



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:12 AM UTC

PDB ID : 1KP8 / pdb_00001kp8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

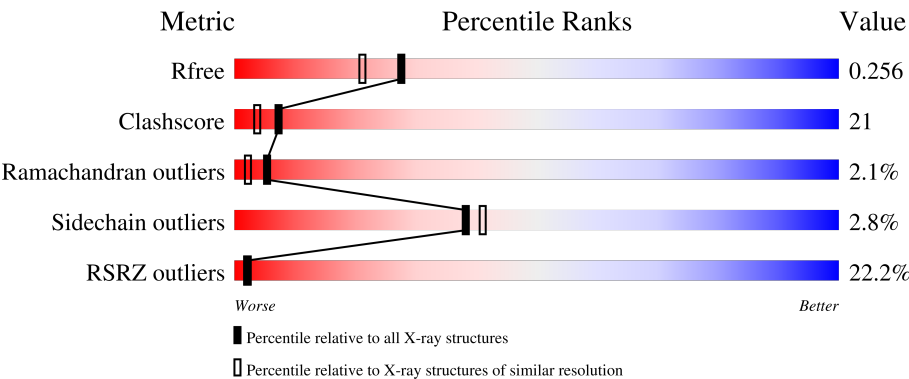
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of 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	19% 61% 31% . .
1	B	547	25% 61% 31% . .
1	C	547	27% 63% 29% . .
1	D	547	11% 64% 29% . .
1	E	547	22% 62% 31% . .

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Mol	Chain	Length	Quality of chain
1	F	547	25% 64% 28%
1	G	547	17% 64% 29%
1	H	547	16% 63% 29%
1	I	547	20% 63% 29%
1	J	547	21% 63% 29%
1	K	547	27% 62% 30%
1	L	547	22% 63% 30%
1	M	547	29% 61% 31%
1	N	547	18% 65% 27%

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 (CCD ID: 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 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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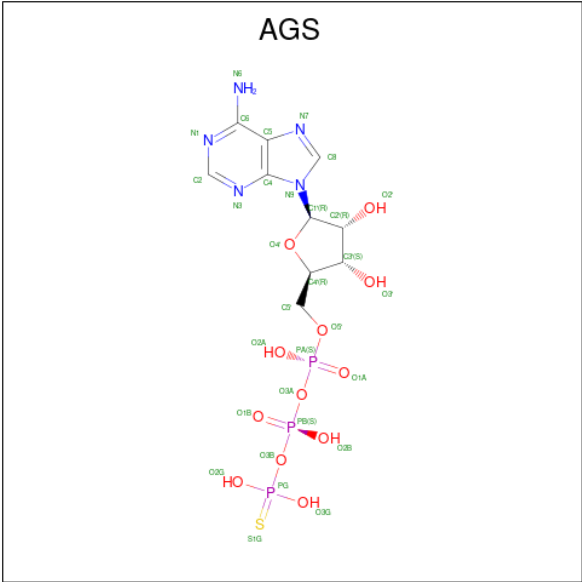
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0
3	N	1	Total 1	Mg 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

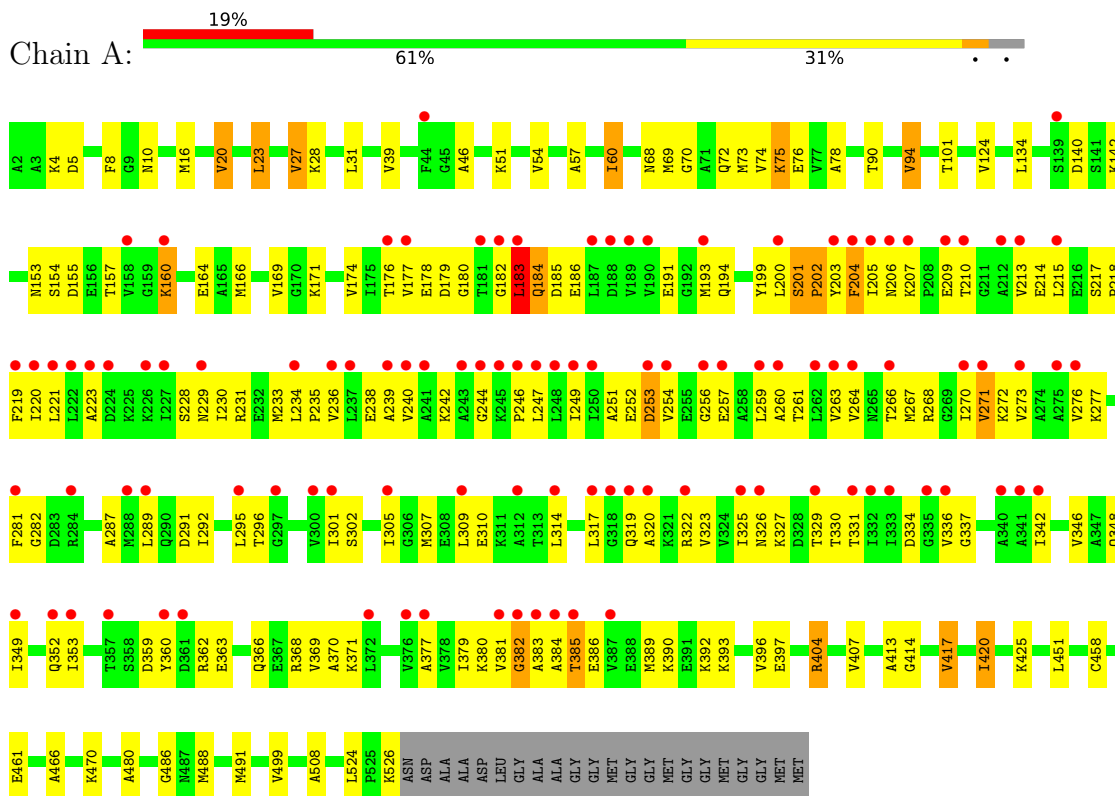
- Molecule 6 is water.

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

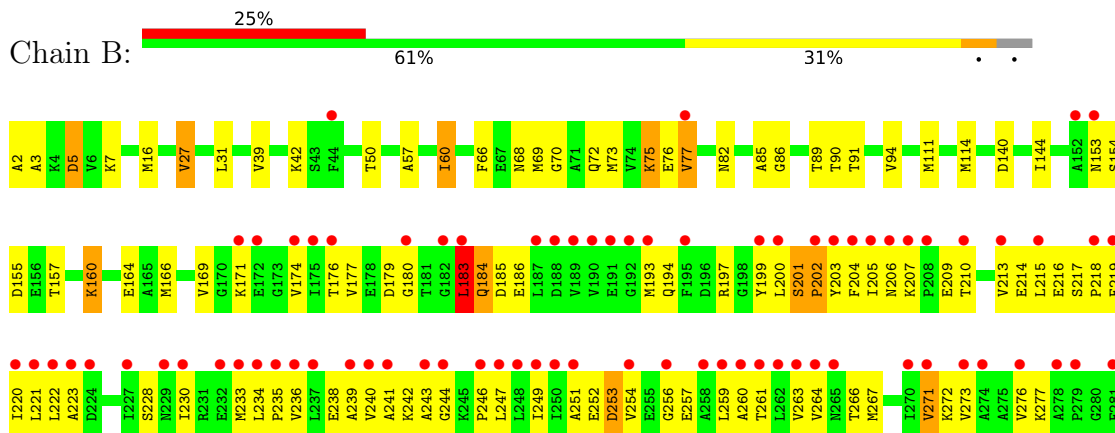
3 Residue-property plots

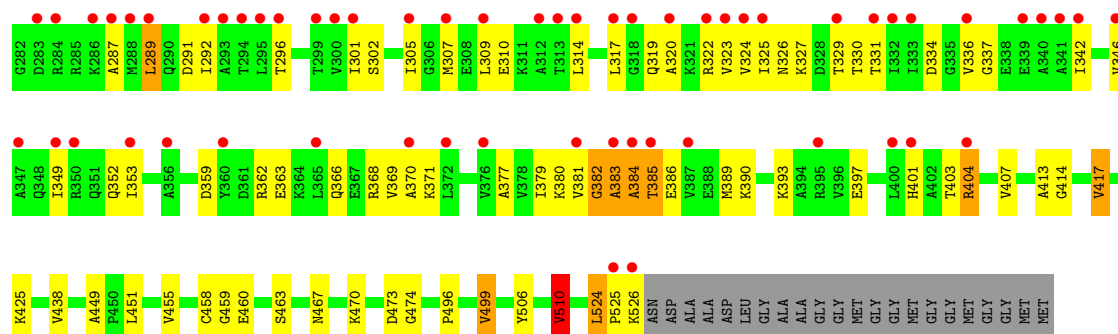
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

