0.99	0.18	43,43,43,43	0
4	K	M	549	1/1	0.99	0.14	45,45,45,45	0

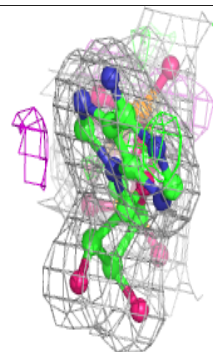
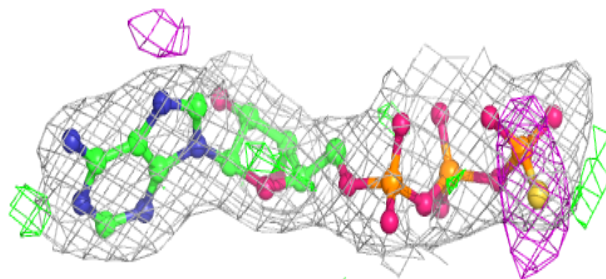
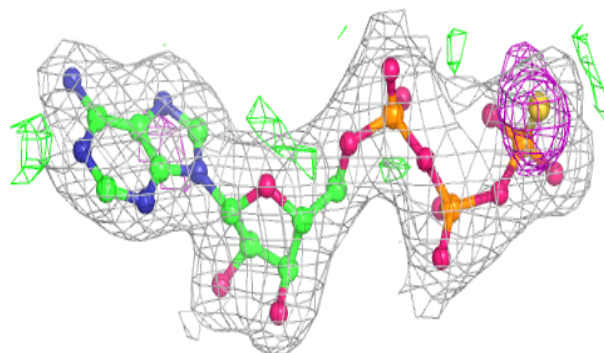
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS D 551:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

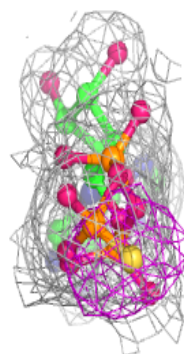
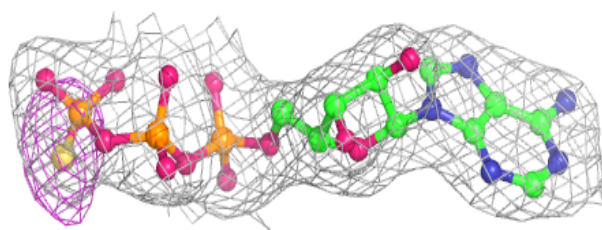
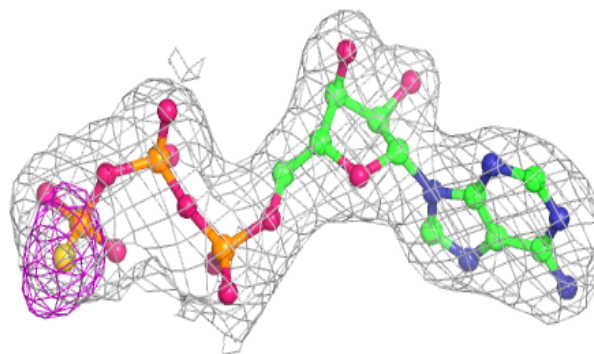
**Electron density around AGS K 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

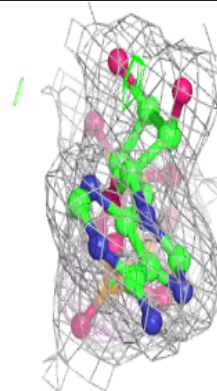
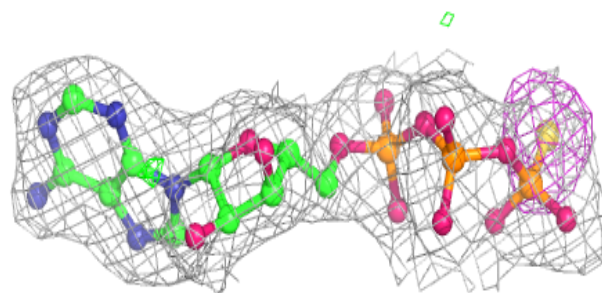
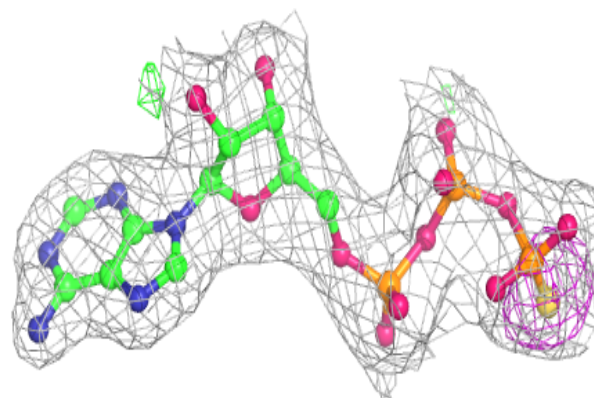