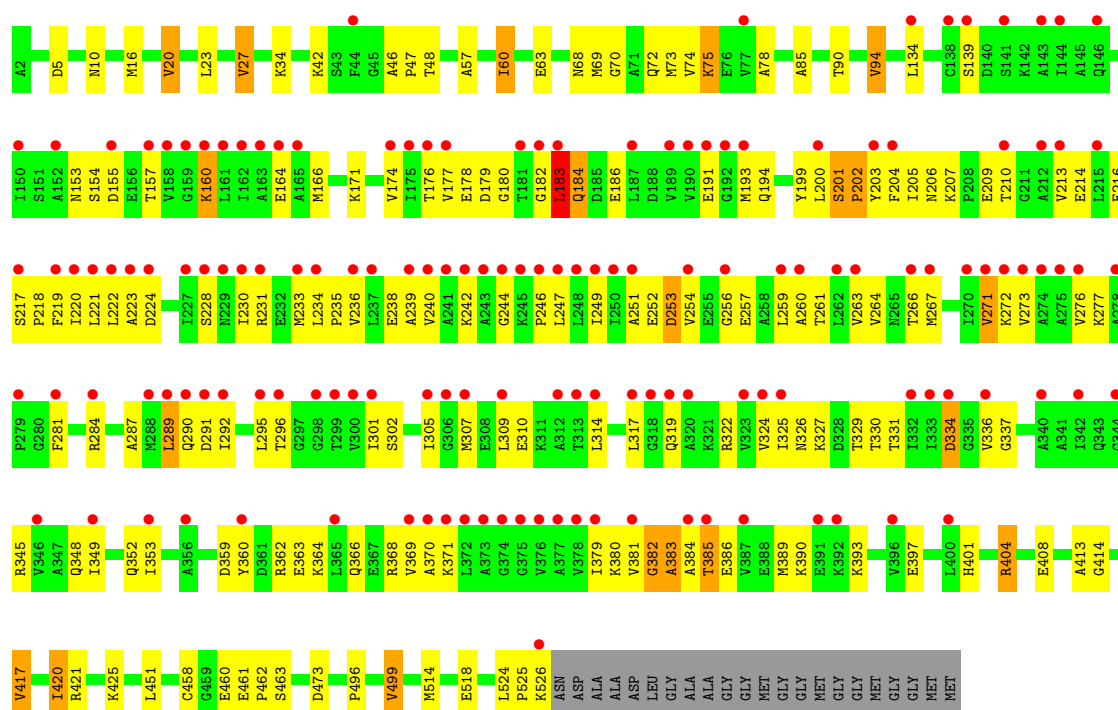


- Molecule 1: groEL protein

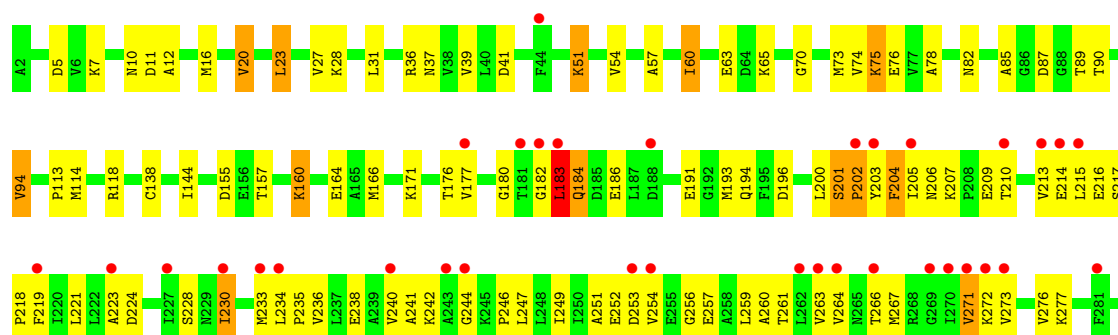


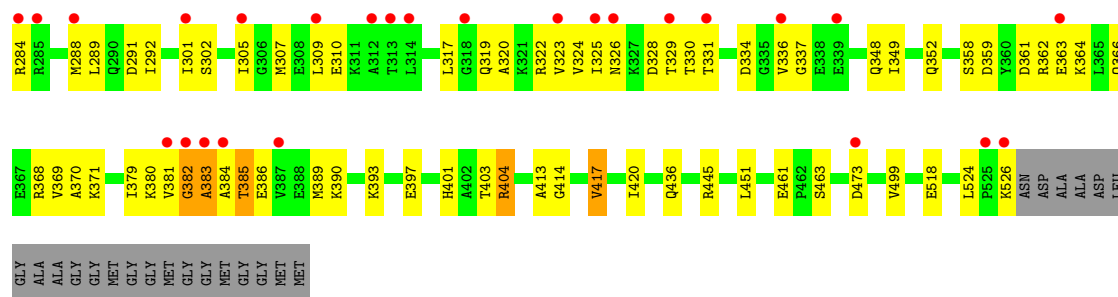


• Molecule 1: groEL protein

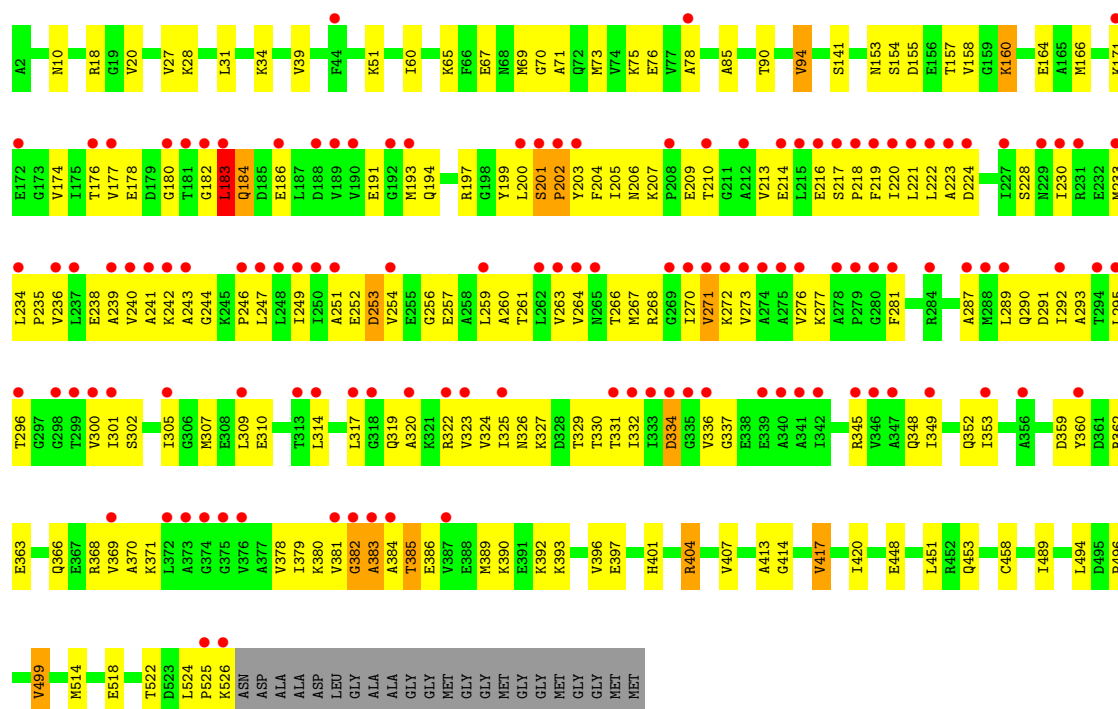


• Molecule 1: groEL protein

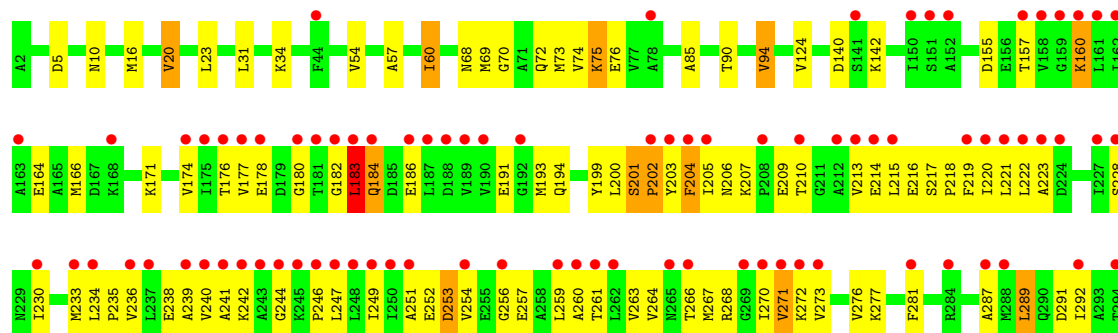


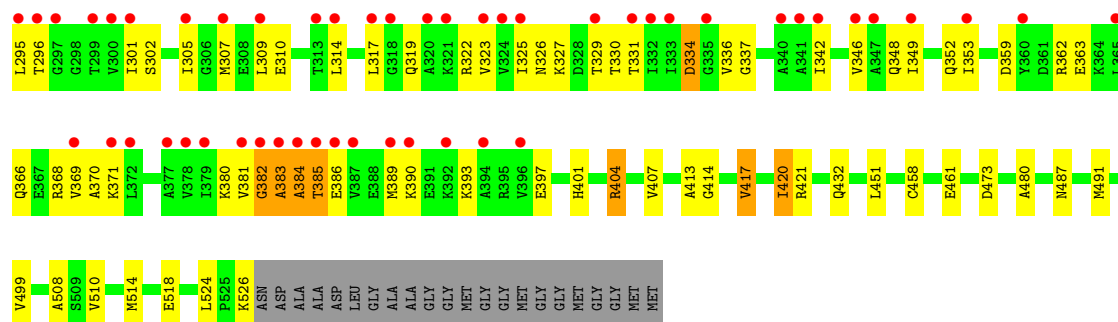


- Molecule 1: groEL protein

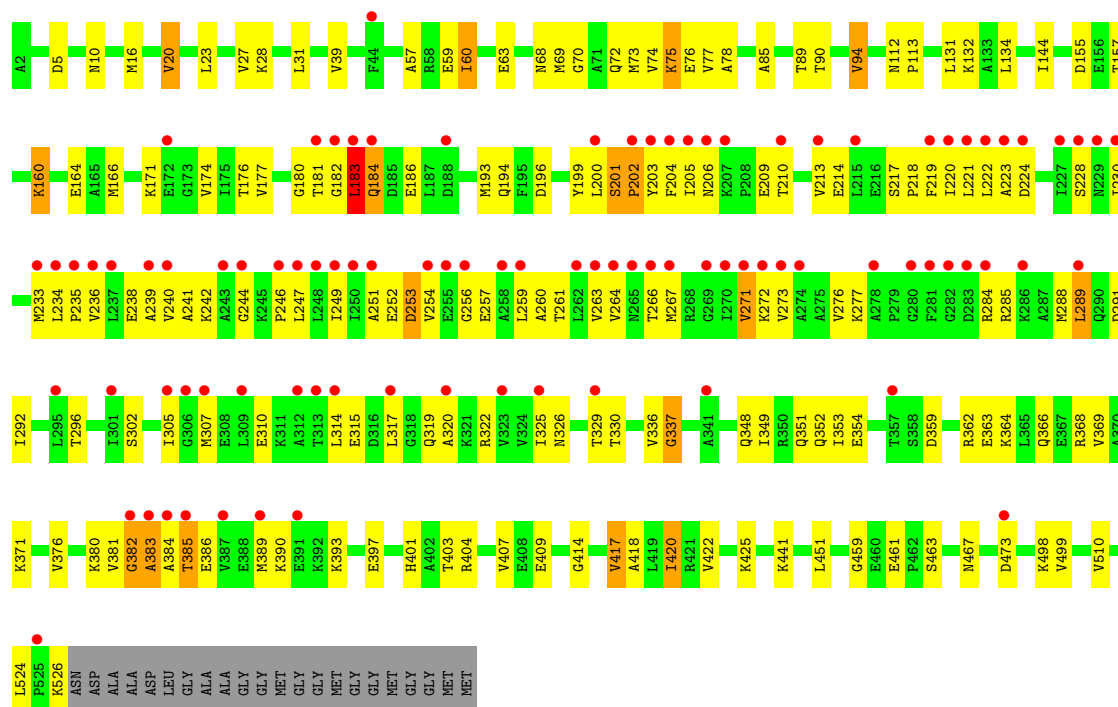


- Molecule 1: groEL protein

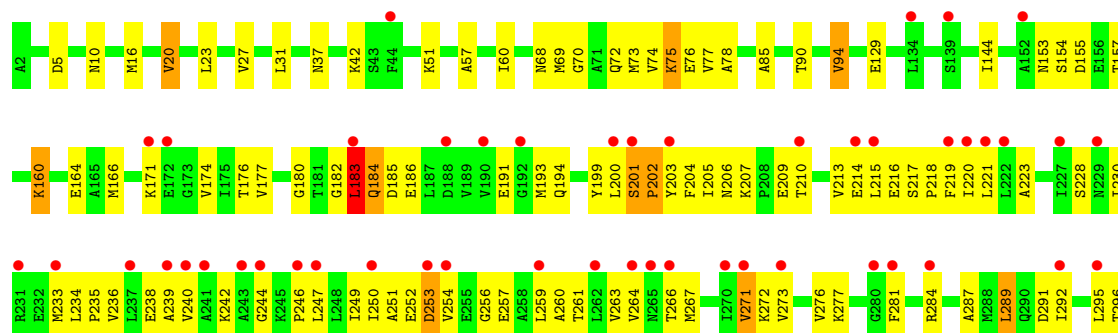


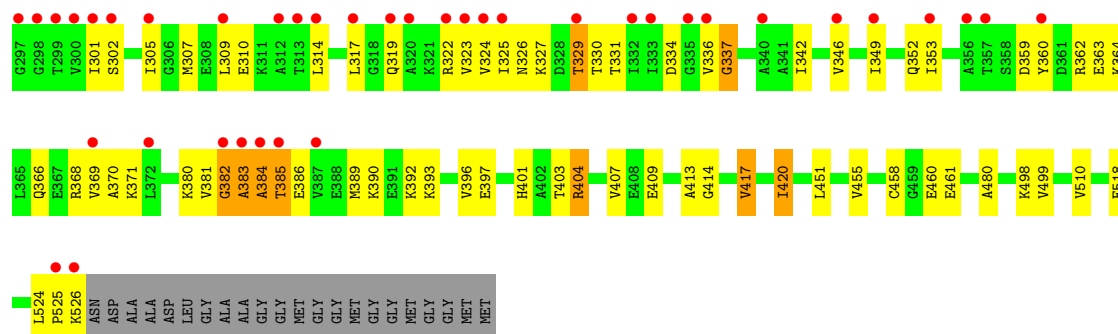


• Molecule 1: groEL protein

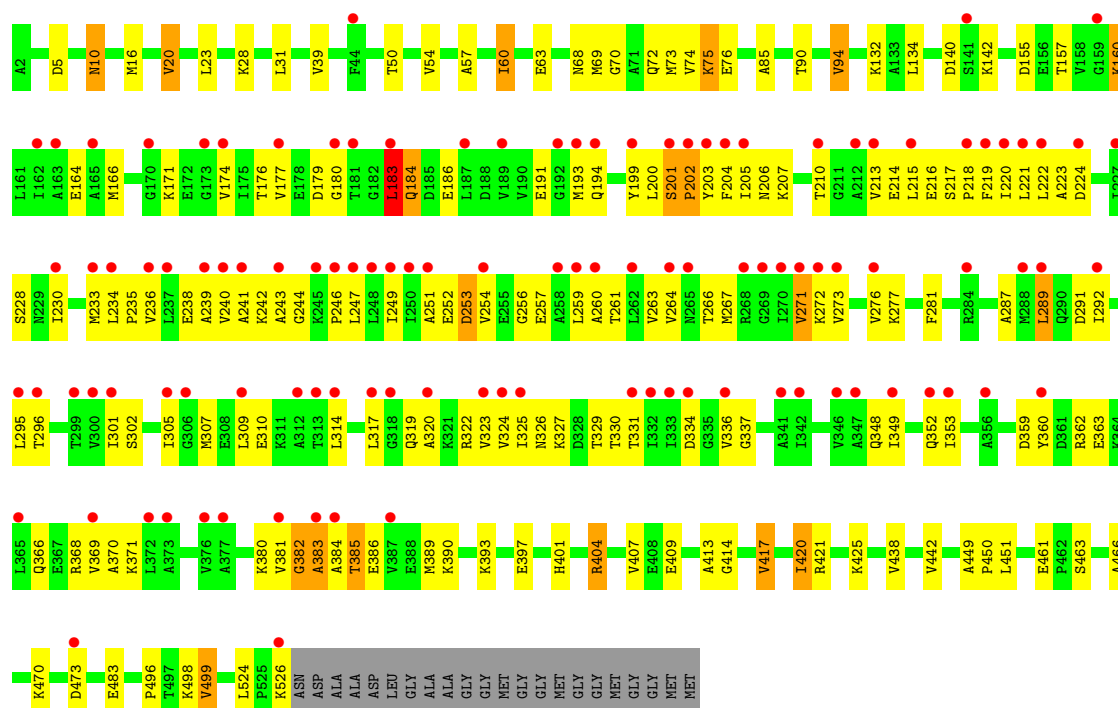


• Molecule 1: groEL protein

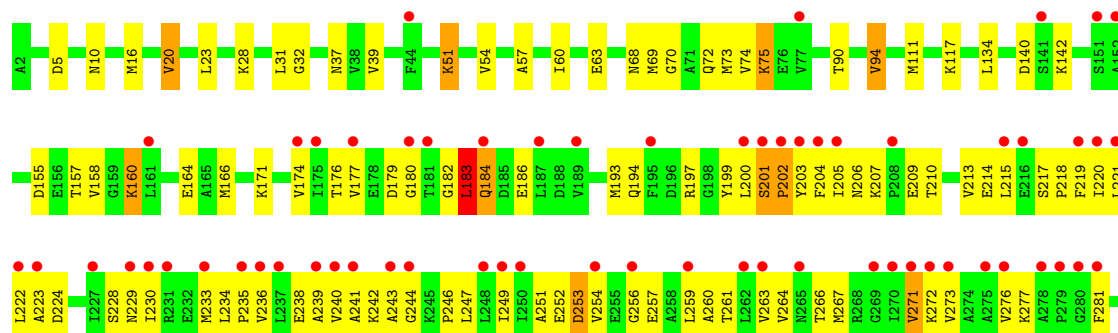


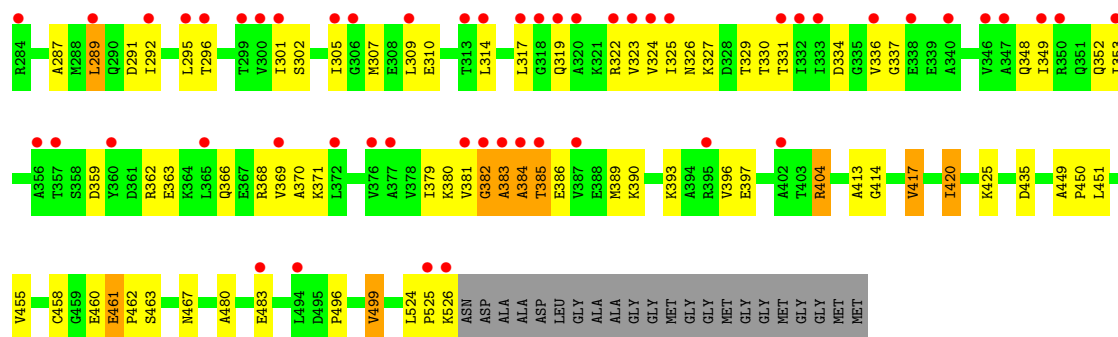


• Molecule 1: groEL protein

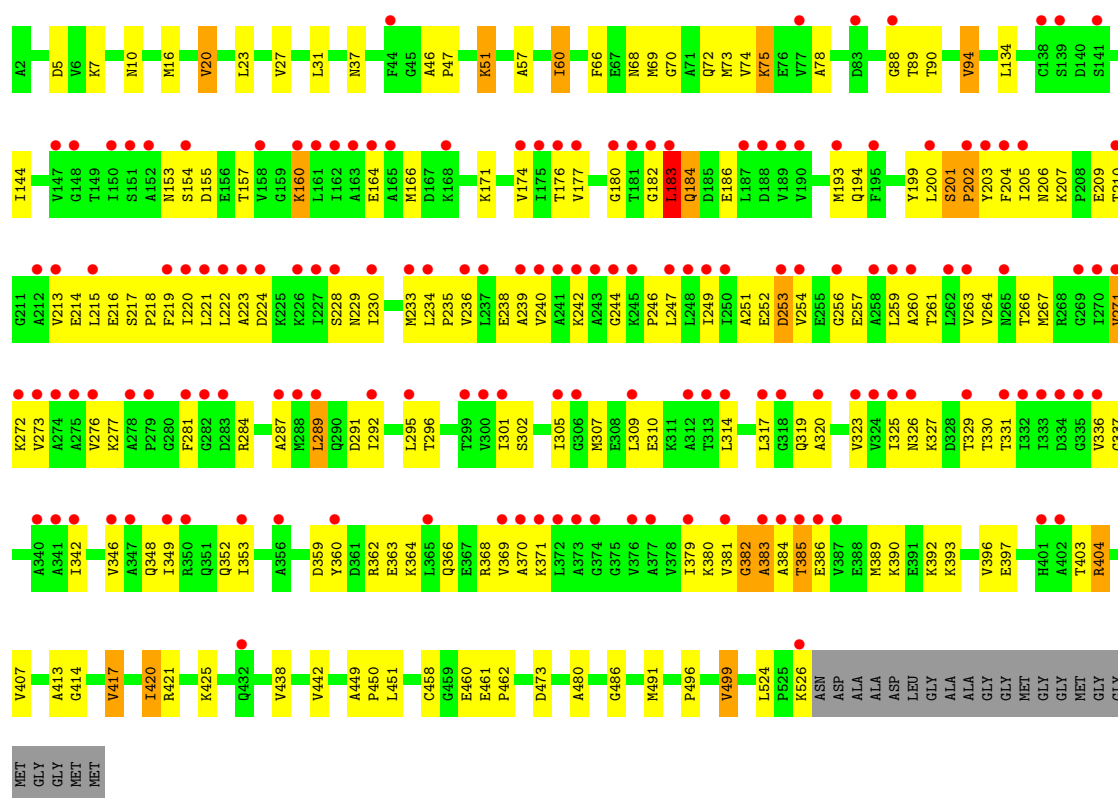


• Molecule 1: groEL protein

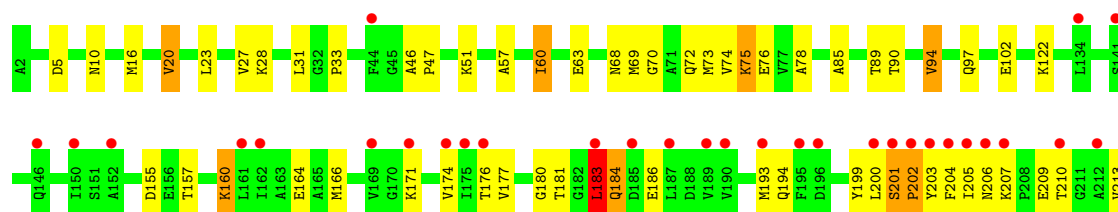


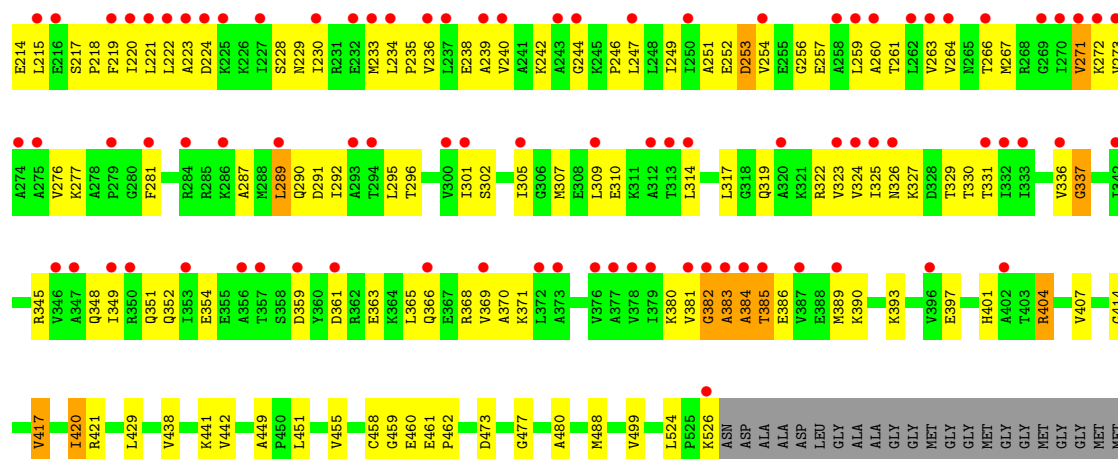


• Molecule 1: groEL protein

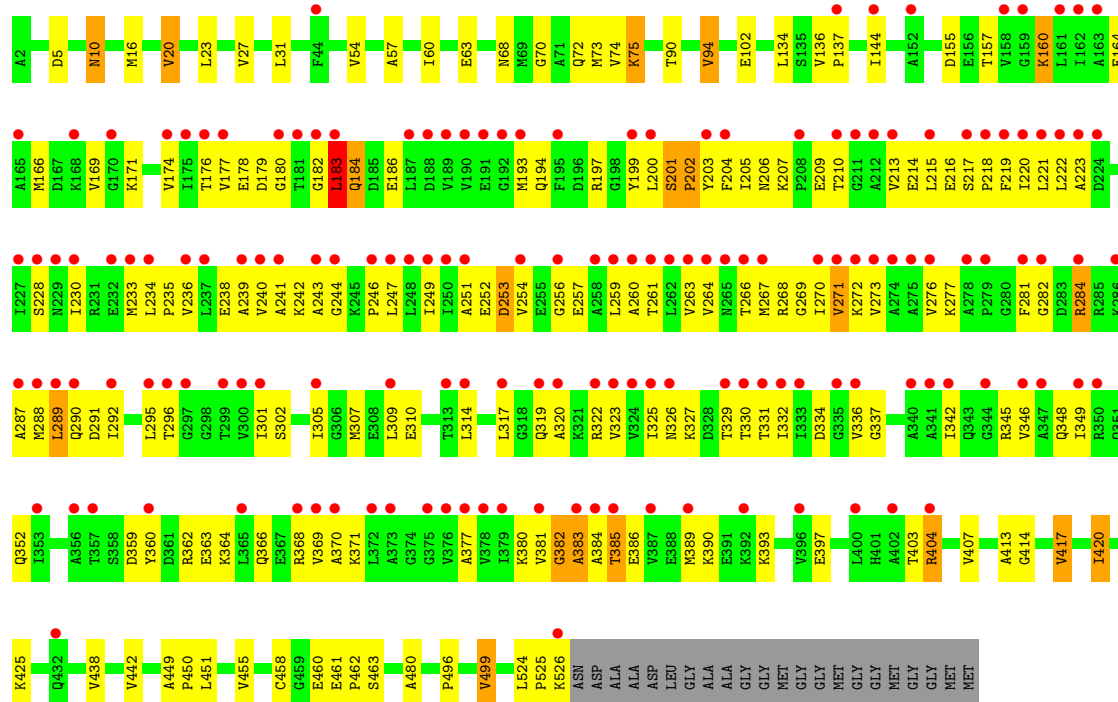


• Molecule 1: groEL protein

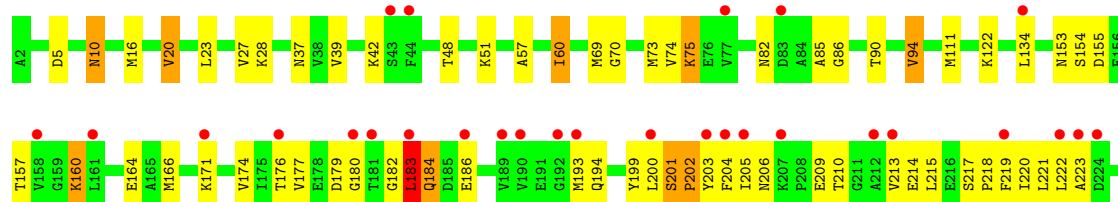


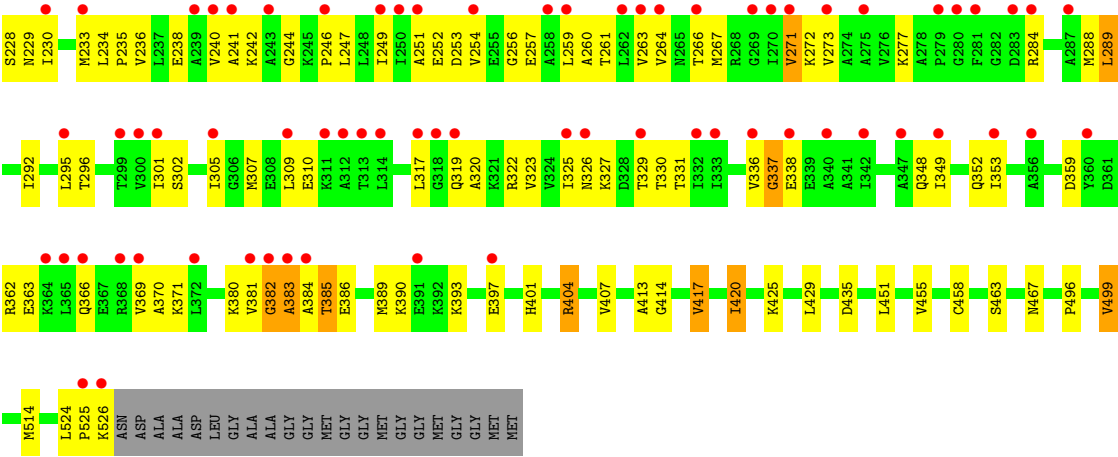


• Molecule 1: groEL protein



• 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) 79.0 (39.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.258 0.241 , 0.256	Depositor DCC
R_{free} test set	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)	0.35 , 57.6	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: AGS, MG, SO4, K

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	0.41	0/3883	0.87	9/5243 (0.2%)
1	B	0.44	0/3883	0.87	7/5243 (0.1%)
1	C	0.41	0/3883	0.87	6/5243 (0.1%)
1	D	0.47	0/3883	0.89	11/5243 (0.2%)
1	E	0.46	0/3883	0.88	3/5243 (0.1%)
1	F	0.42	0/3883	0.85	6/5243 (0.1%)
1	G	0.46	0/3883	0.88	9/5243 (0.2%)
1	H	0.42	0/3883	0.85	6/5243 (0.1%)
1	I	0.39	0/3883	0.86	7/5243 (0.1%)
1	J	0.40	0/3883	0.86	9/5243 (0.2%)
1	K	0.39	0/3883	0.85	7/5243 (0.1%)
1	L	0.42	0/3883	0.85	7/5243 (0.1%)
1	M	0.39	0/3883	0.85	5/5243 (0.1%)
1	N	0.40	0/3883	0.85	4/5243 (0.1%)
All	All	0.42	0/54362	0.86	96/73402 (0.1%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	VAL	CB-CA-C	-8.18	100.94	112.22
1	E	60	ILE	N-CA-C	7.25	118.41	108.84
1	J	461	GLU	CA-C-N	7.17	126.70	119.24
1	J	461	GLU	C-N-CA	7.17	126.70	119.24
1	C	5	ASP	N-CA-C	-7.10	98.15	109.59
1	L	60	ILE	N-CA-C	7.00	118.08	108.84
1	D	60	ILE	N-CA-C	6.94	118.00	108.84
1	C	461	GLU	CA-C-N	6.76	126.27	119.24
1	C	461	GLU	C-N-CA	6.76	126.27	119.24
1	M	60	ILE	N-CA-C	6.68	117.66	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	461	GLU	CA-C-N	6.58	126.08	119.24
1	I	461	GLU	C-N-CA	6.58	126.08	119.24
1	N	60	ILE	N-CA-C	6.54	117.47	108.84
1	C	60	ILE	N-CA-C	6.53	117.46	108.84
1	G	5	ASP	N-CA-C	-6.48	99.16	109.59
1	H	461	GLU	CA-C-N	6.45	125.95	119.24
1	H	461	GLU	C-N-CA	6.45	125.95	119.24
1	E	31	LEU	N-CA-C	6.40	119.56	109.96
1	I	60	ILE	N-CA-C	6.40	117.28	108.84
1	G	60	ILE	N-CA-C	6.39	117.28	108.84
1	A	27	VAL	N-CA-C	6.36	116.51	110.53
1	N	5	ASP	N-CA-C	-6.34	99.38	109.59
1	B	60	ILE	N-CA-C	6.32	117.52	107.98
1	D	5	ASP	N-CA-C	-6.25	99.02	109.07
1	L	31	LEU	N-CA-C	6.18	119.23	109.96
1	A	60	ILE	N-CA-C	6.02	117.45	108.54
1	G	27	VAL	N-CA-C	6.01	116.18	110.53
1	L	5	ASP	N-CA-C	-6.00	99.40	109.07
1	K	31	LEU	N-CA-C	5.97	118.91	109.96
1	A	5	ASP	N-CA-C	-5.94	99.50	109.07
1	H	31	LEU	N-CA-C	5.92	118.85	109.96
1	M	461	GLU	CA-C-N	5.90	125.37	119.24
1	M	461	GLU	C-N-CA	5.90	125.37	119.24
1	G	31	LEU	N-CA-C	5.88	118.78	109.96
1	F	461	GLU	CA-C-N	5.87	125.35	119.24
1	F	461	GLU	C-N-CA	5.87	125.35	119.24
1	D	27	VAL	N-CA-C	5.86	116.04	110.53
1	A	461	GLU	CA-C-N	5.81	125.28	119.24
1	A	461	GLU	C-N-CA	5.81	125.28	119.24
1	H	60	ILE	N-CA-C	5.80	117.13	108.54
1	J	60	ILE	N-CA-C	5.80	117.12	108.54
1	G	461	GLU	CA-C-N	5.77	125.24	119.24
1	G	461	GLU	C-N-CA	5.77	125.24	119.24
1	D	31	LEU	N-CA-C	5.75	118.58	109.96
1	K	461	GLU	CA-C-N	5.71	125.18	119.24
1	K	461	GLU	C-N-CA	5.71	125.18	119.24
1	E	51	LYS	N-CA-C	-5.64	105.07	112.41
1	K	5	ASP	N-CA-C	-5.62	100.02	109.07
1	B	27	VAL	N-CA-C	5.62	115.81	110.53
1	I	31	LEU	N-CA-C	5.58	118.34	109.96
1	A	51	LYS	N-CA-C	-5.58	105.16	112.41
1	J	5	ASP	N-CA-C	-5.58	100.09	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5	ASP	N-CA-C	-5.55	100.14	109.07
1	H	27	VAL	N-CA-C	5.52	115.72	110.53
1	F	60	ILE	N-CA-C	5.51	116.70	108.54
1	C	27	VAL	N-CA-C	5.50	115.70	110.53
1	A	31	LEU	N-CA-C	5.49	118.48	109.76
1	N	28	LYS	N-CA-C	5.48	119.07	112.38
1	D	204	PHE	N-CA-C	-5.48	105.70	112.38
1	L	27	VAL	N-CA-C	5.46	115.67	110.53
1	L	459	GLY	N-CA-C	-5.42	107.73	115.64
1	K	27	VAL	N-CA-C	5.40	115.61	110.53
1	C	408	GLU	N-CA-C	5.40	116.85	111.07
1	J	28	LYS	N-CA-C	5.37	119.45	113.01
1	D	461	GLU	CA-C-N	5.36	126.55	119.84
1	D	461	GLU	C-N-CA	5.36	126.55	119.84
1	A	28	LYS	N-CA-C	5.36	118.92	112.38
1	B	50	THR	N-CA-C	5.35	117.32	109.24
1	K	60	ILE	N-CA-C	5.35	116.46	108.54
1	B	5	ASP	N-CA-C	-5.31	100.52	109.07
1	D	28	LYS	N-CA-C	5.31	118.86	112.38
1	F	204	PHE	N-CA-C	-5.31	105.91	112.38
1	J	31	LEU	N-CA-C	5.28	117.88	109.96
1	B	31	LEU	N-CA-C	5.28	118.15	109.76
1	K	51	LYS	N-CA-C	-5.27	105.13	112.30
1	A	204	PHE	N-CA-C	-5.26	105.96	112.38
1	I	50	THR	N-CA-C	5.23	117.14	109.24
1	I	5	ASP	N-CA-C	-5.22	100.66	109.07
1	N	27	VAL	N-CA-C	5.20	115.42	110.53
1	D	196	ASP	N-CA-C	5.19	117.64	109.39
1	L	51	LYS	N-CA-C	-5.19	105.25	112.30
1	D	328	ASP	N-CA-C	5.18	116.53	110.41
1	G	459	GLY	N-CA-C	-5.18	108.13	115.43
1	B	459	GLY	N-CA-C	-5.14	108.14	115.64
1	J	32	GLY	CA-C-N	5.13	124.92	119.28
1	J	32	GLY	C-N-CA	5.13	124.92	119.28
1	G	28	LYS	N-CA-C	5.10	118.60	112.38
1	J	51	LYS	N-CA-C	-5.09	105.38	112.30
1	M	31	LEU	N-CA-C	5.08	117.58	109.96
1	H	5	ASP	N-CA-C	-5.07	100.90	109.07
1	D	51	LYS	N-CA-C	-5.06	105.83	112.41
1	F	31	LEU	N-CA-C	5.04	117.52	109.96
1	M	5	ASP	N-CA-C	-5.04	100.96	109.07
1	G	196	ASP	N-CA-C	5.01	117.36	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	28	LYS	N-CA-C	5.01	118.49	112.38
1	I	28	LYS	N-CA-C	5.00	118.48	112.38

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	173	0
1	B	3855	0	3982	183	0
1	C	3855	0	3982	164	0
1	D	3855	0	3982	160	0
1	E	3855	0	3982	165	0
1	F	3855	0	3982	151	0
1	G	3855	0	3982	164	1
1	H	3855	0	3982	158	0
1	I	3855	0	3982	165	0
1	J	3855	0	3982	163	0
1	K	3855	0	3982	167	0
1	L	3855	0	3982	162	0
1	M	3855	0	3982	169	0
1	N	3855	0	3982	156	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	5	0
5	H	31	0	12	4	0
5	I	31	0	12	4	0
5	J	31	0	12	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
6	G	269	0	0	12	0
6	H	204	0	0	7	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	2271	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 21.

All (2271) 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:PG	5:A:1:AGS:S1G	1.50	1.49
5:H:1:AGS:S1G	5:H:1:AGS:PG	1.49	1.49
5:M:1:AGS:PG	5:M:1:AGS:S1G	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:PG	5:J:1:AGS:S1G	1.49	1.48
5:L:1:AGS:PG	5:L:1:AGS:S1G	1.49	1.47
5:N:1:AGS:PG	5:N:1:AGS:S1G	1.49	1.47
5: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:I:183:LEU:H	1:I:383:ALA:HB3	1.13	1.10
1:J:183:LEU:H	1:J:383:ALA:HB3	1.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:193:MET:HE1	1:D:292:ILE:HG12	1.41	1.03
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.34	1.02
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.45	0.99
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:193:MET:HE1	1:L:292:ILE:HG12	1.46	0.97
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.46	0.97
1:E:193:MET:HE1	1:E:292:ILE:HG12	1.47	0.96
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:H:193:MET:HE1	1:H:292:ILE:HG12	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:193:MET:HE1	1:F:292:ILE:HG12	1.51	0.92
1:A:193:MET:HE1	1:A:292:ILE:HG12	1.50	0.92
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:J:193:MET:HE1	1:J:292:ILE:HG12	1.51	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:K:193:MET:HE1	1:K:292:ILE:HG12	1.52	0.91
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.52	0.90
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:G:193:MET:HE1	1:G:292:ILE:HG12	1.51	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:B:193:MET:HE1	1:B:292:ILE:HG12	1.50	0.89
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:M:193:MET:HE1	1:M:292:ILE:HG12	1.54	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
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:H:281:PHE:HZ	1:N:383:ALA:HB1	1.38	0.86
1:L:383:ALA:HB1	1:M:281:PHE:CZ	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:70:GLY:HA2	1:B:73:MET:HE3	1.59	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:D:305:ILE:HB	1:D:307:MET:HE2	1.63	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
1:I:305:ILE:HB	1:I:307:MET:HE2	1.64	0.79
1:J:305:ILE:HB	1:J:307:MET:HE2	1.64	0.79
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:B:305:ILE:HB	1:B:307:MET:HE2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:305:ILE:HB	1:K:307:MET:HE2	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:G:305:ILE:HB	1:G:307:MET:HE2	1.66	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:A:305:ILE:HB	1:A:307:MET:HE2	1.67	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:F:305:ILE:HB	1:F:307:MET:HE2	1.67	0.77
1:M:463:SER:HB2	6:M:3029:HOH:O	1.85	0.77
1:C:305:ILE:HB	1:C:307:MET:HE2	1.67	0.76
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:H:305:ILE:HB	1:H:307:MET:HE2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.68	0.75
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:S1G	5:J:1:AGS:O3B	2.45	0.74
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.70	0.74
1:N:305:ILE:HB	1:N:307:MET:HE2	1.70	0.74
1:I:194:GLN:O	1:I:371:LYS:HE3	1.87	0.73
1:L:305:ILE:HB	1:L:307:MET:HE2	1.69	0.73
1:A:359:ASP:O	1:A:363:GLU:HG2	1.88	0.73
1:E:305:ILE:HB	1:E:307:MET:HE2	1.70	0.73
1:C:183:LEU:N	1:C:383:ALA:HB3	2.02	0.73
5:G:1:AGS:S1G	5:G:1:AGS:O3B	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:N:70:GLY:HA2	1:N:73:MET:HE3	1.69	0.73
1:G:473:ASP:HB2	6:G:2130:HOH:O	1.89	0.73
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.68	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
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.68	0.73
1:H:166:MET:HE2	1:H:171:LYS:HA	1.70	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:S1G	5:N:1:AGS:O3G	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:S1G	5:D:551:AGS:O3B	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:70:GLY:HA2	1:A:73:MET:HE3	1.71	0.71
5:I:1:AGS:S1G	5:I:1:AGS:O3B	2.47	0.71
1:A:414:GLY:O	1:A:417:VAL:HG13	1.90	0.71
5:C:1:AGS:S1G	5:C:1:AGS:O3B	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:F:70:GLY:HA2	1:F:73:MET:HE3	1.73	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:S1G	5:E:1:AGS:O3B	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: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: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:G:242:LYS:C	1:G:244:GLY:H	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:414:GLY:O	1:J:417:VAL:HG13	1.92	0.69
5:J:1:AGS:S1G	5:J:1:AGS:O3G	2.47	0.69
1:H:194:GLN:O	1:H:371:LYS:HE3	1.91	0.69
1:M:305:ILE:HB	1:M:307:MET:HE2	1.75	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:K:70:GLY:HA2	1:K:73:MET:HE3	1.74	0.69
1:M:414:GLY:O	1:M:417:VAL:HG13	1.92	0.69
5:N:1:AGS:S1G	5:N:1:AGS:O3B	2.50	0.69
5:A:1:AGS:S1G	5:A:1:AGS:O3B	2.48	0.69
1:C:194:GLN:O	1:C:371:LYS:HE3	1.91	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:N:263:VAL:O	1:N:267:MET:HB2	1.93	0.69
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.23	0.69
5:E:1:AGS:S1G	5:E:1:AGS:O3G	2.46	0.69
5:H:1:AGS:S1G	5:H:1:AGS:O3G	2.48	0.69
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.75	0.69
5:K:1:AGS:S1G	5:K:1:AGS:O3B	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:G:70:GLY:HA2	1:G:73:MET:HE3	1.76	0.68
1:B:414:GLY:O	1:B:417:VAL:HG13	1.93	0.68
1:G:302:SER:H	1:G:307:MET:HE3	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1:AGS:S1G	5:L:1:AGS:O3B	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:I:70:GLY:HA2	1:I:73:MET:HE3	1.74	0.67
1:I:166:MET:HE2	1:I:171:LYS:HA	1.74	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:D:39:VAL:HG12	1:E:69:MET:HE2	1.77	0.67
1:K:383:ALA:HB1	1:L:281:PHE:HZ	1.59	0.67
1:I:263:VAL:O	1:I:267:MET:HB2	1.93	0.67
5:B:1:AGS:S1G	5:B:1:AGS:O3B	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:E:70:GLY:HA2	1:E:73:MET:HE3	1.75	0.67
1:H:177:VAL:HG21	1:H:397:GLU:CG	2.25	0.67
5:B:1:AGS:S1G	5:B:1:AGS:O3G	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:166:MET:HE2	1:N:171:LYS:HA	1.76	0.66
1:G:183:LEU:HD23	1:G:384:ALA:HB2	1.77	0.66
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.75	0.66
1:D:383:ALA:HB1	1:E:281:PHE:CZ	2.29	0.66
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.78	0.66
1:D:414:GLY:O	1:D:417:VAL:HG13	1.96	0.66
1:H:174:VAL:HG22	1:H:194:GLN:HE21	1.61	0.66
5:M:1:AGS:S1G	5:M:1:AGS:O3G	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LYS:C	1:D:244:GLY:H	2.03	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:HH11	1:D:404:ARG:HG2	1.60	0.65
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.78	0.65
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.77	0.65
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:302:SER:H	1:H:307:MET:HE3	1.62	0.65
1:H:404:ARG:HH11	1:H:404:ARG:CG	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:K:213:VAL:HB	1:K:325:ILE:CG1	2.27	0.65
1:F:166:MET:HE2	1:F:171:LYS:HA	1.78	0.65
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.77	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:D:166:MET:HE2	1:D:171:LYS:HA	1.79	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:D:193:MET:HE1	1:D:292:ILE:CG1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:514:MET:HE3	6:C:2670:HOH:O	1.96	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
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.63	0.64
1:D:183:LEU:O	1:D:184:GLN:HB2	1.98	0.64
1:K:183:LEU:HD23	1:K:384:ALA:HB2	1.80	0.64
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.80	0.64
1:D:177:VAL:HG21	1:D:397:GLU:CG	2.27	0.64
1:E:177:VAL:HG21	1:E:397:GLU:CG	2.27	0.64
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.80	0.64
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.63	0.64
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.80	0.64
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.28	0.64
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.28	0.64
1:A:268:ARG:O	1:B:257:GLU:HG3	1.97	0.64
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.64
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.28	0.64
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.80	0.63
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.28	0.63
1:K:183:LEU:H	1:K:383:ALA:CB	2.03	0.63
1:M:166:MET:HE2	1:M:171:LYS:HA	1.80	0.63
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.79	0.63
1:D:302:SER:H	1:D:307:MET:HE3	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:166:MET:HE2	1:A:171:LYS:HA	1.80	0.63
1:C:90:THR:O	1:C:94:VAL:HG13	1.98	0.63
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.79	0.63
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	0.63
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.81	0.63
1:B:166:MET:HE2	1:B:171:LYS:HA	1.80	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:H:362:ARG:O	1:H:366:GLN:HG3	1.99	0.63
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.79	0.63
1:J:54:VAL:HG23	6:J:2067:HOH:O	1.98	0.63
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.81	0.63
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.29	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:HG2	1:J:404:ARG:HH11	1.64	0.62
1:F:302:SER:H	1:F:307:MET:HE3	1.64	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: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:A:360:TYR:OH	1:G:384:ALA:HA	2.00	0.62
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ASN:HA	6:D:2757:HOH:O	1.98	0.62
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.81	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:N	1:N:272:LYS:HD2	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:J:166:MET:HE2	1:J:171:LYS:HA	1.80	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
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:HG2	1:N:404:ARG:HH11	1.65	0.61
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.81	0.61
1:F:16:MET:O	1:F:20:VAL:HG13	2.00	0.61
1:M:525:PRO:HD3	6:M:2817:HOH:O	1.99	0.61
1:N:414:GLY:O	1:N:417:VAL:HG13	2.00	0.61
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.82	0.61
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.82	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.81	0.61
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.01	0.61
1:J:177:VAL:HG21	1:J:397:GLU:CG	2.30	0.61
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.82	0.61
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.83	0.61
1:B:200:LEU:O	1:B:201:SER:HB3	2.00	0.61
1:D:404:ARG:NH1	6:D:2552:HOH:O	2.33	0.61
1:E:78:ALA:HB3	6:E:2338:HOH:O	2.00	0.61
1:G:78:ALA:HB3	6:G:1724:HOH:O	1.98	0.61
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.82	0.61
1:D:183:LEU:HD23	1:D:384:ALA:HB2	1.83	0.61
1:N:200:LEU:O	1:N:201:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:302:SER:H	1:K:307:MET:HE3	1.65	0.61
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.81	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:N	1:C:272:LYS:HD2	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:L:166:MET:HE2	1:L:171:LYS:HA	1.84	0.60
1:N:242:LYS:C	1:N:244:GLY:H	2.07	0.60
1:J:183:LEU:HD12	1:J:184:GLN:HG3	1.83	0.60
1:J:242:LYS:C	1:J:244:GLY:H	2.09	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:C:23:LEU:HD22	1:C:74:VAL:HG13	1.84	0.60
1:C:177:VAL:HG21	1:C:397:GLU:CG	2.31	0.60
1:G:166:MET:HE2	1:G:171:LYS:HA	1.83	0.60
1:H:242:LYS:C	1:H:244:GLY:H	2.09	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:E:242:LYS:C	1:E:244:GLY:H	2.08	0.60
1:I:218:PRO:CB	1:I:246:PRO:HG2	2.28	0.60
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.82	0.60
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.81	0.60
1:M:302:SER:H	1:M:307:MET:HE3	1.67	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:M:242:LYS:C	1:M:244:GLY:H	2.10	0.60
1:A:46:ALA:CB	1:B:76:GLU:HG3	2.31	0.60
1:B:425:LYS:HB2	6:B:2916:HOH:O	2.01	0.60
1:M:200:LEU:O	1:M:201:SER:HB3	1.99	0.60
1:N:302:SER:H	1:N:307:MET:HE3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:SER:H	1:B:307:MET:HE3	1.66	0.60
1:D:272:LYS:N	1:D:272:LYS:HD2	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:L:242:LYS:C	1:L:244:GLY:H	2.06	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:E:221:LEU:HD23	1:E:233:MET:HE1	1.83	0.59
1:F:383:ALA:O	1:F:384:ALA:HB3	2.01	0.59
1:J:272:LYS:HD2	1:J:272:LYS:N	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:E:302:SER:H	1:E:307:MET:HE3	1.68	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: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:K:242:LYS:C	1:K:244:GLY:H	2.08	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:LYS:HD2	1:E:272:LYS:N	2.17	0.59
1:L:90:THR:O	1:L:94:VAL:HG13	2.03	0.59
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.85	0.59
1:A:272:LYS:N	1:A:272:LYS:HD2	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:L:302:SER:H	1:L:307:MET:HE3	1.67	0.58
1:C:155:ASP:OD1	1:C:157:THR:HB	2.03	0.58
1:G:272:LYS:HD2	1:G:272:LYS:N	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:N	1:K:272:LYS:HD2	2.18	0.58
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.69	0.58
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.84	0.58
1:F:242:LYS:C	1:F:244:GLY:H	2.10	0.58
1:F:362:ARG:O	1:F:366:GLN:HG3	2.04	0.58
1:K:166:MET:HE2	1:K:171:LYS:HA	1.84	0.58
1:B:242:LYS:C	1:B:244:GLY:H	2.11	0.58
1:D:11:ASP:HB2	6:D:2704:HOH:O	2.02	0.58
1:H:203:TYR:CD1	1:H:267:MET:HE1	2.39	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:HD2	1:H:272:LYS:N	2.19	0.58
1:K:349:ILE:HA	1:K:352:GLN:CG	2.33	0.58
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:I:242:LYS:C	1:I:244:GLY:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:GLY:O	1:A:389:MET:HG2	2.04	0.57
1:B:272:LYS:HD2	1:B:272:LYS:N	2.19	0.57
1:D:463:SER:HB2	6:D:2645:HOH:O	2.03	0.57
1:H:166:MET:HE2	1:H:171:LYS:CA	2.34	0.57
1:L:272:LYS:N	1:L:272:LYS:HD2	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:85:ALA:O	1:F:401:HIS:HE1	1.88	0.57
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.85	0.57
1:N:183:LEU:HD12	1:N:184:GLN:HG3	1.87	0.57
1:A:326:ASN:HD22	1:A:329:THR:HB	1.70	0.57
1:D:90:THR:O	1:D:94:VAL:HG13	2.05	0.57
1:H:360:TYR:OH	1:N:384:ALA:HA	2.04	0.57
1:I:349:ILE:HA	1:I:352:GLN:CG	2.33	0.57
1:K:183:LEU:HD12	1:K:184:GLN:HG3	1.87	0.57
1:L:386:GLU:O	1:L:390:LYS:HG2	2.04	0.57
1:N:183:LEU:CD1	1:N:184:GLN:HG3	2.34	0.57
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.86	0.57
1:N:362:ARG:O	1:N:366:GLN:HG3	2.05	0.57
1:A:218:PRO:CB	1:A:246:PRO:HG2	2.32	0.57
1:A:235:PRO:CG	1:A:310:GLU:HA	2.29	0.57
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.57
1:I:183:LEU:O	1:I:184:GLN:HB2	2.05	0.57
1:N:206:ASN:HD21	1:N:214:GLU:H	1.50	0.57
1:A:242:LYS:C	1:A:244:GLY:H	2.12	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:302:SER:H	1:I:307:MET:HE3	1.69	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:A:281:PHE:HZ	1:G:383:ALA:CB	2.15	0.57
1:D:160:LYS:HB2	1:D:160:LYS:NZ	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: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:C:242:LYS:C	1:C:244:GLY:H	2.11	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:D:386:GLU:O	1:D:390:LYS:HG2	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:J:383:ALA:O	1:J:384:ALA:HB3	2.05	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:L:384:ALA:HA	1:M:360:TYR:OH	2.05	0.56
1:A:183:LEU:O	1:A:184:GLN:HB2	2.06	0.56
1:J:233:MET:HE1	1:J:249:ILE:HD12	1.87	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:A:200:LEU:O	1:A:201:SER:HB3	2.04	0.56
1:B:183:LEU:HD12	1:B:184:GLN:HG3	1.86	0.56
1:E:71:ALA:O	1:E:75:LYS:HB2	2.05	0.56
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.88	0.56
1:A:282:GLY:HA3	1:G:181:THR:O	2.05	0.56
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.46	0.56
1:H:68:ASN:O	1:H:72:GLN:HG2	2.04	0.56
1:L:155:ASP:OD1	1:L:157:THR:HB	2.05	0.56
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:M:272:LYS:HD2	1:M:272:LYS:N	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:B:349:ILE:HA	1:B:352:GLN:CG	2.34	0.56
1:D:233:MET:HE1	1:D:249:ILE:HD12	1.87	0.56
1:E:300:VAL:HG22	6:E:2717:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.35	0.56
1:M:90:THR:OG1	5:M:1:AGS:S1G	2.63	0.56
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.04	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:J:302:SER:H	1:J:307:MET:HE3	1.70	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:A:69:MET:HE2	1:G:39:VAL:HG12	1.88	0.55
1:A:203:TYR:CD1	1:A:267:MET:HE1	2.42	0.55
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:233:MET:HE1	1:F:249:ILE:HD12	1.88	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:A:302:SER:H	1:A:307:MET:HE3	1.72	0.55
1:H:23:LEU:CD2	1:H:74:VAL:HG13	2.37	0.55
1:H:386:GLU:O	1:H:390:LYS:HG2	2.07	0.55
1:J:326:ASN:HD22	1:J:329:THR:HB	1.71	0.55
1:K: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:I:166:MET:HE2	1:I:171:LYS:CA	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
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:C:166:MET:HE2	1:C:171:LYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ILE:O	1:D:75:LYS:HE3	2.07	0.55
1:D:218:PRO:CB	1:D:246:PRO:HG2	2.33	0.55
1:G:200:LEU:O	1:G: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:L:200:LEU:O	1:L:201:SER:HB3	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:G:252:GLU:O	1:G:253:ASP:HB2	2.06	0.55
1:N:60:ILE:O	1:N:75:LYS:HE3	2.07	0.55
1:A:331:THR:HG22	6:A:2839:HOH:O	2.06	0.55
1:B:362:ARG:O	1:B:366:GLN:HG3	2.07	0.55
1:C:218:PRO:CB	1:C:246:PRO:HG2	2.35	0.55
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.89	0.55
1:G:386:GLU:O	1:G:390:LYS:HG2	2.07	0.55
1:K:362:ARG:O	1:K:366:GLN:HG3	2.07	0.55
1:B:384:ALA:O	1:B:385:THR:HG23	2.08	0.54
1:F:183:LEU:O	1:F:184:GLN:HB2	2.07	0.54
1:F:183:LEU:HD12	1:F:184:GLN:HG3	1.89	0.54
1:F:221:LEU:HD23	1:F:233:MET:HE1	1.88	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
1:K:221:LEU:HD23	1:K:233:MET:HE1	1.88	0.54
1:B:386:GLU:O	1:B:390:LYS:HG2	2.07	0.54
1:C:260:ALA:O	1:C:264:VAL:HG23	2.07	0.54
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:235:PRO:CG	1:B:310:GLU:HA	2.30	0.54
1:G:362:ARG:O	1:G:366:GLN:HG3	2.07	0.54
1:J:221:LEU:HD23	1:J:233:MET:HE1	1.89	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:I:233:MET:HE1	1:I:249:ILE:HD12	1.89	0.54
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.90	0.54
1:L:233:MET:HE1	1:L:249:ILE:HD12	1.89	0.54
1:N:218:PRO:CB	1:N:246:PRO:HG2	2.34	0.54
1:H:305:ILE:HG22	1:H:305:ILE:O	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:HB2	1:F:160:LYS:NZ	2.23	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:C:302:SER:H	1:C:307:MET:HE3	1.72	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:H:200:LEU:O	1:H:201:SER:HB3	2.07	0.54
1:E:166:MET:HE2	1:E:171:LYS:HA	1.88	0.54
1:G:242:LYS:C	1:G:244:GLY:N	2.64	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:L:221:LEU:HD23	1:L:233:MET:HE1	1.89	0.54
1:M:183:LEU:O	1:M:184:GLN:HB2	2.08	0.54
1:B:85:ALA:O	1:B:401:HIS:HE1	1.90	0.53
1:B:383:ALA:O	1:B:384:ALA:HB3	2.08	0.53
1:F:305:ILE:O	1:F:305:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:TYR:CD1	1:K:267:MET:HE1	2.43	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:G:233:MET:HE1	1:G:249:ILE:HD12	1.89	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:90:THR:O	1:J:94:VAL:HG13	2.09	0.53
1:N:203:TYR:CD1	1:N:267:MET:HE1	2.43	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:E:233:MET:HE1	1:E:249:ILE:HD12	1.90	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:M:203:TYR:CD1	1:M:267:MET:HE1	2.44	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:193:MET:HE1	1:G:292:ILE:CG1	2.33	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:G:155:ASP:OD1	1:G:157:THR:HB	2.08	0.53
1:J:310:GLU:OE1	1:J:310:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:ARG:O	1:E:366:GLN:HG3	2.09	0.53
1:I:90:THR:OG1	5:I:1:AGS:S1G	2.65	0.53
1:J:39:VAL:HG12	1:K:69:MET:HE2	1.91	0.53
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.74	0.53
1:L:319:GLN:O	1:L:336:VAL:HG23	2.09	0.53
1:M:155:ASP:OD1	1:M:157:THR:HB	2.08	0.53
1:M:183:LEU:H	1:M:383:ALA:CB	2.10	0.53
1:N:23:LEU:CD2	1:N:74:VAL:HG13	2.38	0.53
1:N:326:ASN:HD22	1:N:329:THR:HB	1.74	0.53
1:B:239:ALA:O	1:B:314:LEU:HD11	2.09	0.53
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.91	0.53
1:B:319:GLN:O	1:B:336:VAL:HG23	2.08	0.53
1:C:236:VAL:O	1:C:240:VAL:HG23	2.09	0.53
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.90	0.53
1:E:386:GLU:O	1:E:390:LYS:HG2	2.09	0.53
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.89	0.53
1:J:183:LEU:O	1:J:184:GLN:HB2	2.08	0.53
1:L:203:TYR:CD1	1:L:267:MET:HE1	2.44	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:D:242:LYS:C	1:D:244:GLY:N	2.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:382:GLY:O	1:I:389:MET:HG2	2.08	0.52
1:J:203:TYR:CD1	1:J:267:MET:HE1	2.44	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:M:319:GLN:HB3	1:M:336:VAL:HG21	1.92	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.39	0.52
1:H:90:THR:OG1	5:H:1:AGS:S1G	2.63	0.52
1:I:221:LEU:HD23	1:I:233:MET:HE1	1.91	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:C:305:ILE:HG22	1:C:305:ILE:O	2.09	0.52
1:G:235:PRO:CG	1:G:310:GLU:HA	2.32	0.52
1:H:383:ALA:O	1:H:384:ALA:HB3	2.09	0.52
1:K:90:THR:O	1:K:94:VAL:HG13	2.09	0.52
1:G:160:LYS:NZ	1:G:160:LYS:HB2	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:B:221:LEU:HD23	1:B:233:MET:HE1	1.92	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:B:160:LYS:HB2	1:B:160:LYS:NZ	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:M:221:LEU:HD23	1:M:233:MET:HE1	1.90	0.52
1:J:496:PRO:HB2	1:J:499:VAL:CG1	2.40	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:90:THR:O	1:M:94:VAL:HG13	2.10	0.52
1:M:134:LEU:HD21	1:M:425:LYS:NZ	2.25	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:27:VAL:HG12	1:E:90:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLU:O	1:E:253:ASP:HB2	2.10	0.52
1:E:319:GLN:O	1:E:336:VAL:HG23	2.10	0.52
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.92	0.52
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.51
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.10	0.51
1:G:305:ILE:O	1:G:305:ILE:HG22	2.10	0.51
1:I:305:ILE:O	1:I:305:ILE:HG22	2.10	0.51
1:K:235:PRO:CG	1:K:310:GLU:HA	2.35	0.51
1:M:284:ARG:NH1	1:M:364:LYS:NZ	2.58	0.51
1:M:305:ILE:O	1:M:305:ILE:HG22	2.09	0.51
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.51
1:B:203:TYR:CD1	1:B:267:MET:HE1	2.45	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:68:ASN:O	1:F:72:GLN:HG2	2.10	0.51
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.92	0.51
1:I:68:ASN:O	1:I:72:GLN:HG2	2.10	0.51
1:A:310:GLU:OE1	1:A:310:GLU:N	2.44	0.51
1:C:134:LEU:HD21	1:C:425:LYS:NZ	2.25	0.51
1:C:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:E:174:VAL:HG22	1:E:194:GLN:HE21	1.74	0.51
1:F:382:GLY:O	1:F:389:MET:HG2	2.10	0.51
1:I:239:ALA:O	1:I:314:LEU:HD11	2.10	0.51
1:K:305:ILE:HG22	1:K:305:ILE:O	2.10	0.51
1:L:242:LYS:C	1:L:244:GLY:N	2.69	0.51
1:A:54:VAL:HG23	6:A:2015:HOH:O	2.10	0.51
1:C:384:ALA:O	1:C:385:THR:HG23	2.11	0.51
1:D:384:ALA:HA	1:E:360:TYR:OH	2.11	0.51
1:E:183:LEU:CD1	1:E:184:GLN:HG3	2.40	0.51
1:F:223:ALA:O	1:F:251:ALA:HA	2.10	0.51
1:I:219:PHE:O	1:I:247:LEU:HD12	2.09	0.51
1:J:16:MET:O	1:J:20:VAL:HG13	2.11	0.51
1:A:160:LYS:HB2	1:A:160:LYS:NZ	2.26	0.51
1:E:305:ILE:HG22	1:E:305:ILE:O	2.10	0.51
1: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:J:252:GLU:O	1:J:253:ASP:HB2	2.10	0.51
1:K:233:MET:HE1	1:K:249:ILE:HD12	1.92	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:N:166:MET:HE2	1:N:171:LYS:CA	2.41	0.51
1:B:305:ILE:O	1:B:305:ILE:HG22	2.11	0.51
1:E:451:LEU:HD23	1:E:451:LEU:C	2.35	0.51
1:H:221:LEU:HD23	1:H:233:MET:HE1	1.93	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: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:M:383:ALA:O	1:M:384:ALA:HB3	2.09	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:90:THR:OG1	5:E:1:AGS:S1G	2.66	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:G:90:THR:OG1	5:G:1:AGS:S1G	2.66	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: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: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:B:271:VAL:HG12	1:B:273:VAL:HG23	1.93	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:OE1	1:M:310:GLU:N	2.44	0.50
1:N:383:ALA:O	1:N:384:ALA:HB3	2.10	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:54:VAL:HG23	6:I:2135:HOH:O	2.11	0.50
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.92	0.50
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.93	0.50
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.93	0.50
1:N:305:ILE:HG22	1:N:305:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:221:LEU:HD23	1:C:233:MET:HE1	1.92	0.50
1:E:413:ALA:CB	1:E:417:VAL:HG22	2.41	0.50
1:F:266:THR:CG2	1:F:273:VAL:H	2.25	0.50
1:G:326:ASN:HD22	1:G:329:THR:HB	1.75	0.50
1:I:193:MET:HE1	1:I:292:ILE:CG1	2.31	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: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:E:203:TYR:CD1	1:E:267:MET:HE1	2.46	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:M:233:MET:HE1	1:M:249:ILE:HD12	1.92	0.50
1:N:514:MET:SD	6:N:2800:HOH:O	2.60	0.50
1:C:203:TYR:CD1	1:C:267:MET:HE1	2.47	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:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.50
1:I:206:ASN:OD1	1:I:207:LYS:HG3	2.11	0.50
1:L:23:LEU:HD22	1:L:74:VAL:HG13	1.93	0.50
1:L:174:VAL:HG22	1:L:194:GLN:HE21	1.75	0.50
1:C:233:MET:HE1	1:C:249:ILE:HD12	1.94	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:M:209:GLU:N	1:M:209:GLU:OE1	2.44	0.50
1:D:271:VAL:HG12	1:D:273:VAL:HG23	1.92	0.50
1:F:203:TYR:CD1	1:F:267:MET:HE1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:310:GLU:N	1:K:310:GLU:OE1	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
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:B:166:MET:HE2	1:B:171:LYS:CA	2.41	0.49
1:B:179:ASP:HB3	1:B:389:MET:HE1	1.94	0.49
1:D:78:ALA:HB1	1:D:89:THR:HB	1.94	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.92	0.49
1:E:236:VAL:O	1:E:240:VAL:HG23	2.12	0.49
1:F:166:MET:HE2	1:F:171:LYS:CA	2.43	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:N:242:LYS:C	1:N:244:GLY:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:O	1:C:72:GLN:HG2	2.12	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.11	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:C:239:ALA:C	1:C:314:LEU:HD21	2.38	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
1:D:202:PRO:O	1:D:203:TYR:HB2	2.12	0.49
1:G:203:TYR:CD1	1:G:267:MET:HE1	2.48	0.49
1:H:336:VAL:O	1:H:337:GLY:C	2.56	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:N:221:LEU:HD23	1:N:233:MET:HE1	1.94	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:5:ASP:HB2	1:B:524:LEU:HD12	1.95	0.49
1:B:223:ALA:O	1:B:251:ALA:HA	2.13	0.49
1:B:524:LEU:C	1:B:526:LYS:H	2.20	0.49
1:B:525:PRO:HD3	6:B:1427:HOH:O	2.13	0.49
1:C:319:GLN:O	1:C:336:VAL:HG23	2.13	0.49
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:60:ILE:O	1:A:75:LYS:HE3	2.13	0.49
1:A:271:VAL:HG12	1:A:273:VAL:HG23	1.94	0.49
1:C:63:GLU:OE2	1:D:526:LYS:HE2	2.13	0.49
1:E:193:MET:HE1	1:E:292:ILE:CG1	2.31	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:L:193:MET:HE1	1:L:292:ILE:CG1	2.31	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:234:LEU:O	1:N:238:GLU:HG3	2.13	0.49
1:A:39:VAL:HG12	1:B:69:MET:HE2	1.95	0.48
1:D:310:GLU:OE1	1:D:310:GLU:N	2.46	0.48
1:E:206:ASN:OD1	1:E:207:LYS:HG3	2.13	0.48
1:F:235:PRO:CG	1:F:310:GLU:HA	2.31	0.48
1:I:203:TYR:CD1	1:I:267:MET:HE1	2.48	0.48
1:I:266:THR:HG22	1:I:271:VAL:O	2.13	0.48
1:I:319:GLN:O	1:I:336:VAL:HG23	2.13	0.48
1:M:223:ALA:O	1:M:251:ALA:HA	2.13	0.48
1:A:233:MET:HE1	1:A:249:ILE:HD12	1.95	0.48
1:B:179:ASP:HB3	1:B:389:MET:CE	2.44	0.48
1:B:404:ARG:HG2	1:B:404:ARG:HH11	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:69:MET:O	1:G:73:MET:HG3	2.13	0.48
1:G:259:LEU:O	1:G:263:VAL:HG23	2.13	0.48
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.95	0.48
1:H:384:ALA:O	1:H:385:THR:HG23	2.13	0.48
1:L:23:LEU:CD2	1:L:74:VAL:HG13	2.42	0.48
1:L:69:MET:O	1:L:73:MET:HG3	2.13	0.48
1:L:326:ASN:HD22	1:L:329:THR:HB	1.77	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:B:233:MET:HE1	1:B:249:ILE:HD12	1.95	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:73:MET:O	1:F:76:GLU:HB2	2.13	0.48
1:F:319:GLN:O	1:F:336:VAL:HG23	2.12	0.48
1:G:336:VAL:O	1:G:337:GLY:C	2.55	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:K:202:PRO:O	1:K:203:TYR:HB2	2.12	0.48
1:K:242:LYS:C	1:K:244:GLY:N	2.71	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:77:VAL:HG11	1:B:510:VAL:CG2	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:O	1:C:526:LYS:N	2.45	0.48
1:E:242:LYS:C	1:E:244:GLY:N	2.71	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:H:242:LYS:C	1:H:244:GLY:N	2.70	0.48
1:I:73:MET:O	1:I:76:GLU:HB2	2.13	0.48
1:J:206:ASN:OD1	1:J:207:LYS:HG3	2.13	0.48
1:J:496:PRO:HB2	1:J:499:VAL:HG12	1.94	0.48
1:K:160:LYS:O	1:K:164:GLU:HG3	2.12	0.48
1:L:176:THR:HG22	1:L:177:VAL:N	2.28	0.48
1:L:384:ALA:O	1:L:385:THR:HG23	2.14	0.48
1:M:281:PHE:H	1:M:284:ARG:HD2	1.76	0.48
1: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:B:384:ALA:C	1:B:385:THR:HG23	2.38	0.48
1:B:451:LEU:HD23	1:B:451:LEU:C	2.39	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:63:GLU:OE2	1:E:526:LYS:HE2	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
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:242:LYS:C	1:J:244:GLY:N	2.71	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:46:ALA:HB2	1:B:76:GLU:HG2	1.93	0.48
1:A:166:MET:HE2	1:A:171:LYS:CA	2.44	0.48
1:A:176:THR:HG21	1:A:322:ARG:HH12	1.79	0.48
1:A:206:ASN:OD1	1:A:207:LYS:HG3	2.13	0.48
1:B:200:LEU:HG	1:B:276:VAL:HA	1.96	0.48
1:G:166:MET:HE2	1:G:171:LYS:CA	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:384:ALA:C	1:H:385:THR:HG23	2.39	0.48
1:J:166:MET:HE2	1:J:171:LYS:CA	2.43	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:242:LYS:C	1:C:244:GLY:N	2.72	0.48
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	0.48
1:D:113:PRO:HD2	6:D:2375:HOH:O	2.14	0.48
1:D:524:LEU:O	1:D:526:LYS:N	2.46	0.48
1:E:259:LEU:O	1:E:263:VAL:HG23	2.14	0.48
1:F:180:GLY:HA3	1:F:381:VAL:O	2.13	0.48
1:F:252:GLU:O	1:F:253:ASP:HB2	2.14	0.48
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.93	0.48
1:H:219:PHE:O	1:H:247:LEU:HD12	2.13	0.48