Electron density around AGS J 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

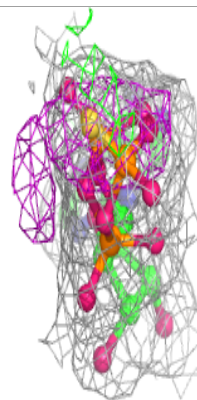
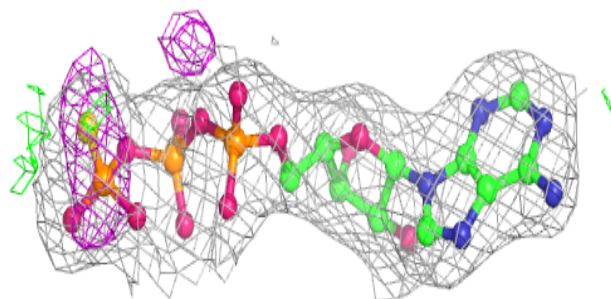
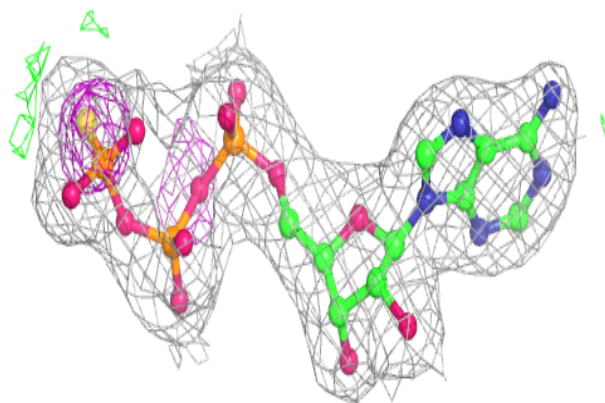
**Electron density around AGS F 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

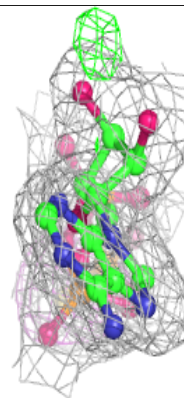
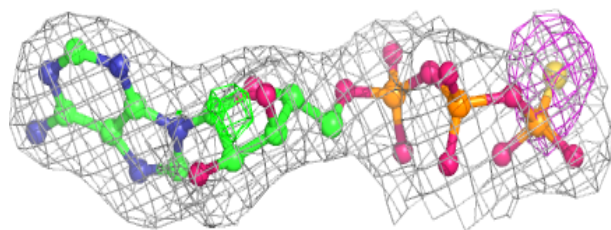
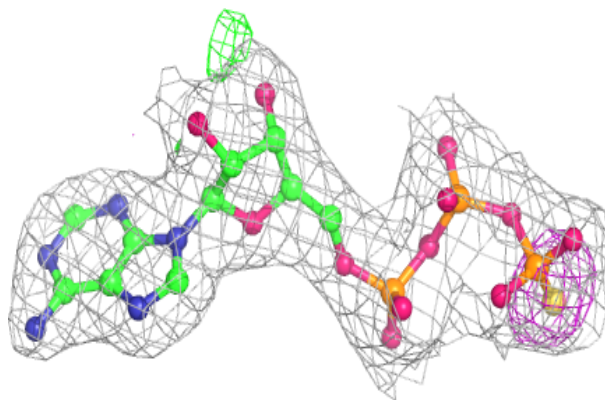


Electron density around AGS L 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