1:H:252:GLU:O	1:H:253:ASP:HB2	2.12	0.48
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.49	0.48
1:J:193:MET:HE1	1:J:292:ILE:CG1	2.36	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:D:166:MET:HE2	1:D:171:LYS:CA	2.42	0.48
1:F:222:LEU:HB3	1:F:289:LEU:CD2	2.44	0.48
1:G:73:MET:O	1:G:76:GLU:HB2	2.13	0.48
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.96	0.48
1:H:266:THR:HG22	1:H:271:VAL:O	2.14	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ALA:O	1:G:314:LEU:HD11	2.14	0.47
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.96	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.95	0.47
1:A: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:37:ASN:HD21	1:K:51:LYS:HE3	1.80	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: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:OE1	1:G:209:GLU:N	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
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.50	0.47
1:A:209:GLU:OE1	1:A:209:GLU:N	2.44	0.47
1:A:231:ARG:NH1	1:G:242:LYS:HG2	2.28	0.47
1:B:206:ASN:OD1	1:B:207:LYS:HG3	2.13	0.47
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	0.47
1:D:217:SER:N	1:D:218:PRO:CD	2.78	0.47
1:H: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:384:ALA:C	1:C:385:THR:HG23	2.39	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:N:336:VAL:O	1:N:337:GLY:C	2.58	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:D:252:GLU:O	1:D:253:ASP:HB2	2.15	0.47
1:F:384:ALA:C	1:F:385:THR:HG23	2.40	0.47
1:H:206:ASN:OD1	1:H:207:LYS:HG3	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:176:THR:HG22	1:J:177:VAL:N	2.29	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:L:366:GLN:HA	1:L:369:VAL:HG22	1.95	0.47
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.50	0.47
1:M: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:N:183:LEU:HD13	1:N:184:GLN:N	2.29	0.47
1:A:134:LEU:HD21	1:A:425:LYS:NZ	2.30	0.47
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.50	0.47
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.96	0.47
1:D:382:GLY:O	1:D:389:MET:HG2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:THR:O	1:E:94:VAL:HG13	2.14	0.47
1:E:260:ALA:O	1:E:264:VAL:HG23	2.15	0.47
1:I:336:VAL:O	1:I:337:GLY:C	2.58	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:K:384:ALA:C	1:K:385:THR:HG23	2.39	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:HB2	1:M:160:LYS:NZ	2.29	0.47
1:M:166:MET:HE2	1:M:171:LYS:CA	2.44	0.47
1:A:236:VAL:O	1:A:240:VAL:HG23	2.15	0.47
1:C:23:LEU:CD2	1:C:74:VAL:HG13	2.45	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:D:193:MET:CE	1:D:292:ILE:HG12	2.28	0.47
1:D:206:ASN:HD21	1:D:214:GLU:H	1.63	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: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:A:169:VAL:HG13	1:A:377:ALA:HB2	1.97	0.46
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.98	0.46
1:C:60:ILE:O	1:C:75:LYS:HE3	2.15	0.46
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.81	0.46
1:G:384:ALA:O	1:G:385:THR:HG23	2.15	0.46
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:I:260:ALA:O	1:I:264:VAL:HG23	2.14	0.46
1:I:325:ILE:HG22	1:I:330:THR:HA	1.98	0.46
1:M:63:GLU:OE2	1:N:526:LYS:HE2	2.15	0.46
1:N:155:ASP:OD1	1:N:157:THR:HB	2.14	0.46
1:A:336:VAL:O	1:A:337:GLY:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:LYS:C	1:F:244:GLY:N	2.73	0.46
1:G:78:ALA:HB1	1:G:89:THR:HB	1.96	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.46
5:G:1:AGS:S1G	5:G:1:AGS:O2G	2.53	0.46
1:H:233:MET:HE1	1:H:249:ILE:HD12	1.96	0.46
1:I:463:SER:HB2	6:I:2586:HOH:O	2.14	0.46
1:K:166:MET:HE2	1:K:171:LYS:CA	2.45	0.46
1:K:239:ALA:C	1:K:314:LEU:HD21	2.41	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:OE1	1:D:209:GLU:N	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:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.98	0.46
1:J:384:ALA:O	1:J:385:THR:OG1	2.33	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:G:202:PRO:C	1:G:204:PHE:H	2.23	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:J:336:VAL:O	1:J:337:GLY:C	2.58	0.46
1:K:16:MET:SD	1:K:73:MET:HE1	2.55	0.46
1:K:60:ILE:O	1:K:75:LYS:HE3	2.16	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: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:M:242:LYS:C	1:M:244:GLY:N	2.72	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:OE1	1:C:209:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:LEU:N	1:F:235:PRO:HD2	2.30	0.46
1:F:383:ALA:O	1:F:384:ALA:CB	2.63	0.46
1:G:384:ALA:C	1:G:385:THR:HG23	2.40	0.46
1:H:250:ILE:HG22	6:H:2938:HOH:O	2.15	0.46
1:H:404:ARG:NH1	1:H:404:ARG:CG	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:B:242:LYS:C	1:B:244:GLY:N	2.73	0.46
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.79	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:H:295:LEU:HD13	1:H:295:LEU:C	2.41	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:69:MET:HE2	1:G:39:VAL:CG1	2.46	0.46
1:A:78:ALA:HB3	6:A:2430:HOH:O	2.15	0.46
1:B:336:VAL:O	1:B:337:GLY:C	2.59	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:K:204:PHE:C	1:K:213:VAL:HG22	2.41	0.46
1:L:384:ALA:C	1:L:385:THR:HG23	2.40	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:D:203:TYR:CD1	1:D:267:MET:HE1	2.51	0.46
1:E:234:LEU:N	1:E:235:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.98	0.46
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.97	0.46
1:H:183:LEU:CD2	1:H:384:ALA:HB2	2.45	0.46
1:H:353:ILE:HD13	1:H:366:GLN:HG2	1.98	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:78:ALA:HB1	1:K:89:THR:HB	1.98	0.46
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.98	0.46
1:L:68:ASN:O	1:L:72:GLN:HG2	2.16	0.46
1:A:242:LYS:C	1:A:244:GLY:N	2.73	0.46
1:A:325:ILE:HG22	1:A:330:THR:HA	1.98	0.46
1:A:486:GLY:C	1:A:491:MET:HE2	2.41	0.46
1:A:524:LEU:O	1:A:526:LYS:N	2.48	0.46
1:D:41:ASP:CA	1:E:69:MET:HE3	2.46	0.46
1:E:336:VAL:O	1:E:337:GLY:C	2.58	0.46
1:I:69:MET:O	1:I:73:MET:HG3	2.15	0.46
1:K:234:LEU:N	1:K:235:PRO:HD2	2.31	0.46
1:L:90:THR:OG1	5:L:1:AGS:S1G	2.65	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:D:263:VAL:HG12	1:D:267:MET:HE2	1.98	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: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:G:384:ALA:O	1:G:385:THR:OG1	2.32	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:215:LEU:HB2	1:N:323:VAL:CG2	2.47	0.45
1:N:271:VAL:HG12	1:N:273:VAL:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ILE:HG21	1:D:309:LEU:HD23	1.98	0.45
1:E:202:PRO:C	1:E:204:PHE:H	2.23	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:217:SER:N	1:F:218:PRO:CD	2.79	0.45
1:H:216:GLU:C	1:H:218:PRO:HD3	2.41	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
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:37:ASN:ND2	1:K:51:LYS:HE3	2.32	0.45
1:K:217:SER:N	1:K:218:PRO:CD	2.80	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:M:384:ALA:C	1:M:385:THR:HG23	2.42	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: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:K:451:LEU:HD23	1:K:451:LEU:C	2.41	0.45
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.99	0.45
1:N:384:ALA:C	1:N:385:THR:HG23	2.41	0.45
1:A:185:ASP:OD1	1:A:382:GLY:N	2.48	0.45
1:C:336:VAL:O	1:C:337:GLY:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:VAL:HG12	1:B:69:MET:CE	2.47	0.45
1:A:295:LEU:HD13	1:A:295:LEU:C	2.42	0.45
1:A:369:VAL:HG23	1:A:370:ALA:N	2.32	0.45
1:B:39:VAL:CG1	1:C:69:MET:HE2	2.47	0.45
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.17	0.45
1:C:206:ASN:OD1	1:C:207:LYS:HG3	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:E:369:VAL:HG23	1:E:370:ALA:N	2.30	0.45
1:E:384:ALA:C	1:E:385:THR:HG23	2.42	0.45
1:G:238:GLU:O	1:G:241:ALA:HB3	2.16	0.45
1:H:202:PRO:C	1:H:204:PHE:H	2.24	0.45
1:I:384:ALA:C	1:I:385:THR:HG23	2.41	0.45
1:K:486:GLY:C	1:K:491:MET:HE2	2.42	0.45
1:L:222:LEU:HB3	1:L:289:LEU:CD2	2.46	0.45
1:L:524:LEU:HD12	1:L:524:LEU:HA	1.87	0.45
1:M:222:LEU:HB3	1:M:289:LEU:CD2	2.47	0.45
1:E:210:THR:HG22	1:E:210:THR:O	2.17	0.45
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.47	0.45
1:F:325:ILE:HG22	1:F:330:THR:HA	1.98	0.45
1:F:366:GLN:O	1:F:369:VAL:HG22	2.16	0.45
1:G:463:SER:O	1:G:467:ASN:HB2	2.17	0.45
1:I:242:LYS:C	1:I:244:GLY:N	2.73	0.45
1:K:295:LEU:HD13	1:K:295:LEU:C	2.42	0.45
1:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.45
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.99	0.45
1:N:90:THR:O	1:N:94:VAL:HG13	2.16	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: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:F:325:ILE:HA	1:F:329:THR:O	2.17	0.45
1:J:160:LYS:HB2	1:J:160:LYS:NZ	2.32	0.45
1:J:239:ALA:O	1:J:314:LEU:HD11	2.16	0.45
1:J:272:LYS:NZ	1:K:229:ASN:OD1	2.50	0.45
1:K:88:GLY:HA2	5:K:1:AGS:PB	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:260:ALA:O	1:K:264:VAL:HG23	2.16	0.45
1:K:342:ILE:O	1:K:346:VAL:HG23	2.16	0.45
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.98	0.45
1:L:369:VAL:HG23	1:L:370:ALA:N	2.32	0.45
1:M:295:LEU:C	1:M:295:LEU:HD13	2.42	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:39:VAL:HG12	1:C:69:MET:CE	2.47	0.45
1:B:342:ILE:O	1:B:346:VAL:HG23	2.17	0.45
1:C:179:ASP:HB3	1:C:389:MET:HE1	1.99	0.45
1:C:210:THR:O	1:C:210:THR:HG22	2.17	0.45
1:D:451:LEU:C	1:D:451:LEU:HD23	2.42	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: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:N:233:MET:HE1	1:N:249:ILE:HD12	1.99	0.45
1:A:384:ALA:C	1:A:385:THR:HG23	2.41	0.44
1:C:182:GLY:HA2	1:C:383:ALA:HB3	1.97	0.44
1:C:381:VAL:O	1:C:382:GLY:O	2.36	0.44
1:D:39:VAL:CG1	1:E:69:MET:HE2	2.46	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:I:295:LEU:HD13	1:I:295:LEU:C	2.42	0.44
1:J:37:ASN:HD21	1:J:51:LYS:HE3	1.80	0.44
1:K:209:GLU:OE1	1:K:209:GLU:N	2.47	0.44
1: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:16:MET:SD	1:B:73:MET:HE1	2.57	0.44
1:B:209:GLU:OE1	1:B:209:GLU:N	2.48	0.44
1:B:384:ALA:HA	1:C:360:TYR:OH	2.17	0.44
1:B:455:VAL:O	1:B:458:CYS:HB2	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:N:301:ILE:HG21	1:N:309:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:353:ILE:HD13	1:N:366:GLN:HG2	1.99	0.44
1:B:204:PHE:C	1:B:213:VAL:HG22	2.41	0.44
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.00	0.44
1:D:202:PRO:C	1:D:204:PHE:H	2.24	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:F:336:VAL:O	1:F:337:GLY:C	2.60	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:J:295:LEU:C	1:J:295:LEU:HD13	2.43	0.44
1:K:182:GLY:HA2	1:K:383:ALA:HB3	1.99	0.44
1:L:336:VAL:O	1:L:337:GLY:C	2.59	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:F:383:ALA:C	6:F:2746:HOH:O	2.60	0.44
1:H:155:ASP:OD1	1:H:157:THR:HB	2.18	0.44
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.99	0.44
1: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:210:THR:O	1:K:210:THR:HG22	2.16	0.44
1:K:222:LEU:HB3	1:K:289:LEU:CD2	2.48	0.44
1:K:266:THR:HG22	1:K:271:VAL:O	2.17	0.44
1: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: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:D:384:ALA:C	1:D:385:THR:HG23	2.42	0.44
1:E:239:ALA:C	1:E:314:LEU:HD21	2.43	0.44
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.99	0.44
1:G:210:THR:O	1:G:210:THR:HG22	2.17	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.18	0.44
1:J:217:SER:N	1:J:218:PRO:HD3	2.32	0.44
1:J:324:VAL:O	1:J:331:THR:HG22	2.18	0.44
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.44
1:K:134:LEU:HD21	1:K:425:LYS:NZ	2.32	0.44
1:K:413:ALA:HB3	1:K:417:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:1:AGS:S1G	5:K:1:AGS:O2G	2.55	0.44
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.99	0.44
1:M:73:MET:HB3	6:M:2221:HOH:O	2.18	0.44
1:M:290:GLN:HB3	1:M:345:ARG:NH2	2.31	0.44
1:N:384:ALA:O	1:N:385:THR:HG23	2.17	0.44
1:B:239:ALA:C	1:B:314:LEU:HD21	2.43	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:183:LEU:CD2	1:F:384:ALA:HB2	2.47	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: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:68:ASN:O	1:J:72:GLN:HG2	2.17	0.44
1:J:217:SER:N	1:J:218:PRO:CD	2.81	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:202:PRO:C	1:C:204:PHE:H	2.25	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:202:PRO:C	1:I:204:PHE:H	2.25	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:K:216:GLU:C	1:K:218:PRO:HD3	2.43	0.44
1:N:252:GLU:O	1:N:253:ASP:HB2	2.16	0.44
1:A:69:MET:CE	1:G:39:VAL:HG12	2.47	0.44
1:C:179:ASP:HB3	1:C:389:MET:CE	2.48	0.44
1:E:234:LEU:O	1:E:238:GLU:HG3	2.17	0.44
1:F:389:MET:N	6:F:2746:HOH:O	2.50	0.44
1:J:384:ALA:C	1:J:385:THR:HG23	2.42	0.44
1:M:369:VAL:HG23	1:M:370:ALA:N	2.32	0.44
1:M:384:ALA:O	1:M:385:THR:OG1	2.33	0.44
1:N:42:LYS:HE3	1:N:48:THR:OG1	2.18	0.44
1:N:217:SER:N	1:N:218:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:TYR:CZ	1:F:327:LYS:HA	2.53	0.43
1:F:260:ALA:O	1:F:264:VAL:HG23	2.18	0.43
1:G:381:VAL:O	1:G:382:GLY:O	2.36	0.43
1:H:69:MET:HE2	1:N:39:VAL:HG12	2.00	0.43
1:H:217:SER:N	1:H:218:PRO:HD3	2.33	0.43
1:I:239:ALA:C	1:I:314:LEU:HD21	2.42	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.17	0.43
1:M:210:THR:HG22	1:M:210:THR:O	2.18	0.43
1:M:268:ARG:C	1:M:270:ILE:H	2.25	0.43
1:M:336:VAL:O	1:M:337:GLY:C	2.60	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:263:VAL:HG12	1:F:267:MET:HE2	2.00	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:160:LYS:HB2	1:H:160:LYS:HZ3	1.83	0.43
1:H:518:GLU:HG2	6:N:1187:HOH:O	2.18	0.43
1:K:336:VAL:O	1:K:337:GLY:C	2.61	0.43
1:L:199:TYR:CZ	1:L:327:LYS:HA	2.53	0.43
1:L:295:LEU:C	1:L:295:LEU:HD13	2.42	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:D:216:GLU:C	1:D:218:PRO:HD3	2.44	0.43
1:E:73:MET:O	1:E:76:GLU:HB2	2.18	0.43
1:F:295:LEU:HD13	1:F:295:LEU:C	2.43	0.43
1:F:451:LEU:HD23	1:F:451:LEU:C	2.43	0.43
1:G:351:GLN:HA	1:G:354:GLU:HG2	1.99	0.43
1:H:260:ALA:O	1:H:264:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:179:ASP:HB3	1:M:389:MET:HE1	2.00	0.43
1:N:210:THR:O	1:N:210:THR:HG22	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:O	1:A:210:THR:HG22	2.18	0.43
1:A:221:LEU:HD23	1:A:233:MET:HE1	1.99	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:M:239:ALA:C	1:M:314:LEU:HD21	2.43	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:2:ALA:O	1:B:3:ALA:C	2.61	0.43
1:B:218:PRO:HD2	1:B:320:ALA:O	2.18	0.43
1:B:266:THR:HG22	1:B:271:VAL:O	2.19	0.43
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.01	0.43
1:D:203:TYR:CG	1:D:267:MET:HE1	2.53	0.43
1:G:224:ASP:HB3	1:G:302:SER:HB3	2.00	0.43
1:J:69:MET:O	1:J:73:MET:HG3	2.19	0.43
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.54	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:263:VAL:HG12	1:N:267:MET:HE2	2.01	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:D:325:ILE:HG22	1:D:330:THR:HG23	1.99	0.43
1:F:178:GLU:OE2	1:F:322:ARG:NH1	2.51	0.43
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.00	0.43
1:H:183:LEU:HD13	1:H:184:GLN:N	2.33	0.43
1:H:409:GLU:OE2	1:H:498:LYS:HG3	2.19	0.43
1:I:210:THR:O	1:I:210:THR:HG22	2.19	0.43
1:J:210:THR:HG22	1:J:210:THR:O	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:L:204:PHE:C	1:L:213:VAL:HG22	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:82:ASN:O	1:N:86:GLY:N	2.49	0.43
1:A:194:GLN:OE1	1:A:329:THR:HG21	2.18	0.43
1:A:384:ALA:O	1:A:385:THR:OG1	2.33	0.43
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.52	0.43
1:B:202:PRO:C	1:B:204:PHE:H	2.26	0.43
1:B:234:LEU:O	1:B:238:GLU:HG3	2.18	0.43
1:E:18:ARG:HG2	1:E:67:GLU:CD	2.44	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:G:302:SER:H	1:G:307:MET:CE	2.28	0.43
1:H:369:VAL:HG23	1:H:370:ALA:N	2.34	0.43
1:J:209:GLU:OE1	1:J:209:GLU:N	2.47	0.43
1:L:85:ALA:O	1:L:401:HIS:HE1	2.01	0.43
1:N:153:ASN:O	1:N:154:SER:HB2	2.18	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:I:263:VAL:HG12	1:I:267:MET:HE2	2.01	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:N:233:MET:C	1:N:235:PRO:HD2	2.44	0.43
1:C:295:LEU:HD13	1:C:295:LEU:C	2.44	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:239:ALA:C	1:F:314:LEU:HD21	2.44	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:I:179:ASP:HB3	1:I:389:MET:HE1	2.00	0.43
1:K:384:ALA:O	1:K:385:THR:OG1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:LEU:HB3	1:N:289:LEU:HD21	2.01	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.43
1:A:417:VAL:HG11	1:A:488:MET:HG3	2.00	0.43
1:B:241:ALA:HB1	1:C:231:ARG:NH1	2.33	0.43
1:C:204:PHE:C	1:C:213:VAL:HG22	2.44	0.43
1:D:65:LYS:HG2	6:D:1200:HOH:O	2.19	0.43
1:D:234:LEU:O	1:D:238:GLU:HG3	2.18	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
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:193:MET:HE1	1:C:292:ILE:CG1	2.33	0.42
1:C:421:ARG:CZ	1:C:473:ASP:HA	2.49	0.42
1:D:384:ALA:O	1:D:385:THR:OG1	2.35	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:G:451:LEU:HD23	1:G:451:LEU:C	2.44	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:263:VAL:HG12	1:K:267:MET:HE2	2.02	0.42
1:L:60:ILE:O	1:L:75:LYS:HE3	2.19	0.42
1:L:383:ALA:O	1:L:384:ALA:CB	2.66	0.42
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.00	0.42
1:M:284:ARG:HH11	1:M:364:LYS:CE	2.32	0.42
5:N:1:AGS:S1G	5:N:1:AGS:O2G	2.54	0.42
1:A:204:PHE:C	1:A:213:VAL:HG22	2.44	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: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:J:239:ALA:C	1:J:314:LEU:HD21	2.44	0.42
1:K:319:GLN:HB3	1:K:336:VAL:HG21	2.00	0.42
1:M:496:PRO:O	1:M:499:VAL:HG13	2.19	0.42
1:A:202:PRO:C	1:A:204:PHE:H	2.24	0.42
1:A:253:ASP:OD1	1:A:277:LYS:HE2	2.19	0.42
1:C:496:PRO:O	1:C:499:VAL:HG13	2.19	0.42
1:D:37:ASN:HD21	1:D:51:LYS:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:O	1:D:288:MET:HG3	2.19	0.42
1:E:220:ILE:CD1	1:E:296:THR:HG21	2.48	0.42
1:E:295:LEU:C	1:E:295:LEU:HD13	2.45	0.42
1:F:204:PHE:C	1:F:213:VAL:HG22	2.44	0.42
1:H:233:MET:C	1:H:235:PRO:HD2	2.45	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:N	1:N:272:LYS:CD	2.83	0.42
1:A:8:PHE:HB3	6:A:1960:HOH:O	2.20	0.42
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	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:36:ARG:HG3	1:E:518:GLU:HG2	2.00	0.42
1:D:206:ASN:OD1	1:D:207:LYS:HG3	2.19	0.42
1:D:336:VAL:O	1:D:337:GLY:C	2.61	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:G:85:ALA:O	1:G:401:HIS:HE1	2.02	0.42
1:G:302:SER:N	1:G:307:MET:HE3	2.31	0.42
1:G:524:LEU:O	1:G:526:LYS:N	2.52	0.42
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.42
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.02	0.42
1:L:94:VAL:HB	6:L:2642:HOH:O	2.20	0.42
1:M:288:MET:HA	1:M:291:ASP:OD2	2.19	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:N:206:ASN:ND2	1:N:214:GLU:H	2.16	0.42
1: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:60:ILE:O	1:F:75:LYS:HE3	2.19	0.42
1:F:183:LEU:HD13	1:F:184:GLN:N	2.34	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:215:LEU:HB2	1:J:323:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:GLU:O	1:J:241:ALA:HB3	2.20	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:L:202:PRO:C	1:L:204:PHE:H	2.25	0.42
1:M:284:ARG:HH11	1:M:364:LYS:NZ	2.18	0.42
6:C:2549:HOH:O	1:J:463:SER:HB2	2.19	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:305:ILE:HD12	1:F:307:MET:HE2	2.01	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:I:233:MET:C	1:I:235:PRO:HD2	2.45	0.42
1:J:182:GLY:HA2	1:J:383:ALA:HB3	2.02	0.42
1:J:348:GLN:O	1:J:352:GLN:HG2	2.19	0.42
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.60	0.42
1:K:460:GLU:O	1:K:462:PRO:HD3	2.18	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:F:268:ARG:C	1:F:270:ILE:H	2.27	0.42
1:H:182:GLY:HA2	1:H:383:ALA:HB3	2.02	0.42
1:I:179:ASP:HB3	1:I:389:MET:CE	2.49	0.42
1:J:206:ASN:ND2	1:J:214:GLU:H	2.17	0.42
1: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: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:B:216:GLU:C	1:B:218:PRO:HD3	2.45	0.42
1:E:216:GLU:C	1:E:218:PRO:HD3	2.45	0.42
1:F:206:ASN:ND2	1:F:214:GLU:H	2.16	0.42
1:H:210:THR:O	1:H:210:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:384:ALA:O	1:I:385:THR:OG1	2.36	0.42
1:J:90:THR:OG1	5:J:1:AGS:S1G	2.75	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:HD12	1:M:524:LEU:HA	1.87	0.42
1:A:4:LYS:HG3	1:G:59:GLU:O	2.19	0.42
1:B:77:VAL:HG11	1:B:506:TYR:O	2.18	0.42
1:B:324:VAL:O	1:B:331:THR:HG22	2.20	0.42
1:C:166:MET:HE2	1:C:171:LYS:CA	2.49	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:369:VAL:HG23	1:N:370:ALA:N	2.35	0.42
1:B:473:ASP:CG	1:B:474:GLY:H	2.28	0.42
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:F:384:ALA:O	1:F:385:THR:OG1	2.36	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:M:204:PHE:C	1:M:213:VAL:HG22	2.45	0.42
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.35	0.42
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:216:GLU:C	1:F:218:PRO:HD3	2.45	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:183:LEU:CD2	1:N:384:ALA:HB2	2.49	0.41
1:N:325:ILE:HA	1:N:329:THR:O	2.18	0.41
1:A:176:THR:HG22	1:A:177:VAL:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASP:HB3	1:A:389:MET:HE1	2.01	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: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
1:J:202:PRO:C	1:J:204:PHE:H	2.27	0.41
1:L:97:GLN:HG2	6:L:2018:HOH:O	2.19	0.41
1:L:263:VAL:HG12	1:L:267:MET:HE2	2.02	0.41
5:L:1:AGS:S1G	5:L:1:AGS:O2G	2.55	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
1:E:183:LEU:CD2	1:E:384:ALA:HB2	2.50	0.41
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: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:239:ALA:C	1:G:314:LEU:HD21	2.45	0.41
1:L:122:LYS:HE2	1:L:429:LEU:HD11	2.02	0.41
1:L:210:THR:O	1:L:210:THR:HG22	2.20	0.41
1:L:384:ALA:O	1:L:385:THR:OG1	2.32	0.41
1:N:69:MET:O	1:N:73:MET:HG3	2.19	0.41
1:N:209:GLU:OE1	1:N:209:GLU:N	2.48	0.41
1:N:524:LEU:HD12	1:N:524:LEU:HA	1.91	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:204:PHE:C	1:H:213:VAL:HG22	2.45	0.41
1:I:217:SER:HA	1:I:320:ALA:O	2.20	0.41
1:J:177:VAL:HA	1:J:379:ILE:O	2.20	0.41
1:J:295:LEU:HD13	1:J:295:LEU:O	2.20	0.41
1:K: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:MET:HE1	1:M:292:ILE:CG1	2.39	0.41
1:N:176:THR:HG22	1:N:177:VAL:N	2.35	0.41
1:N:451:LEU:HD23	1:N:451:LEU:C	2.46	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:182:GLY:HA2	1:D:383:ALA:HB3	2.03	0.41
1:D:284:ARG:NH1	1:D:364:LYS:NZ	2.67	0.41
1:E:28:LYS:HD2	1:E:453:GLN:NE2	2.36	0.41
1:E:178:GLU:OE1	1:E:378:VAL:HG11	2.20	0.41
1:E:182:GLY:HA2	1:E:383:ALA:HB3	2.02	0.41
1:E:204:PHE:C	1:E:213:VAL:HG22	2.46	0.41
1:E:325:ILE:HG22	1:E:330:THR:HG23	2.02	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:I:305:ILE:HD12	1:I:307:MET:HE2	2.02	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
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:C:182:GLY:HA2	1:C:383:ALA:CB	2.50	0.41
1:C:216:GLU:C	1:C:218:PRO:HD3	2.46	0.41
1:D:200:LEU:HG	1:D:276:VAL:HA	2.01	0.41
1:D:210:THR:O	1:D:210:THR:HG22	2.19	0.41
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.41
1:G:263:VAL:HG12	1:G:267:MET:HE2	2.01	0.41
1:H:85:ALA:O	1:H:401:HIS:HE1	2.03	0.41
1:I:324:VAL:O	1:I:331:THR:HG22	2.21	0.41
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.56	0.41
1:K:295:LEU:HD13	1:K:295:LEU:O	2.20	0.41
1:K:366:GLN:O	1:K:369:VAL:HG22	2.20	0.41
1:L:239:ALA:C	1:L:314:LEU:HD21	2.46	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:N:179:ASP:HB3	1:N:389:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:NH1	1:G:242:LYS:HA	2.35	0.41
1:A:266:THR:HG21	1:A:273:VAL:H	1.86	0.41
1:B:69:MET:O	1:B:73:MET:HG3	2.20	0.41
1:B:199:TYR:C	1:B:201:SER:H	2.29	0.41
1:N:455:VAL:O	1:N:458:CYS:HB2	2.21	0.41
1:A:268:ARG:C	1:A:270:ILE:H	2.29	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: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:183:LEU:CD2	1:G:384:ALA:HB2	2.48	0.41
1:G:266:THR:HG22	1:G:273:VAL:H	1.86	0.41
1:I:242:LYS:O	1:I:243:ALA:HB3	2.20	0.41
1:J:140:ASP:OD2	1:J:142:LYS:HB3	2.21	0.41
1:K:381:VAL:O	1:K:382:GLY:O	2.39	0.41
1:L:194:GLN:HG3	1:L:331:THR:HB	2.03	0.41
1:M:134:LEU:HD21	1:M:425:LYS:HZ2	1.86	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:N:295:LEU:HD13	1:N:295:LEU:C	2.45	0.41
1:A:194:GLN:HG3	1:A:331:THR:HB	2.02	0.41
1:A:239:ALA:C	1:A:314:LEU:HD21	2.46	0.41
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.41
1:B:174:VAL:HG22	1:B:194:GLN:NE2	2.36	0.41
1:B:177:VAL:HA	1:B:379:ILE:O	2.21	0.41
1:B:194:GLN:HG3	1:B:331:THR:HB	2.03	0.41
1:B:205:ILE:CA	1:B:213:VAL:HG22	2.50	0.41
1:C:496:PRO:HB2	1:C:499:VAL:CG1	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:F:421:ARG:CZ	1:F:473:ASP:HA	2.51	0.41
1:G:77:VAL:CG2	1:G:510:VAL:HG21	2.51	0.41
1:G:200:LEU:HG	1:G:276:VAL:HA	2.02	0.41
1:G:221:LEU:HD23	1:G:233:MET:HE1	2.02	0.41
1:G:284:ARG:O	1:G:288:MET:HG3	2.21	0.41
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.19	0.41
1:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:324:VAL:O	1:H:331:THR:HG22	2.21	0.41
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.60	0.41
1:I:63:GLU:HB2	1:J:524:LEU:CD2	2.50	0.41
1: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:182:GLY:HA2	1:J:383:ALA:CB	2.50	0.41
1:J:381:VAL:O	1:J:382:GLY:O	2.39	0.41
1:K:272:LYS:HZ3	1:L:229:ASN:HD21	1.68	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:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.41
1:L:46:ALA:HA	1:L:47:PRO:HD3	1.93	0.41
1:L:183:LEU:CD2	1:L:384:ALA:HB2	2.49	0.41
1:L:200:LEU:HG	1:L:276:VAL:HA	2.02	0.41
1:L:215:LEU:HB2	1:L:323:VAL:HG22	2.03	0.41
1:L:235:PRO:CG	1:L:310:GLU:HA	2.34	0.41
1:L:290:GLN:HB3	1:L:345:ARG:NH2	2.35	0.41
1:L:351:GLN:HA	1:L:354:GLU:HG2	2.02	0.41
1:L:477:GLY:HA2	6:L:2905:HOH:O	2.20	0.41
1:M:202:PRO:C	1:M:204:PHE:H	2.27	0.41
1:M:233:MET:C	1:M:235:PRO:HD2	2.45	0.41
1:M:253:ASP:OD1	1:M:277:LYS:HE2	2.20	0.41
1:M:449:ALA:HB3	1:M:450:PRO:HD3	2.03	0.41
1:N:85:ALA:O	1:N:401:HIS:HE1	2.03	0.41
1:N:134:LEU:HD21	1:N:425:LYS:NZ	2.35	0.41
1:N:194:GLN:OE1	1:N:329:THR:HG21	2.21	0.41
1:N:202:PRO:C	1:N:204:PHE:H	2.27	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: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:I:216:GLU:C	1:I:218:PRO:HD3	2.46	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:F:202:PRO:C	1:F:204:PHE:H	2.28	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:K:193:MET:HE1	1:K:292:ILE:CG1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LYS:HB2	1:L:160:LYS:NZ	2.36	0.40
1:M:205:ILE:CA	1:M:213:VAL:HG22	2.48	0.40
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.03	0.40
1:B:233:MET:C	1:B:235:PRO:HD2	2.46	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: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:242:LYS:O	1:J:243:ALA:HB3	2.20	0.40
1:J:366:GLN:O	1:J:369:VAL:HG22	2.20	0.40
1:K:7:LYS:HE2	1:K:66:PHE:CE2	2.56	0.40
1:K:194:GLN:OE1	1:K:329:THR:HG21	2.21	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:404:ARG:HH11	1:K:404:ARG:CG	2.31	0.40
1:M:197:ARG:HD2	1:M:277:LYS:HB2	2.04	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:199:TYR:CZ	1:C:327:LYS:HA	2.56	0.40
1:C:295:LEU:HD13	1:C:295:LEU:O	2.21	0.40
1:E:268:ARG:C	1:E:270:ILE:H	2.30	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:204:PHE:C	1:I:213:VAL:HG22	2.46	0.40
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.02	0.40
1:J:204:PHE:C	1:J:213:VAL:HG22	2.46	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:B:111:MET:SD	1:B:438:VAL:HG21	2.62	0.40
1:B:253:ASP:OD1	1:B:277:LYS:HE2	2.21	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:LEU:HB2	1:F:323:VAL:HG22	2.03	0.40
1:G:233:MET:C	1:G:235:PRO:HD2	2.47	0.40
1:H:239:ALA:C	1:H:314:LEU:HD21	2.45	0.40
1:H:451:LEU:HD23	1:H:451:LEU:C	2.47	0.40
1:I:194:GLN:HG3	1:I:331:THR:HB	2.02	0.40
1:I:438:VAL:O	1:I:442:VAL:HG23	2.21	0.40
1:I:524:LEU:HD12	1:I:524:LEU:HA	1.93	0.40
1:K:153:ASN:O	1:K:154:SER:HB2	2.20	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:N:302:SER:N	1:N:307:MET:HE3	2.35	0.40
1:B:42:LYS:HB3	1:B:42:LYS:HE2	1.95	0.40
1:C:206:ASN:ND2	1:C:214:GLU:H	2.18	0.40
1:C:331:THR:HG23	1:C:331:THR:O	2.22	0.40
1:C:451:LEU:C	1:C:451:LEU:HD23	2.46	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
1:H:266:THR:HG21	1:H:273:VAL:H	1.85	0.40
1:H:302:SER:N	1:H:307:MET:HE3	2.33	0.40
1:H:326:ASN:HD22	1:H:329:THR:HB	1.86	0.40
1:I:39:VAL:HG12	1:J:69:MET:HE2	2.04	0.40
1:I:85:ALA:O	1:I:401:HIS:HE1	2.04	0.40
1:I:132:LYS:HE2	6:I:1912:HOH:O	2.21	0.40
1:J:253:ASP:OD1	1:J:277:LYS:HE2	2.22	0.40
1:K:194:GLN:HG3	1:K:331:THR:HB	2.03	0.40
1:K:217:SER:HA	1:K:320:ALA:O	2.21	0.40
1:L:305:ILE:HD12	1:L:307:MET:HE2	2.04	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
1:M:216:GLU:C	1:M:218:PRO:HD3	2.47	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%)	7	3
1	B	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5	2
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	5	2
1	D	523/547 (96%)	492 (94%)	22 (4%)	9 (2%)	7	3
1	E	523/547 (96%)	485 (93%)	27 (5%)	11 (2%)	5	2
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5	2
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	5	2
1	H	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5	2
1	I	523/547 (96%)	486 (93%)	27 (5%)	10 (2%)	6	3
1	J	523/547 (96%)	486 (93%)	25 (5%)	12 (2%)	5	2
1	K	523/547 (96%)	484 (92%)	29 (6%)	10 (2%)	6	3
1	L	523/547 (96%)	488 (93%)	23 (4%)	12 (2%)	5	2
1	M	523/547 (96%)	487 (93%)	25 (5%)	11 (2%)	5	2
1	N	523/547 (96%)	487 (93%)	26 (5%)	10 (2%)	6	3
All	All	7322/7658 (96%)	6820 (93%)	350 (5%)	152 (2%)	5	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	392 (97%)	12 (3%)	36	38
1	B	404/413 (98%)	394 (98%)	10 (2%)	42	45
1	C	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	D	404/413 (98%)	391 (97%)	13 (3%)	34	35
1	E	404/413 (98%)	395 (98%)	9 (2%)	45	50
1	F	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	G	404/413 (98%)	393 (97%)	11 (3%)	39	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	I	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	J	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	K	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	L	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	M	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	N	404/413 (98%)	393 (97%)	11 (3%)	39	42
All	All	5656/5782 (98%)	5497 (97%)	159 (3%)	38	41

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	20	VAL
1	A	23	LEU
1	A	75	LYS
1	A	94	VAL
1	A	160	LYS
1	A	183	LEU
1	A	289	LEU
1	A	404	ARG
1	A	417	VAL
1	A	420	ILE
1	A	499	VAL
1	B	75	LYS
1	B	77	VAL
1	B	160	LYS
1	B	183	LEU
1	B	289	LEU
1	B	404	ARG
1	B	417	VAL
1	B	499	VAL
1	B	510	VAL
1	B	524	LEU
1	C	10	ASN
1	C	20	VAL
1	C	75	LYS
1	C	94	VAL
1	C	160	LYS
1	C	183	LEU

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Mol	Chain	Res	Type
1	C	289	LEU
1	C	404	ARG
1	C	417	VAL
1	C	420	ILE
1	C	499	VAL
1	D	10	ASN
1	D	20	VAL
1	D	23	LEU
1	D	75	LYS
1	D	94	VAL
1	D	160	LYS
1	D	183	LEU
1	D	230	ILE
1	D	289	LEU
1	D	404	ARG
1	D	417	VAL
1	D	473	ASP
1	D	499	VAL
1	E	20	VAL
1	E	94	VAL
1	E	160	LYS
1	E	183	LEU
1	E	289	LEU
1	E	404	ARG
1	E	417	VAL
1	E	499	VAL
1	E	514	MET
1	F	10	ASN
1	F	20	VAL
1	F	75	LYS
1	F	94	VAL
1	F	160	LYS
1	F	183	LEU
1	F	289	LEU
1	F	404	ARG
1	F	417	VAL
1	F	420	ILE
1	F	499	VAL
1	F	514	MET
1	G	10	ASN
1	G	20	VAL
1	G	75	LYS

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Mol	Chain	Res	Type
1	G	94	VAL
1	G	160	LYS
1	G	183	LEU
1	G	289	LEU
1	G	404	ARG
1	G	417	VAL
1	G	420	ILE
1	G	499	VAL
1	H	10	ASN
1	H	20	VAL
1	H	75	LYS
1	H	94	VAL
1	H	160	LYS
1	H	183	LEU
1	H	289	LEU
1	H	329	THR
1	H	404	ARG
1	H	417	VAL
1	H	420	ILE
1	H	499	VAL
1	I	10	ASN
1	I	20	VAL
1	I	75	LYS
1	I	94	VAL
1	I	160	LYS
1	I	183	LEU
1	I	289	LEU
1	I	404	ARG
1	I	417	VAL
1	I	420	ILE
1	I	483	GLU
1	I	499	VAL
1	J	10	ASN
1	J	20	VAL
1	J	75	LYS
1	J	94	VAL
1	J	160	LYS
1	J	183	LEU
1	J	289	LEU
1	J	404	ARG
1	J	417	VAL
1	J	420	ILE

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Mol	Chain	Res	Type
1	J	483	GLU
1	J	499	VAL
1	K	10	ASN
1	K	20	VAL
1	K	75	LYS
1	K	94	VAL
1	K	160	LYS
1	K	183	LEU
1	K	289	LEU
1	K	404	ARG
1	K	417	VAL
1	K	420	ILE
1	K	499	VAL
1	L	10	ASN
1	L	20	VAL
1	L	75	LYS
1	L	94	VAL
1	L	160	LYS
1	L	183	LEU
1	L	289	LEU
1	L	404	ARG
1	L	417	VAL
1	L	420	ILE
1	L	499	VAL
1	M	10	ASN
1	M	20	VAL
1	M	75	LYS
1	M	94	VAL
1	M	160	LYS
1	M	183	LEU
1	M	284	ARG
1	M	289	LEU
1	M	404	ARG
1	M	417	VAL
1	M	420	ILE
1	M	499	VAL
1	N	10	ASN
1	N	20	VAL
1	N	75	LYS
1	N	94	VAL
1	N	160	LYS
1	N	183	LEU

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Mol	Chain	Res	Type
1	N	289	LEU
1	N	404	ARG
1	N	417	VAL
1	N	420	ILE
1	N	499	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) 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	A	453	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	401	HIS
1	C	37	ASN
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	265	ASN
1	D	319	GLN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	401	HIS
1	D	453	GLN