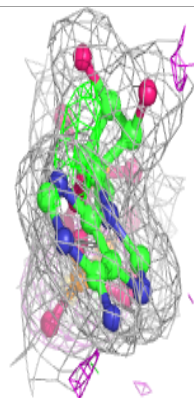
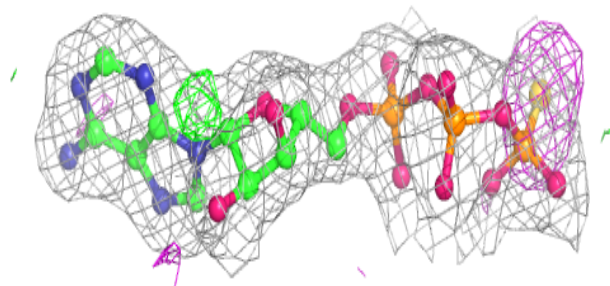
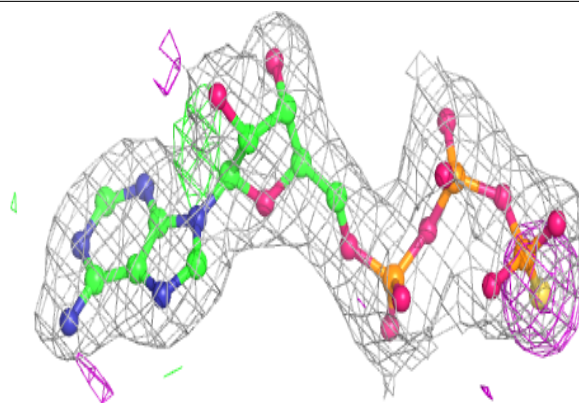
**Electron density around AGS M 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

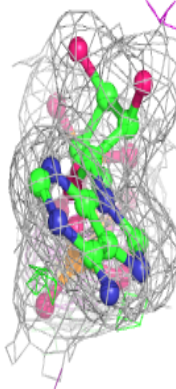
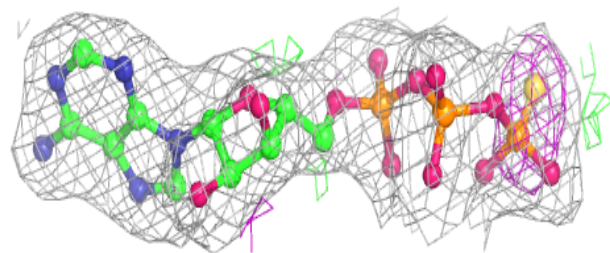
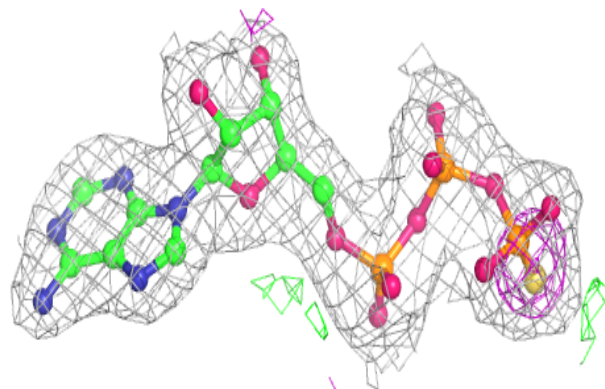


Electron density around AGS G 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

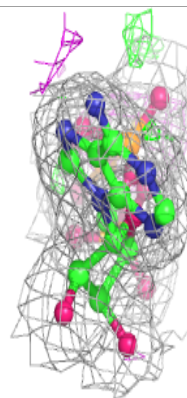
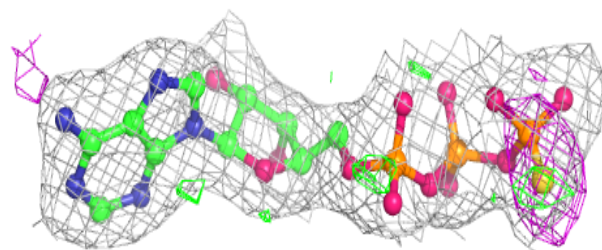
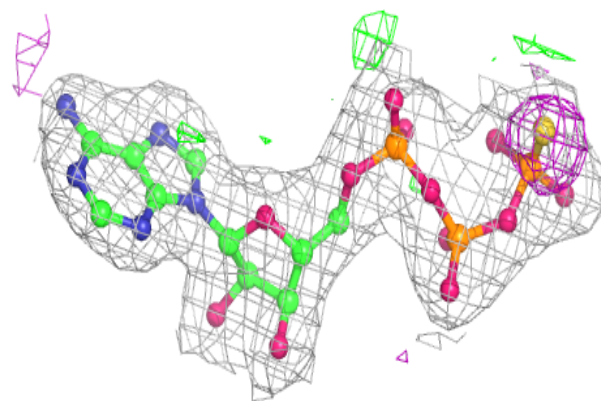
**Electron density around AGS B 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

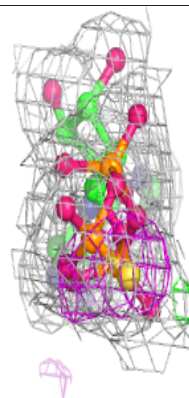
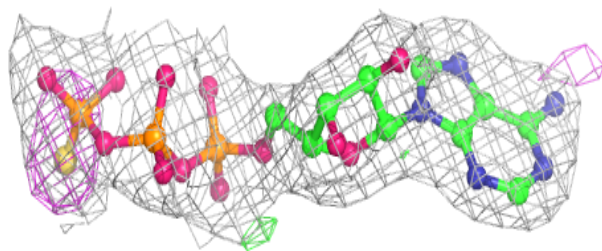
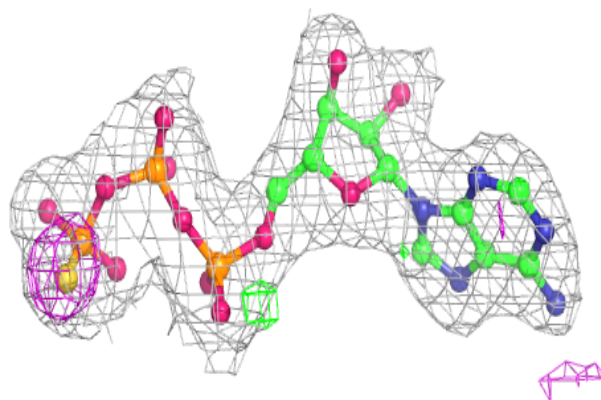


Electron density around AGS I 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

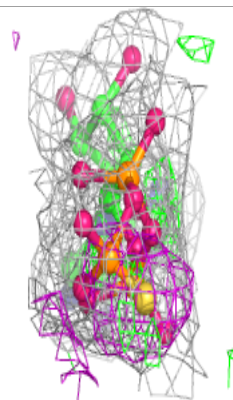
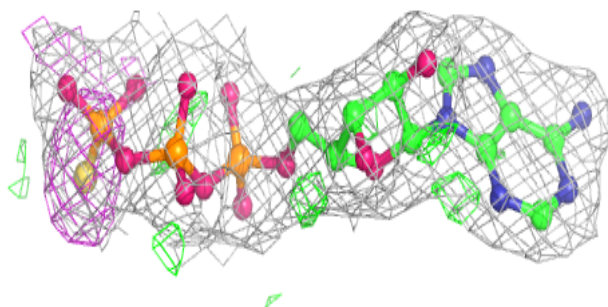
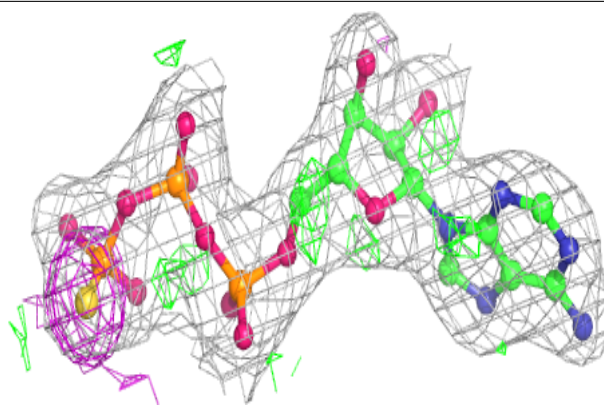
**Electron density around AGS C 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