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

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Mol	Chain	Res	Type
1	I	453	GLN
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
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	N	37	ASN
1	N	146	GLN
1	N	265	ASN
1	N	319	GLN
1	N	326	ASN
1	N	348	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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	L	4003	-	4,4,4	1.51	1 (25%)	6,6,6	1.13	0
2	SO4	A	4001	-	4,4,4	1.51	1 (25%)	6,6,6	1.14	0
5	AGS	N	1	3,4	32,33,33	3.59	4 (12%)	45,52,52	1.00	2 (4%)
5	AGS	J	1	3,4	32,33,33	3.49	2 (6%)	45,52,52	0.96	1 (2%)
2	SO4	F	4004	-	4,4,4	1.45	1 (25%)	6,6,6	1.15	0
2	SO4	C	4012	-	4,4,4	1.54	1 (25%)	6,6,6	1.13	0
2	SO4	K	4022	-	4,4,4	1.50	1 (25%)	6,6,6	1.12	0
5	AGS	B	1	3,4	32,33,33	3.58	4 (12%)	45,52,52	1.05	1 (2%)
2	SO4	M	4014	-	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	K	4021	-	4,4,4	1.54	1 (25%)	6,6,6	1.12	0
2	SO4	A	4007	-	4,4,4	1.49	1 (25%)	6,6,6	1.13	0
5	AGS	I	1	3,4	32,33,33	3.56	3 (9%)	45,52,52	1.02	2 (4%)
2	SO4	B	4010	-	4,4,4	1.53	1 (25%)	6,6,6	1.11	0
2	SO4	A	4008	-	4,4,4	1.51	1 (25%)	6,6,6	1.11	0
2	SO4	H	4017	-	4,4,4	1.52	1 (25%)	6,6,6	1.12	0
5	AGS	L	1	3,4	32,33,33	3.54	3 (9%)	45,52,52	1.02	1 (2%)
5	AGS	H	1	3,4	32,33,33	3.57	3 (9%)	45,52,52	1.09	2 (4%)
5	AGS	F	1	3,4	32,33,33	3.48	2 (6%)	45,52,52	0.97	1 (2%)
5	AGS	M	1	3,4	32,33,33	3.57	4 (12%)	45,52,52	1.05	3 (6%)
2	SO4	E	4006	-	4,4,4	1.52	1 (25%)	6,6,6	1.10	0
2	SO4	E	4005	-	4,4,4	1.43	1 (25%)	6,6,6	1.14	0
2	SO4	H	4018	-	4,4,4	1.51	1 (25%)	6,6,6	1.09	0
2	SO4	N	4016	-	4,4,4	1.51	1 (25%)	6,6,6	1.12	0
2	SO4	C	4011	-	4,4,4	1.51	1 (25%)	6,6,6	1.11	0
2	SO4	N	4015	-	4,4,4	1.52	1 (25%)	6,6,6	1.13	0
5	AGS	K	1	3,4	32,33,33	3.56	4 (12%)	45,52,52	1.01	2 (4%)
5	AGS	E	1	3,4	32,33,33	3.63	5 (15%)	45,52,52	1.10	1 (2%)
5	AGS	A	1	3,4	32,33,33	3.54	4 (12%)	45,52,52	1.06	2 (4%)
5	AGS	C	1	3,4	32,33,33	3.57	4 (12%)	45,52,52	1.05	1 (2%)
2	SO4	J	4020	-	4,4,4	1.52	1 (25%)	6,6,6	1.11	0
2	SO4	J	4019	-	4,4,4	1.51	1 (25%)	6,6,6	1.10	0
5	AGS	G	1	3,4	32,33,33	3.63	2 (6%)	45,52,52	1.07	1 (2%)
5	AGS	D	551	3,4	32,33,33	3.57	3 (9%)	45,52,52	1.01	1 (2%)
2	SO4	M	4013	-	4,4,4	1.56	1 (25%)	6,6,6	1.12	0
2	SO4	G	4002	-	4,4,4	1.51	1 (25%)	6,6,6	1.14	0
2	SO4	B	4009	-	4,4,4	1.50	1 (25%)	6,6,6	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	F	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	G	1	3,4	-	3/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	M	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	D	551	3,4	-	3/21/38/38	0/3/3/3
5	AGS	N	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	J	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	K	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	B	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	E	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	I	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	H	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	A	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	L	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	C	1	3,4	-	3/21/38/38	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-19.61	1.48	1.90
5	E	1	AGS	PG-S1G	-19.53	1.48	1.90
5	D	551	AGS	PG-S1G	-19.43	1.48	1.90
5	N	1	AGS	PG-S1G	-19.13	1.49	1.90
5	I	1	AGS	PG-S1G	-19.13	1.49	1.90
5	H	1	AGS	PG-S1G	-19.03	1.49	1.90
5	C	1	AGS	PG-S1G	-19.02	1.49	1.90
5	J	1	AGS	PG-S1G	-19.01	1.49	1.90
5	K	1	AGS	PG-S1G	-18.99	1.49	1.90
5	M	1	AGS	PG-S1G	-18.96	1.49	1.90
5	F	1	AGS	PG-S1G	-18.87	1.49	1.90
5	L	1	AGS	PG-S1G	-18.86	1.49	1.90
5	B	1	AGS	PG-S1G	-18.70	1.50	1.90
5	A	1	AGS	PG-S1G	-18.59	1.50	1.90
5	A	1	AGS	PA-O3A	4.52	1.64	1.59
5	B	1	AGS	PB-O3A	4.11	1.63	1.59
5	H	1	AGS	PA-O3A	3.87	1.63	1.59
5	L	1	AGS	PB-O3A	3.82	1.63	1.59
5	B	1	AGS	PA-O3A	3.72	1.63	1.59
5	H	1	AGS	PB-O3A	3.56	1.63	1.59
5	A	1	AGS	PB-O3A	3.53	1.63	1.59
5	C	1	AGS	PA-O3A	3.43	1.63	1.59
5	C	1	AGS	PB-O3A	3.25	1.63	1.59
5	G	1	AGS	PA-O3A	3.21	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	AGS	PB-O3B	3.14	1.62	1.59
5	N	1	AGS	PA-O3A	3.10	1.62	1.59
5	M	1	AGS	PB-O3A	3.09	1.62	1.59
5	N	1	AGS	PB-O3A	3.04	1.62	1.59
5	I	1	AGS	PB-O3A	3.04	1.62	1.59
5	M	1	AGS	PA-O3A	3.04	1.62	1.59
2	M	4013	SO4	O1-S	3.01	1.62	1.44
5	K	1	AGS	PB-O3B	3.00	1.62	1.59
2	K	4021	SO4	O1-S	2.95	1.62	1.44
2	C	4012	SO4	O1-S	2.94	1.62	1.44
2	B	4010	SO4	O1-S	2.93	1.62	1.44
2	M	4014	SO4	O1-S	2.93	1.62	1.44
2	N	4015	SO4	O1-S	2.92	1.62	1.44
2	C	4011	SO4	O1-S	2.91	1.62	1.44
2	H	4018	SO4	O1-S	2.91	1.62	1.44
2	J	4019	SO4	O1-S	2.91	1.62	1.44
2	J	4020	SO4	O1-S	2.91	1.62	1.44
2	E	4006	SO4	O1-S	2.91	1.62	1.44
2	H	4017	SO4	O1-S	2.90	1.62	1.44
2	B	4009	SO4	O1-S	2.90	1.62	1.44
2	N	4016	SO4	O1-S	2.90	1.62	1.44
2	A	4008	SO4	O1-S	2.90	1.62	1.44
2	A	4001	SO4	O1-S	2.89	1.62	1.44
2	G	4002	SO4	O1-S	2.89	1.62	1.44
2	L	4003	SO4	O1-S	2.87	1.61	1.44
2	K	4022	SO4	O1-S	2.87	1.61	1.44
2	A	4007	SO4	O1-S	2.83	1.61	1.44
5	K	1	AGS	PB-O3A	2.80	1.62	1.59
2	F	4004	SO4	O1-S	2.76	1.61	1.44
5	B	1	AGS	PB-O3B	2.76	1.62	1.59
2	E	4005	SO4	O1-S	2.72	1.61	1.44
5	K	1	AGS	PA-O3A	2.71	1.62	1.59
5	E	1	AGS	PB-O3A	2.59	1.62	1.59
5	L	1	AGS	PA-O3A	2.55	1.62	1.59
5	M	1	AGS	PB-O3B	2.48	1.62	1.59
5	I	1	AGS	PA-O3A	2.43	1.62	1.59
5	N	1	AGS	PB-O3B	2.31	1.62	1.59
5	A	1	AGS	PB-O3B	2.24	1.61	1.59
5	E	1	AGS	PA-O3A	2.19	1.61	1.59
5	D	551	AGS	C4-N3	2.15	1.38	1.34
5	F	1	AGS	PG-O3G	-2.15	1.47	1.54
5	J	1	AGS	PB-O3A	2.04	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	551	AGS	PG-O3G	-2.03	1.48	1.54
5	C	1	AGS	PB-O3B	2.01	1.61	1.59
5	E	1	AGS	PG-O3G	-2.01	1.48	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	AGS	O4'-C1'-N9	3.93	115.64	108.09
5	B	1	AGS	O4'-C1'-N9	3.69	115.17	108.09
5	C	1	AGS	O4'-C1'-N9	3.43	114.68	108.09
5	H	1	AGS	O4'-C1'-N9	3.39	114.59	108.09
5	L	1	AGS	O4'-C1'-N9	3.35	114.53	108.09
5	I	1	AGS	O4'-C1'-N9	3.25	114.34	108.09
5	D	551	AGS	O4'-C1'-N9	3.23	114.28	108.09
5	G	1	AGS	O4'-C1'-N9	3.19	114.22	108.09
5	M	1	AGS	O4'-C1'-N9	3.17	114.17	108.09
5	K	1	AGS	O4'-C1'-N9	3.12	114.09	108.09
5	F	1	AGS	O4'-C1'-N9	2.88	113.61	108.09
5	A	1	AGS	O4'-C1'-N9	2.67	113.21	108.09
5	N	1	AGS	O4'-C1'-N9	2.61	113.11	108.09
5	J	1	AGS	O4'-C1'-N9	2.59	113.06	108.09
5	M	1	AGS	C1'-N9-C8	2.20	131.99	127.09
5	I	1	AGS	PB-O3B-PG	-2.13	125.38	133.17
5	N	1	AGS	PB-O3B-PG	-2.06	125.63	133.17
5	A	1	AGS	C1'-N9-C8	2.05	131.64	127.09
5	K	1	AGS	PB-O3B-PG	-2.02	125.76	133.17
5	H	1	AGS	O2A-PA-O3A	2.02	112.73	107.27
5	M	1	AGS	PB-O3B-PG	-2.00	125.84	133.17

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C	1	AGS	PB-O3B-PG-O2G
5	C	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

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

There are no ring outliers.

15 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1	AGS	4	0
5	J	1	AGS	4	0
5	B	1	AGS	4	0
5	I	1	AGS	4	0

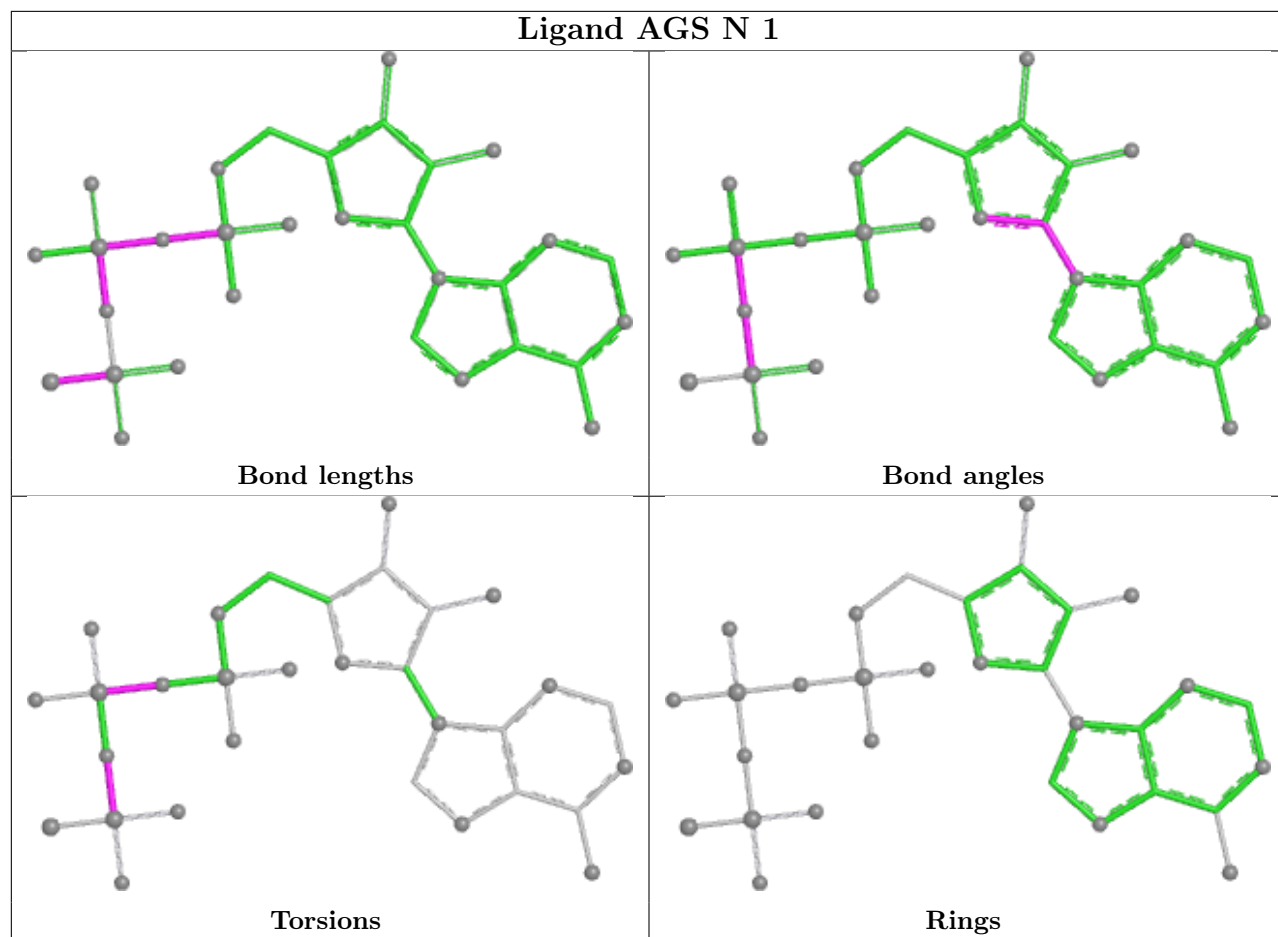
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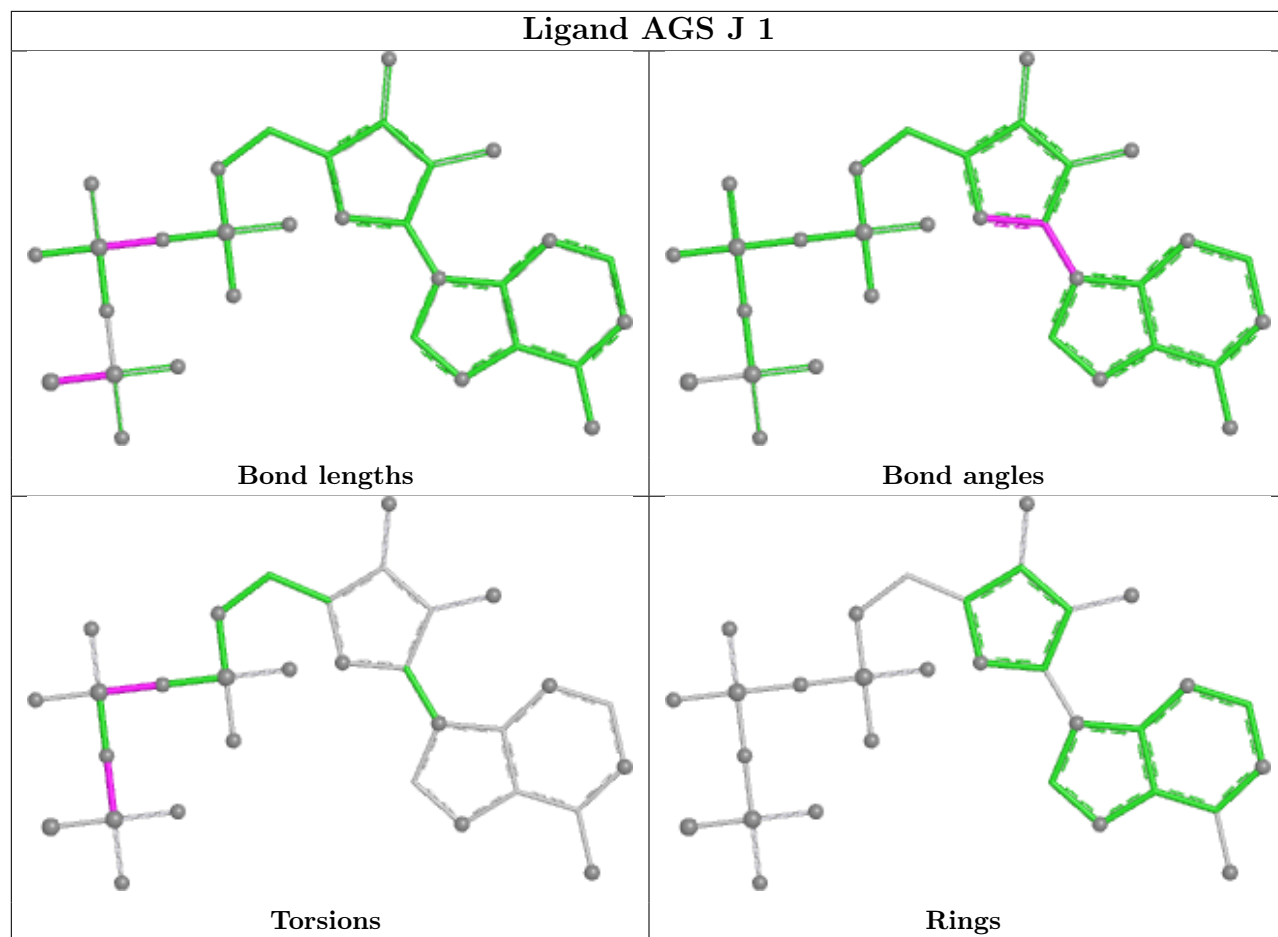
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1	AGS	5	0
5	H	1	AGS	4	0
5	F	1	AGS	3	0
5	M	1	AGS	5	0
2	E	4005	SO4	1	0
5	K	1	AGS	5	0
5	E	1	AGS	4	0
5	A	1	AGS	3	0
5	C	1	AGS	3	0
5	G	1	AGS	5	0
5	D	551	AGS	4	0

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.

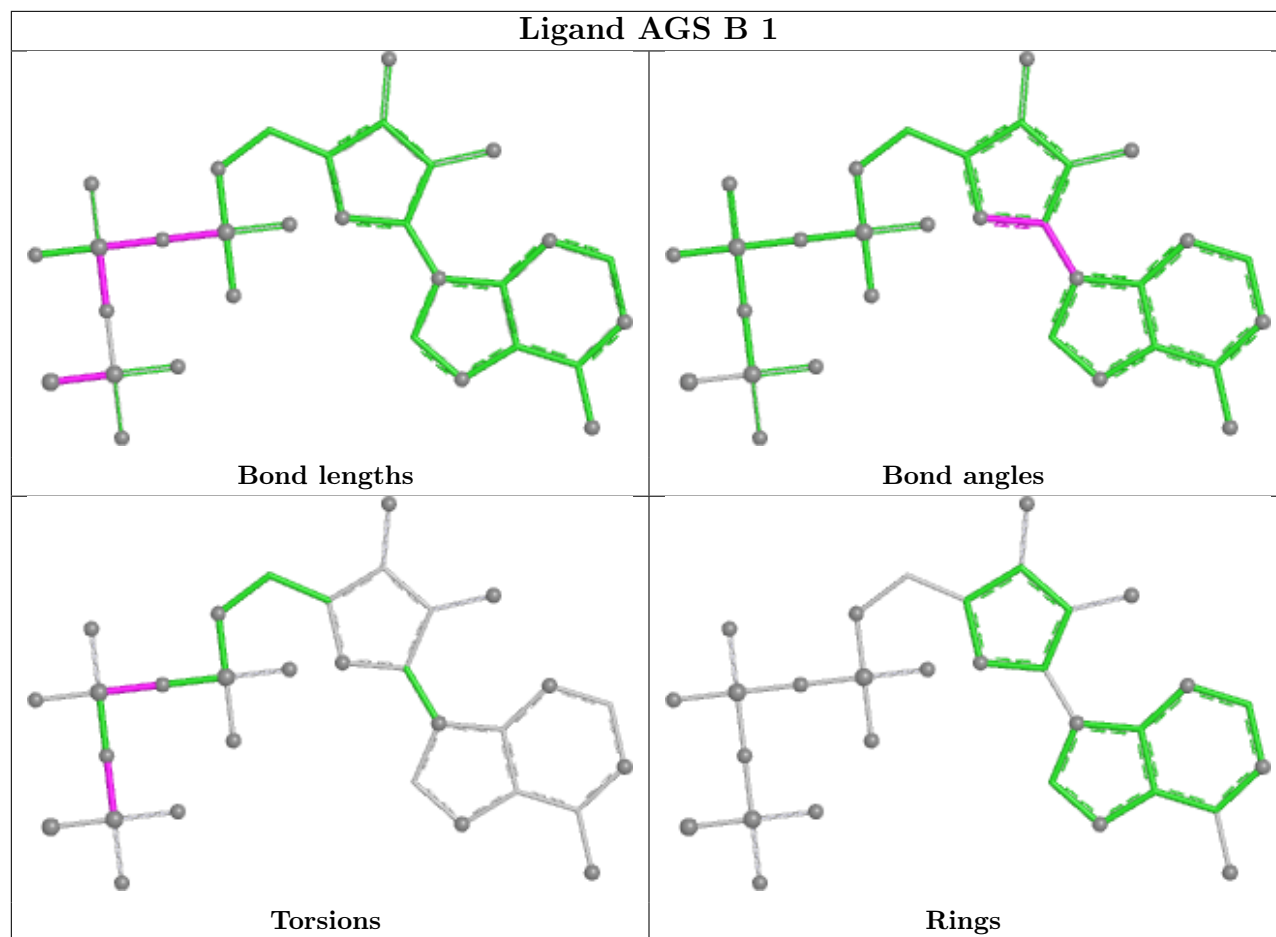
Ligand AGS N 1

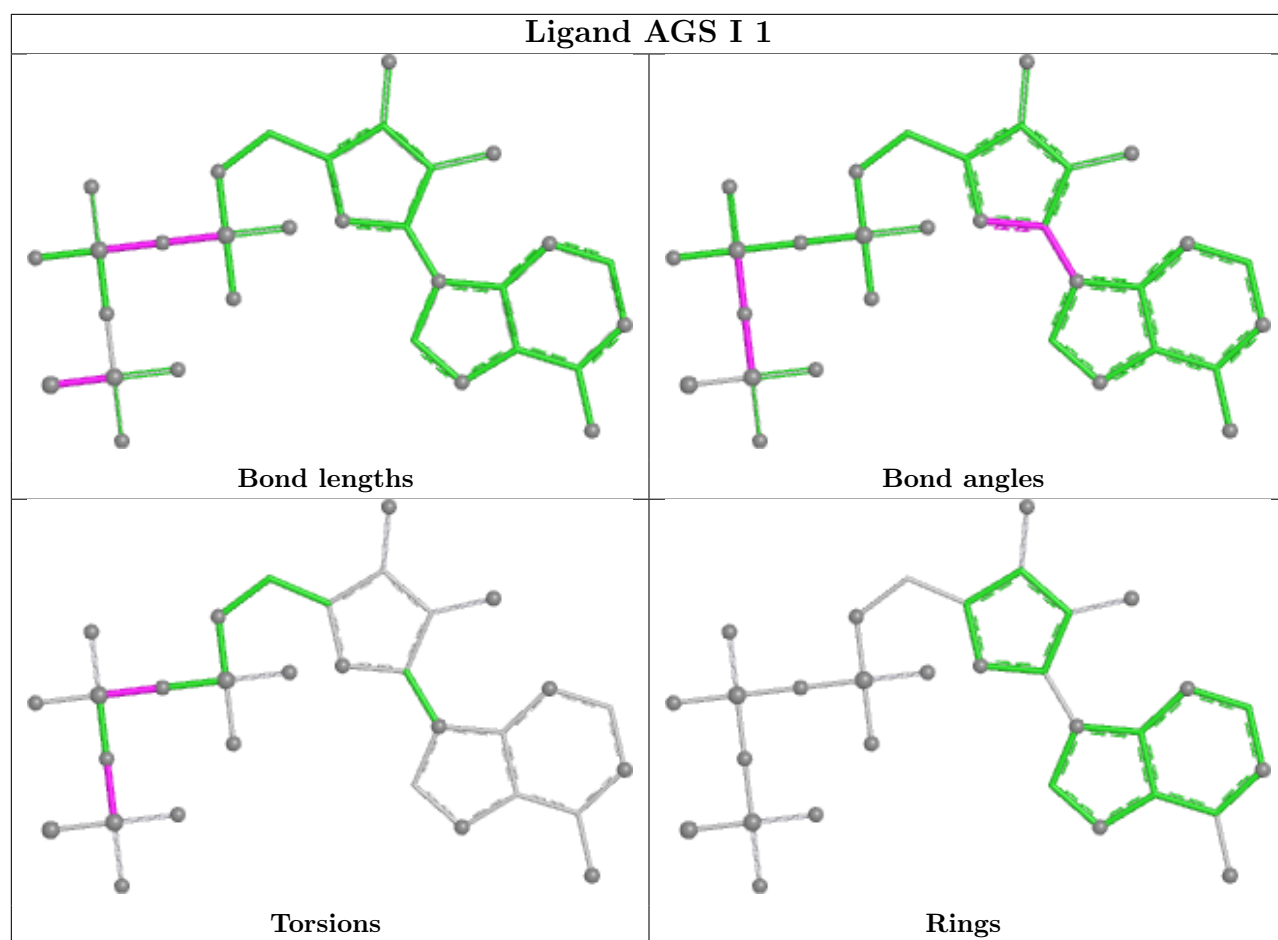


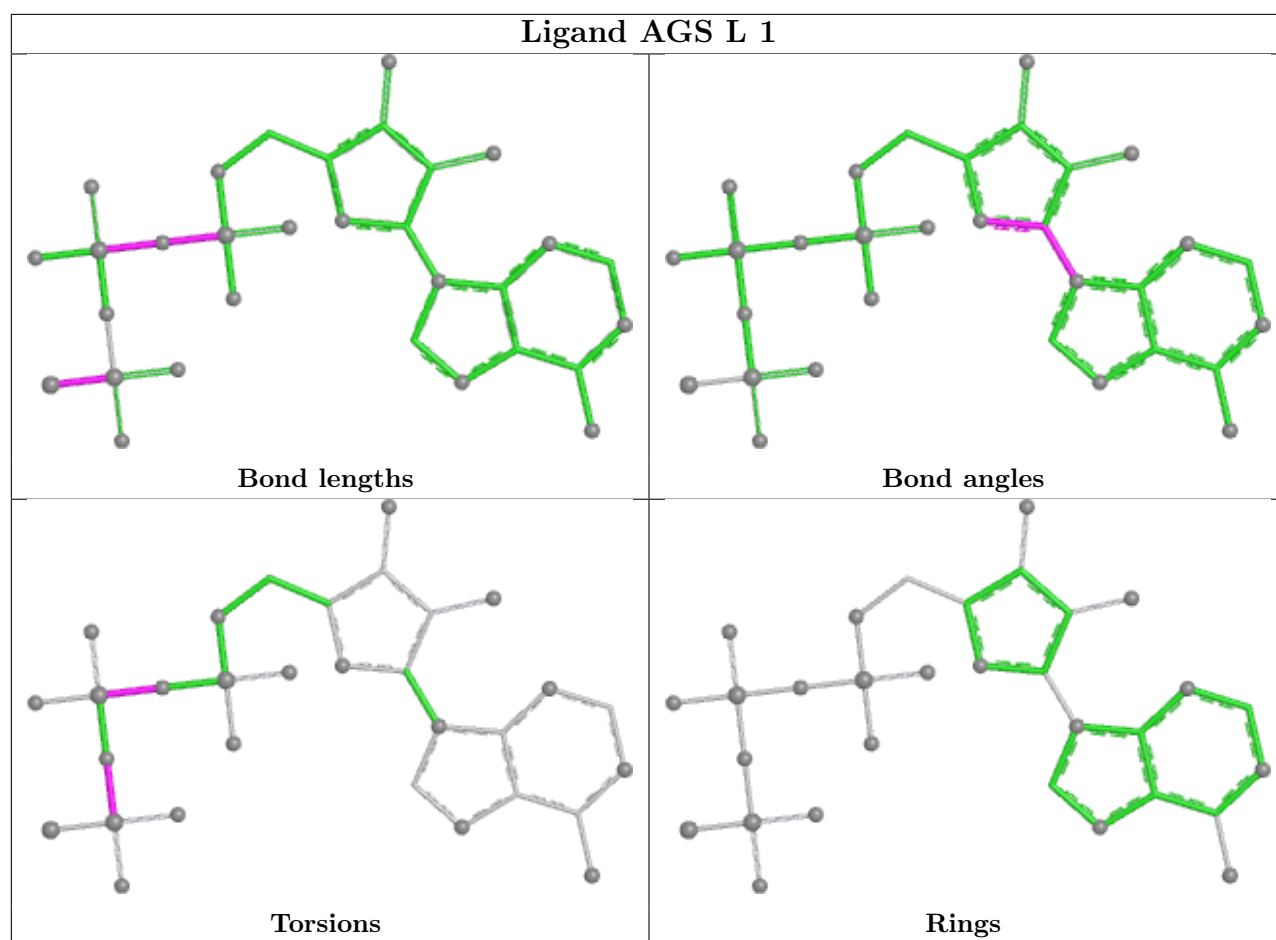
Ligand AGS J 1



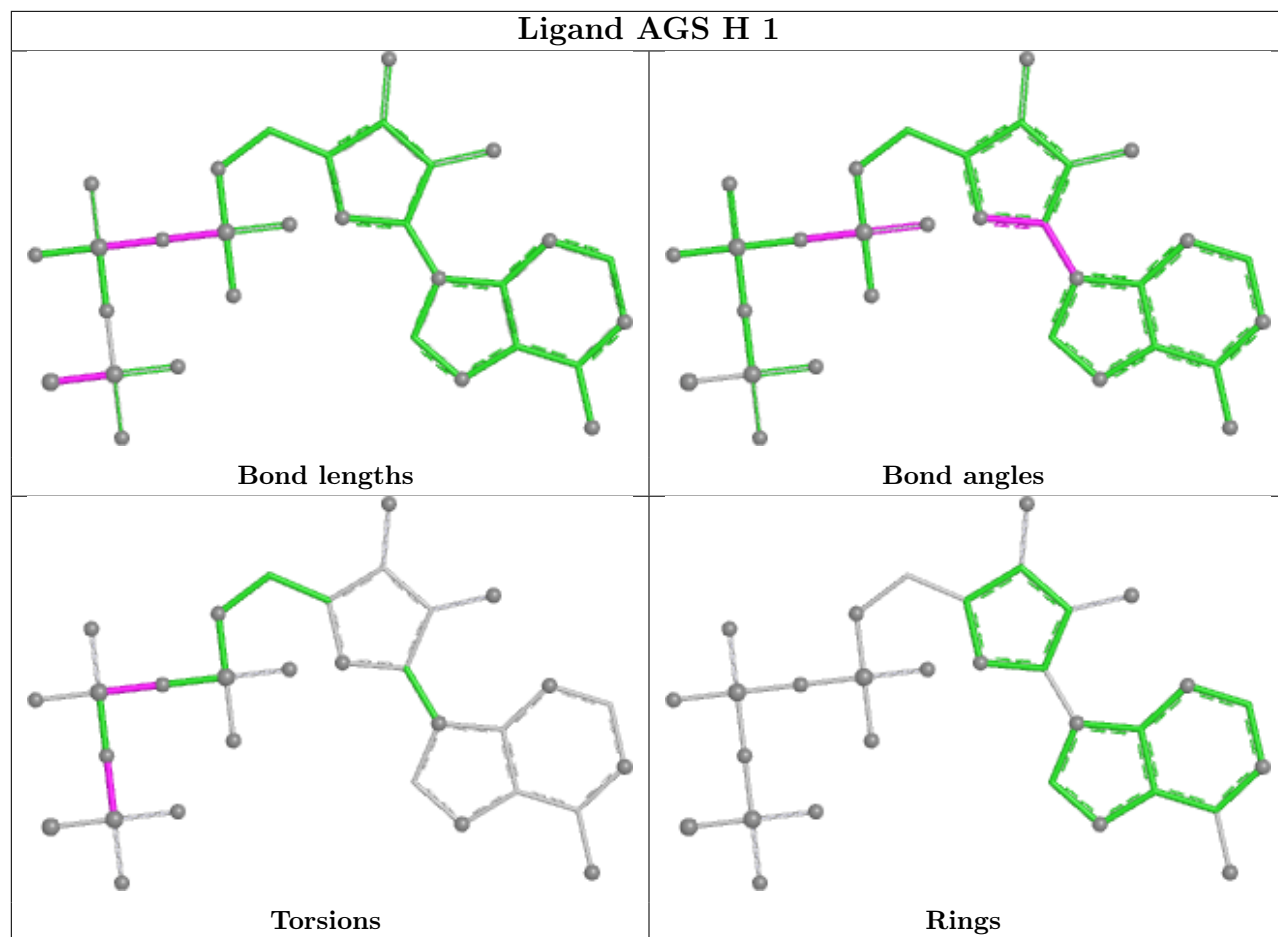
Ligand AGS B 1



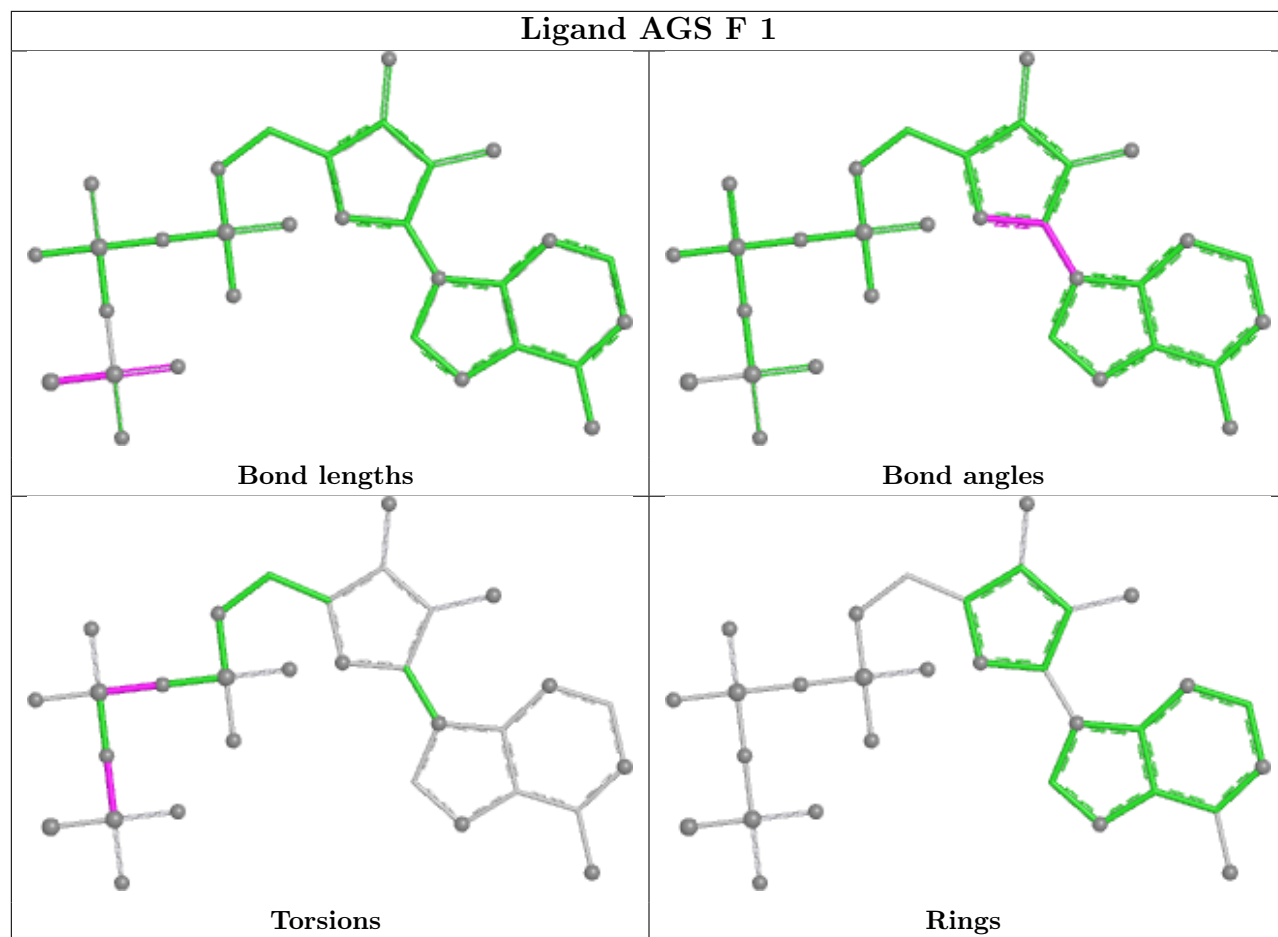




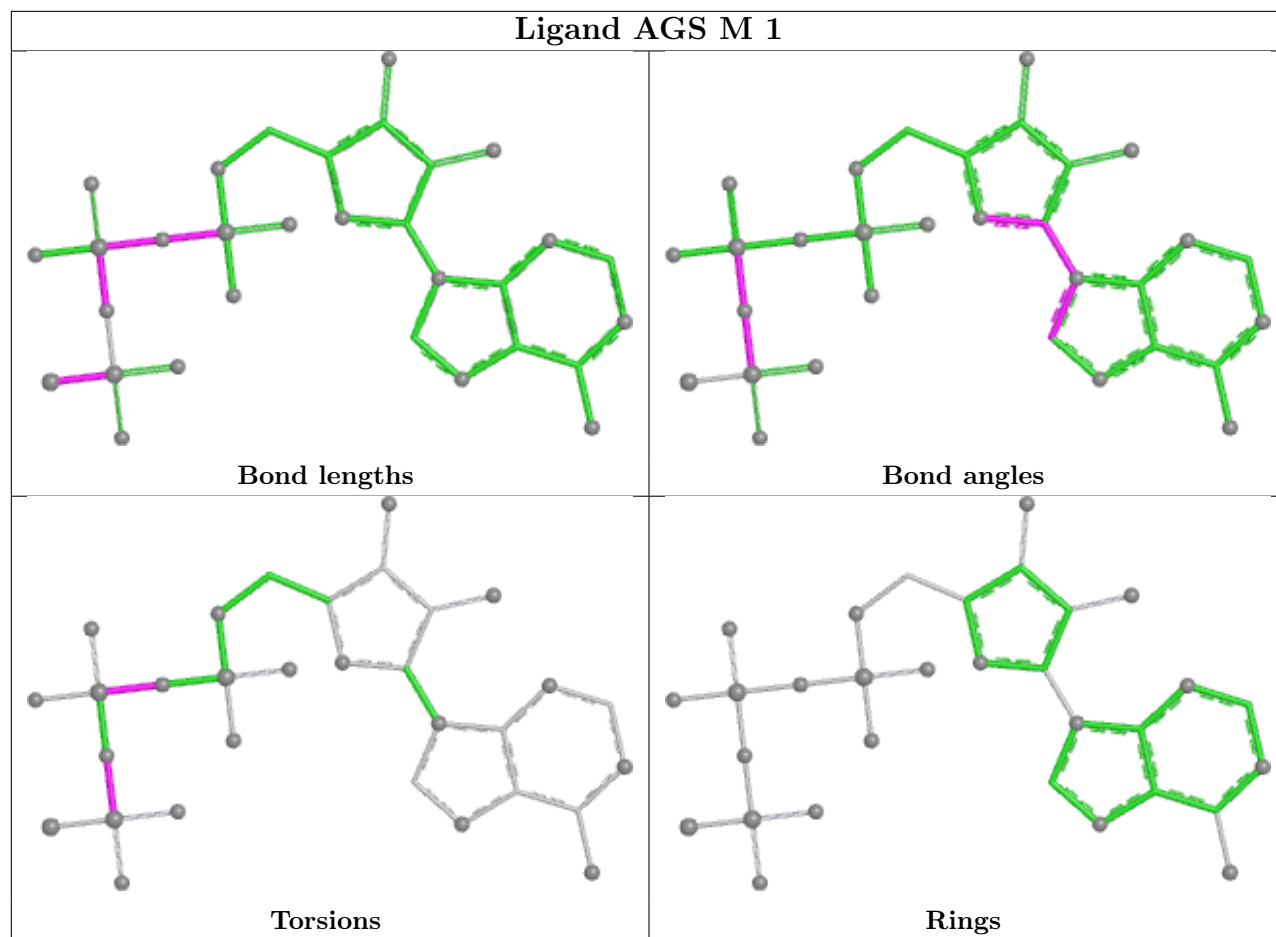
Ligand AGS H 1



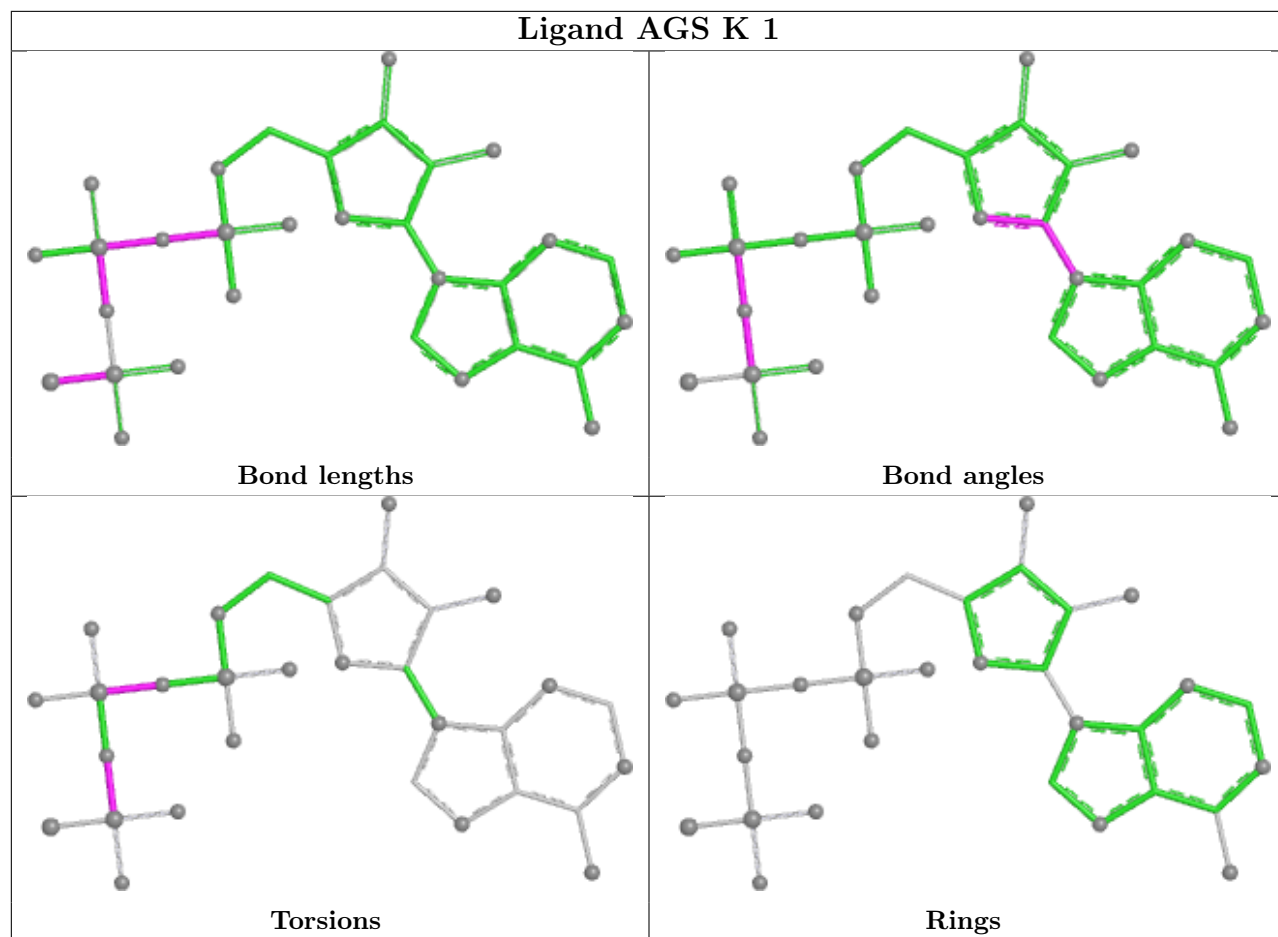
Ligand AGS F 1



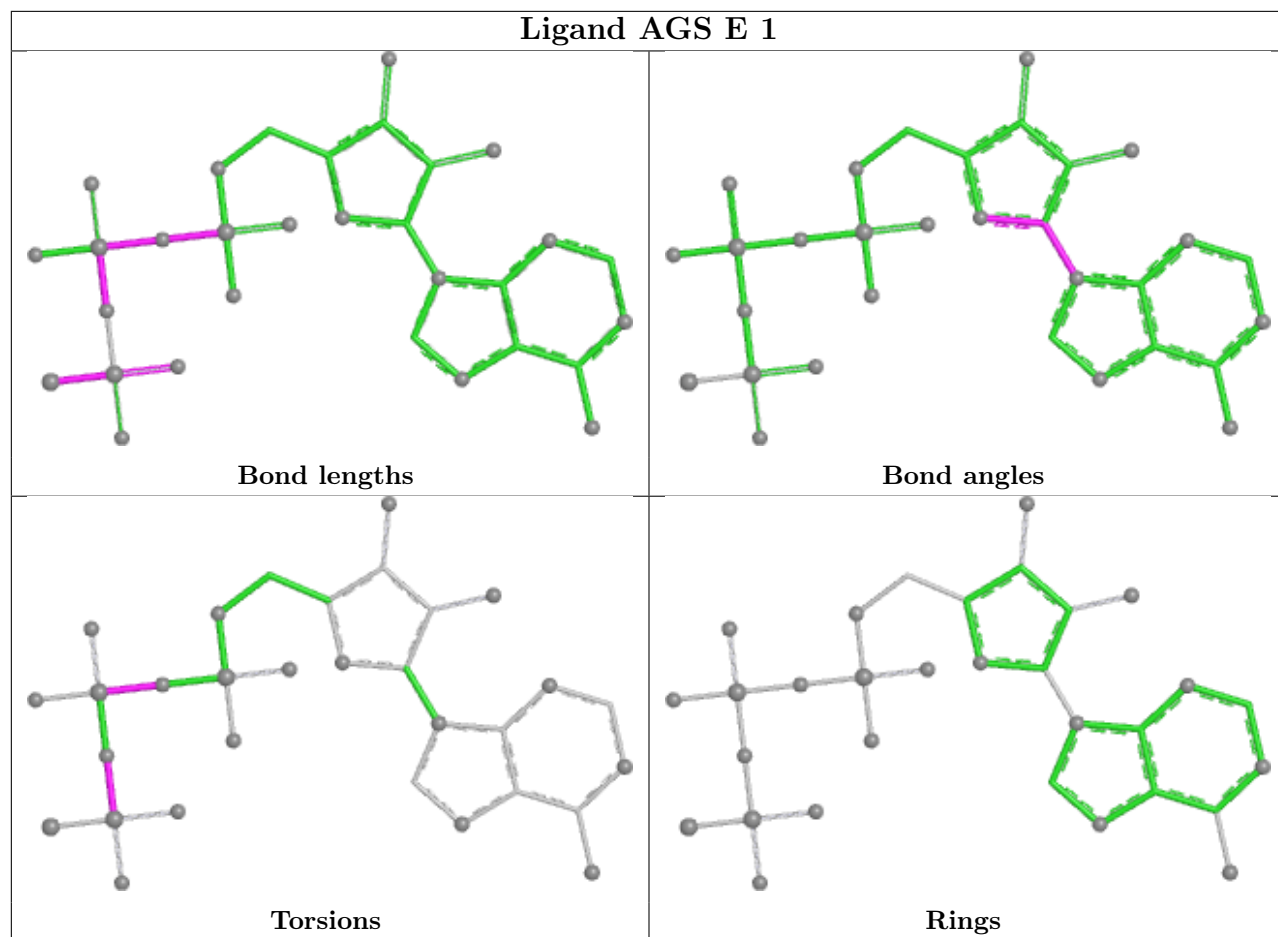
Ligand AGS M 1



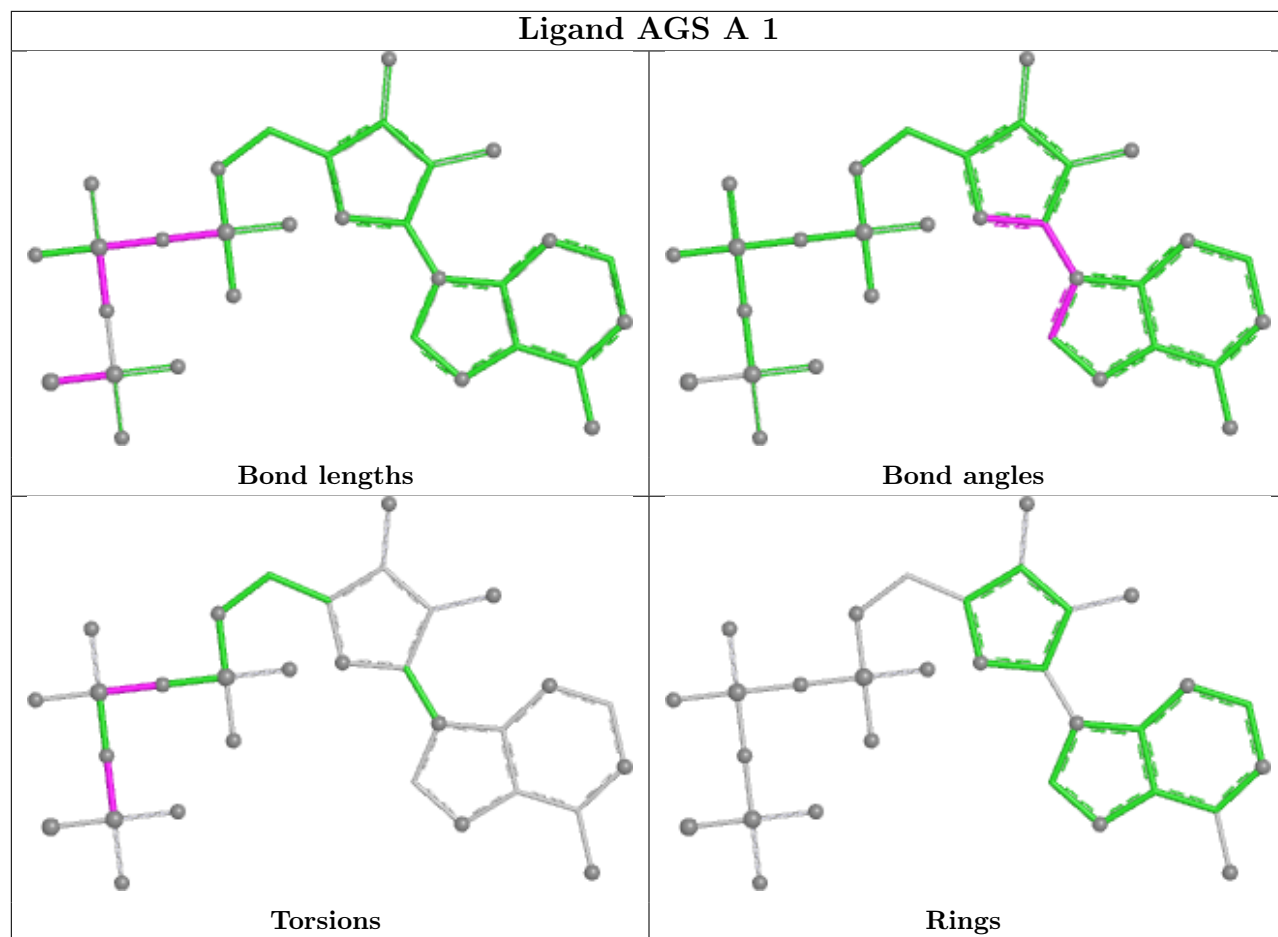
Ligand AGS K 1



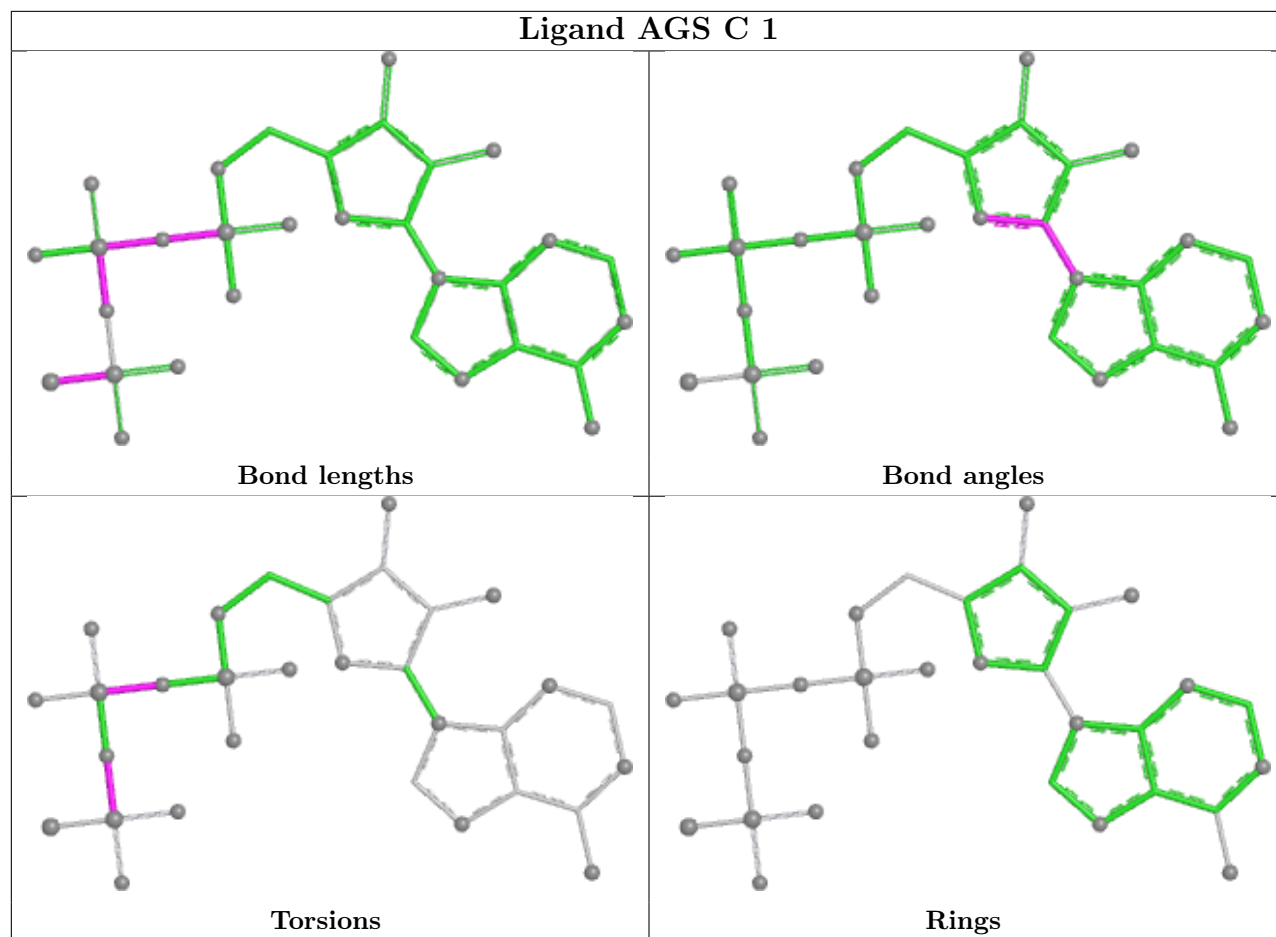
Ligand AGS E 1



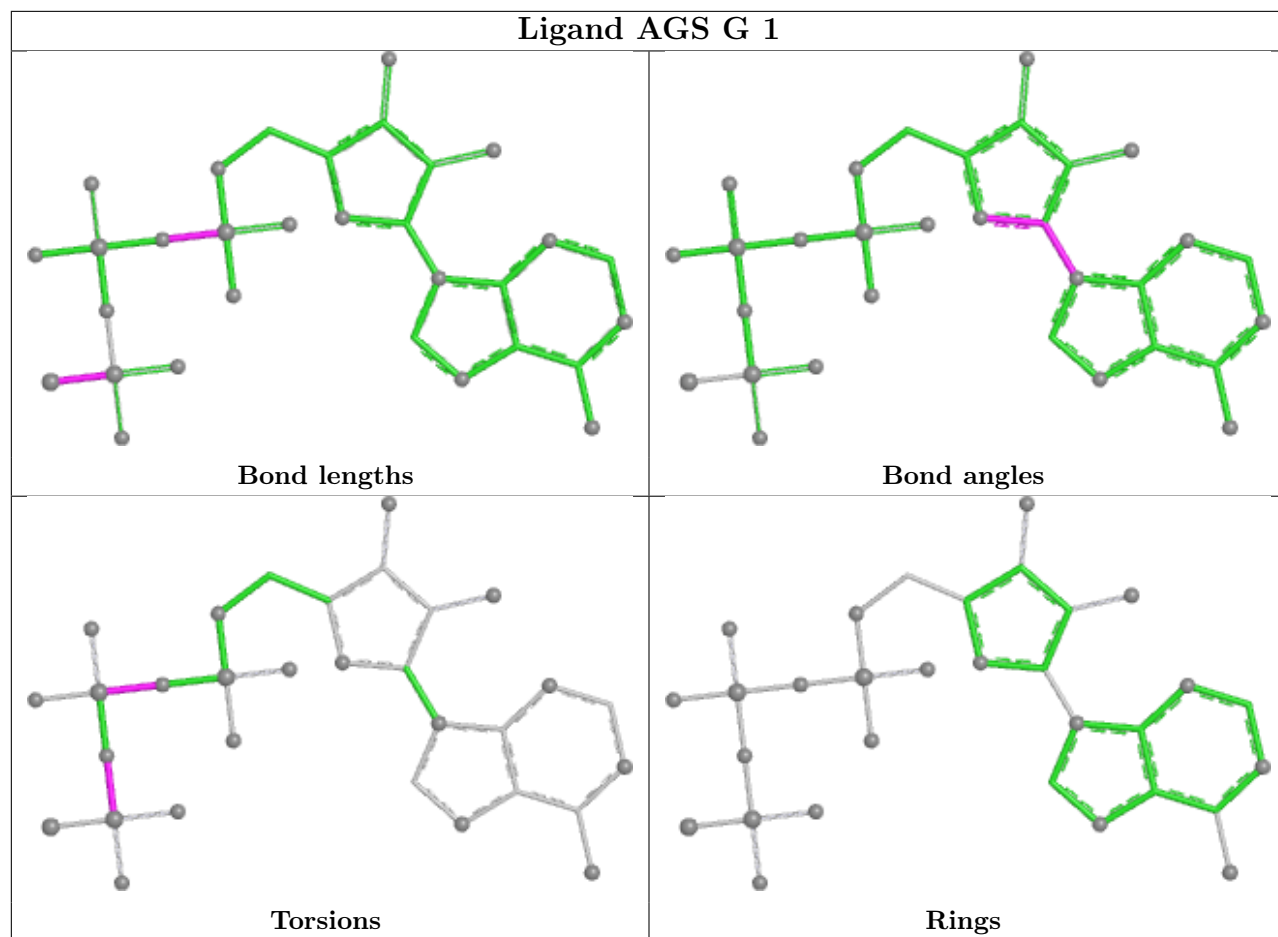
Ligand AGS A 1

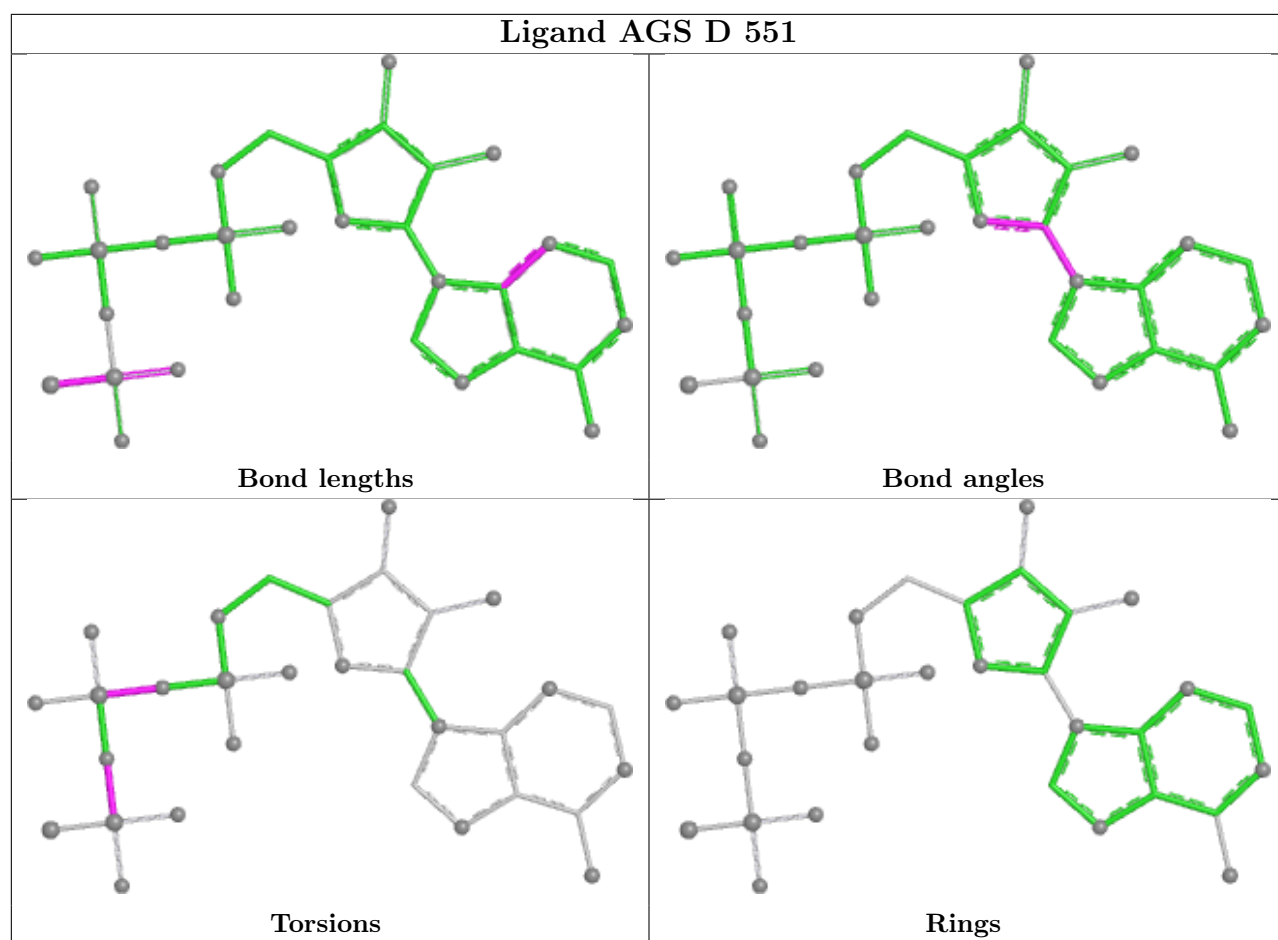


Ligand AGS C 1



Ligand AGS G 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%)	0.97	106 (20%) 3 2	28, 64, 121, 132	0
1	B	525/547 (95%)	1.04	135 (25%) 1 1	24, 59, 149, 159	0
1	C	525/547 (95%)	1.27	147 (28%) 1 1	29, 71, 141, 152	0
1	D	525/547 (95%)	0.66	60 (11%) 10 9	25, 48, 99, 115	0
1	E	525/547 (95%)	0.90	123 (23%) 2 2	23, 55, 134, 145	0
1	F	525/547 (95%)	1.15	135 (25%) 1 1	27, 66, 150, 159	0
1	G	525/547 (95%)	0.81	92 (17%) 4 3	26, 50, 113, 126	0
1	H	525/547 (95%)	0.82	87 (16%) 4 4	26, 56, 118, 130	0
1	I	525/547 (95%)	1.00	112 (21%) 2 2	31, 69, 132, 143	0
1	J	525/547 (95%)	1.11	114 (21%) 2 2	31, 73, 138, 146	0
1	K	525/547 (95%)	1.32	149 (28%) 1 1	31, 78, 151, 159	0
1	L	525/547 (95%)	1.04	119 (22%) 2 2	29, 66, 136, 149	0
1	M	525/547 (95%)	1.29	157 (29%) 1 1	30, 77, 152, 160	0
1	N	525/547 (95%)	0.95	97 (18%) 3 3	28, 65, 118, 129	0
All	All	7350/7658 (95%)	1.02	1633 (22%) 2 2	23, 60, 140, 160	0

All (1633) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	233	MET	6.4
1	M	259	LEU	6.3
1	M	223	ALA	6.3
1	M	346	VAL	6.0
1	K	349	ILE	5.9
1	E	223	ALA	5.9
1	L	383	ALA	5.8
1	D	271	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	309	LEU	5.7
1	K	271	VAL	5.6
1	B	227	ILE	5.6
1	C	349	ILE	5.6
1	M	233	MET	5.6
1	K	341	ALA	5.5
1	M	262	LEU	5.4
1	K	227	ILE	5.4
1	F	349	ILE	5.4
1	F	240	VAL	5.4
1	M	195	PHE	5.3
1	F	233	MET	5.2
1	A	263	VAL	5.2
1	K	331	THR	5.2
1	B	349	ILE	5.2
1	B	243	ALA	5.2
1	E	309	LEU	5.2
1	K	237	LEU	5.2
1	M	237	LEU	5.2
1	J	333	ILE	5.1
1	E	271	VAL	5.1
1	B	239	ALA	5.0
1	J	349	ILE	5.0
1	M	349	ILE	5.0
1	C	372	LEU	5.0
1	J	222	LEU	5.0
1	N	349	ILE	5.0
1	F	259	LEU	5.0
1	M	222	LEU	5.0
1	E	349	ILE	5.0
1	F	387	VAL	4.9
1	J	271	VAL	4.9
1	E	270	ILE	4.9
1	M	249	ILE	4.9
1	F	381	VAL	4.9
1	J	305	ILE	4.9
1	G	383	ALA	4.8
1	B	222	LEU	4.8
1	C	161	LEU	4.8
1	C	270	ILE	4.8
1	A	271	VAL	4.8
1	I	250	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	189	VAL	4.8
1	K	222	LEU	4.7
1	M	263	VAL	4.7
1	M	320	ALA	4.7
1	F	314	LEU	4.7
1	M	218	PRO	4.7
1	B	342	ILE	4.7
1	K	305	ILE	4.7
1	B	190	VAL	4.7
1	J	381	VAL	4.7
1	K	387	VAL	4.7
1	J	223	ALA	4.7
1	L	356	ALA	4.7
1	B	262	LEU	4.7
1	F	389	MET	4.7
1	C	263	VAL	4.6
1	H	317	LEU	4.6
1	C	305	ILE	4.6
1	L	227	ILE	4.6
1	F	222	LEU	4.6
1	F	332	ILE	4.6
1	F	353	ILE	4.6
1	C	300	VAL	4.6
1	M	273	VAL	4.6
1	M	314	LEU	4.6
1	B	250	ILE	4.6
1	C	249	ILE	4.6
1	G	270	ILE	4.6
1	M	333	ILE	4.6
1	M	251	ALA	4.5
1	G	314	LEU	4.5
1	F	270	ILE	4.5
1	C	44	PHE	4.5
1	C	292	ILE	4.5
1	F	227	ILE	4.5
1	N	325	ILE	4.5
1	B	233	MET	4.5
1	G	271	VAL	4.5
1	C	250	ILE	4.4
1	G	205	ILE	4.4
1	K	299	THR	4.4
1	C	271	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	237	LEU	4.4
1	C	230	ILE	4.4
1	F	230	ILE	4.4
1	F	202	PRO	4.4
1	C	222	LEU	4.4
1	F	360	TYR	4.4
1	H	44	PHE	4.4
1	K	275	ALA	4.4
1	M	387	VAL	4.4
1	M	332	ILE	4.4
1	M	372	LEU	4.3
1	H	233	MET	4.3
1	L	323	VAL	4.3
1	M	221	LEU	4.3
1	J	249	ILE	4.3
1	K	250	ILE	4.3
1	M	353	ILE	4.3
1	C	387	VAL	4.3
1	J	309	LEU	4.3
1	M	189	VAL	4.3
1	M	336	VAL	4.3
1	N	77	VAL	4.3
1	M	377	ALA	4.2
1	B	365	LEU	4.2
1	J	215	LEU	4.2
1	K	158	VAL	4.2
1	K	175	ILE	4.2
1	I	360	TYR	4.2
1	F	44	PHE	4.2
1	M	270	ILE	4.2
1	B	314	LEU	4.2
1	J	314	LEU	4.2
1	B	210	THR	4.2
1	A	301	ILE	4.2
1	E	353	ILE	4.2
1	G	325	ILE	4.2
1	K	332	ILE	4.2