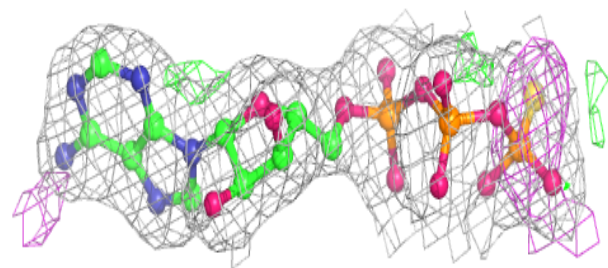
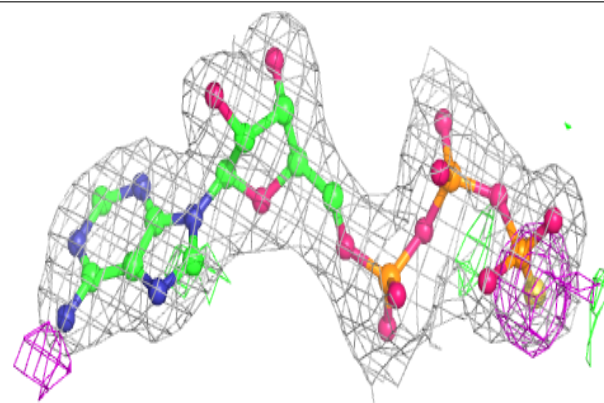


Electron density around AGS E 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

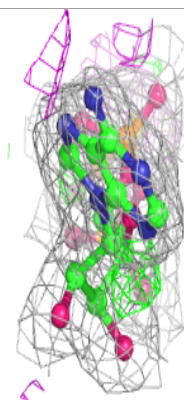
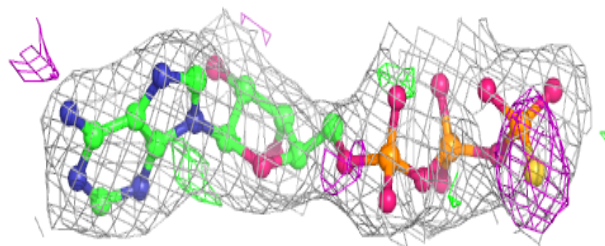
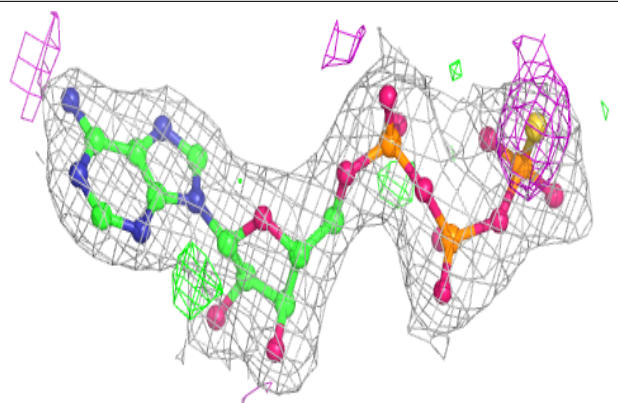
**Electron density around AGS H 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

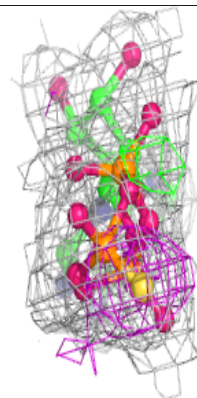
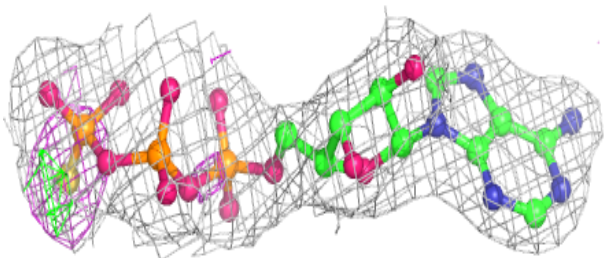
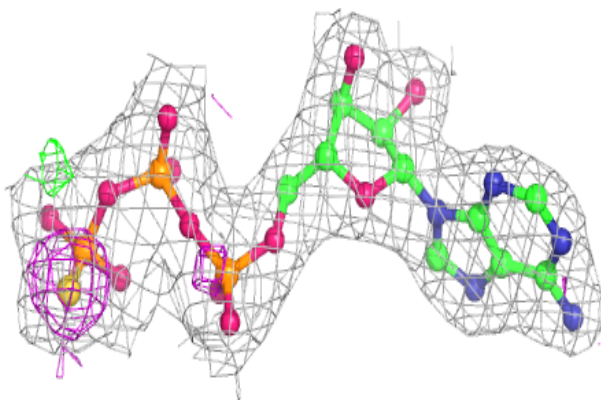


Electron density around AGS N 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AGS A 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.