1	M	250	ILE	4.2
1	F	241	ALA	4.2
1	G	243	ALA	4.2
1	C	237	LEU	4.2
1	F	215	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	44	PHE	4.2
1	K	309	LEU	4.2
1	M	309	LEU	4.2
1	D	323	VAL	4.2
1	M	323	VAL	4.2
1	H	335	GLY	4.1
1	A	305	ILE	4.1
1	J	250	ILE	4.1
1	E	233	MET	4.1
1	C	274	ALA	4.1
1	B	289	LEU	4.1
1	C	187	LEU	4.1
1	E	222	LEU	4.1
1	M	219	PHE	4.1
1	D	387	VAL	4.1
1	J	336	VAL	4.1
1	B	188	ASP	4.1
1	I	305	ILE	4.1
1	J	353	ILE	4.1
1	M	305	ILE	4.1
1	J	317	LEU	4.1
1	L	382	GLY	4.1
1	C	320	ALA	4.1
1	I	341	ALA	4.1
1	B	223	ALA	4.0
1	B	237	LEU	4.0
1	F	237	LEU	4.0
1	C	360	TYR	4.0
1	C	346	VAL	4.0
1	D	44	PHE	4.0
1	L	381	VAL	4.0
1	K	241	ALA	4.0
1	D	253	ASP	4.0
1	F	234	LEU	4.0
1	C	190	VAL	4.0
1	I	324	VAL	4.0
1	K	369	VAL	4.0
1	N	271	VAL	4.0
1	A	353	ILE	4.0
1	B	230	ILE	4.0
1	B	305	ILE	4.0
1	F	250	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	223	ALA	4.0
1	H	383	ALA	4.0
1	E	314	LEU	4.0
1	A	276	VAL	4.0
1	K	281	PHE	4.0
1	E	301	ILE	4.0
1	D	382	GLY	4.0
1	M	258	ALA	3.9
1	C	314	LEU	3.9
1	H	314	LEU	3.9
1	K	259	LEU	3.9
1	N	222	LEU	3.9
1	J	376	VAL	3.9
1	L	271	VAL	3.9
1	K	270	ILE	3.9
1	M	335	GLY	3.9
1	K	377	ALA	3.9
1	K	372	LEU	3.9
1	C	177	VAL	3.9
1	F	271	VAL	3.9
1	K	254	VAL	3.9
1	B	220	ILE	3.9
1	B	301	ILE	3.9
1	C	221	LEU	3.9
1	M	248	LEU	3.9
1	L	353	ILE	3.9
1	M	182	GLY	3.9
1	E	243	ALA	3.9
1	K	340	ALA	3.9
1	B	295	LEU	3.9
1	C	247	LEU	3.9
1	H	222	LEU	3.9
1	H	271	VAL	3.8
1	M	271	VAL	3.8
1	D	270	ILE	3.8
1	G	183	LEU	3.8
1	H	309	LEU	3.8
1	M	324	VAL	3.8
1	M	192	GLY	3.8
1	D	325	ILE	3.8
1	N	205	ILE	3.8
1	C	377	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	262	LEU	3.8
1	M	266	THR	3.8
1	E	346	VAL	3.8
1	C	342	ILE	3.8
1	A	360	TYR	3.8
1	K	239	ALA	3.8
1	M	243	ALA	3.8
1	B	259	LEU	3.8
1	J	248	LEU	3.8
1	F	300	VAL	3.8
1	G	254	VAL	3.8
1	M	376	VAL	3.8
1	A	44	PHE	3.8
1	C	220	ILE	3.7
1	A	187	LEU	3.7
1	L	314	LEU	3.7
1	B	254	VAL	3.7
1	C	174	VAL	3.7
1	C	273	VAL	3.7
1	K	336	VAL	3.7
1	C	301	ILE	3.7
1	E	230	ILE	3.7
1	G	220	ILE	3.7
1	J	270	ILE	3.7
1	A	223	ALA	3.7
1	A	237	LEU	3.7
1	C	248	LEU	3.7
1	C	295	LEU	3.7
1	K	187	LEU	3.7
1	M	317	LEU	3.7
1	C	160	LYS	3.7
1	B	202	PRO	3.7
1	C	189	VAL	3.7
1	E	300	VAL	3.7
1	F	346	VAL	3.7
1	K	189	VAL	3.7
1	B	219	PHE	3.7
1	L	305	ILE	3.7
1	B	293	ALA	3.7
1	J	239	ALA	3.7
1	K	203	TYR	3.7
1	L	526	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	202	PRO	3.7
1	F	273	VAL	3.7
1	M	254	VAL	3.7
1	I	44	PHE	3.7
1	E	220	ILE	3.7
1	K	342	ILE	3.7
1	J	526	LYS	3.7
1	K	320	ALA	3.7
1	N	275	ALA	3.7
1	M	217	SER	3.6
1	B	174	VAL	3.6
1	B	240	VAL	3.6
1	B	271	VAL	3.6
1	G	273	VAL	3.6
1	G	387	VAL	3.6
1	M	190	VAL	3.6
1	A	250	ILE	3.6
1	B	332	ILE	3.6
1	H	270	ILE	3.6
1	N	270	ILE	3.6
1	I	193	MET	3.6
1	J	360	TYR	3.6
1	G	240	VAL	3.6
1	K	346	VAL	3.6
1	E	292	ILE	3.6
1	I	249	ILE	3.6
1	J	227	ILE	3.6
1	F	385	THR	3.6
1	C	317	LEU	3.6
1	J	262	LEU	3.6
1	K	317	LEU	3.6
1	K	164	GLU	3.6
1	A	387	VAL	3.6
1	E	263	VAL	3.6
1	C	332	ILE	3.6
1	I	219	PHE	3.6
1	I	333	ILE	3.6
1	K	383	ALA	3.6
1	A	259	LEU	3.6
1	B	247	LEU	3.6
1	F	365	LEU	3.6
1	N	372	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	180	GLY	3.6
1	C	369	VAL	3.5
1	F	378	VAL	3.5
1	H	300	VAL	3.5
1	G	301	ILE	3.5
1	I	331	THR	3.5
1	N	353	ILE	3.5
1	E	320	ALA	3.5
1	H	241	ALA	3.5
1	A	314	LEU	3.5
1	J	365	LEU	3.5
1	N	314	LEU	3.5
1	F	203	TYR	3.5
1	E	264	VAL	3.5
1	K	381	VAL	3.5
1	A	270	ILE	3.5
1	E	242	LYS	3.5
1	F	272	LYS	3.5
1	J	230	ILE	3.5
1	M	230	ILE	3.5
1	J	44	PHE	3.5
1	A	241	ALA	3.5
1	G	258	ALA	3.5
1	K	243	ALA	3.5
1	L	275	ALA	3.5
1	N	525	PRO	3.5
1	J	372	LEU	3.5
1	M	234	LEU	3.5
1	N	134	LEU	3.5
1	C	318	GLY	3.5
1	E	284	ARG	3.5
1	K	276	VAL	3.5
1	K	323	VAL	3.5
1	C	227	ILE	3.5
1	L	325	ILE	3.5
1	B	44	PHE	3.5
1	C	281	PHE	3.5
1	G	223	ALA	3.5
1	K	370	ALA	3.5
1	L	384	ALA	3.5
1	G	244	GLY	3.5
1	M	360	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	240	VAL	3.5
1	A	254	VAL	3.5
1	B	189	VAL	3.5
1	E	387	VAL	3.5
1	I	276	VAL	3.5
1	N	240	VAL	3.5
1	N	273	VAL	3.5
1	I	270	ILE	3.4
1	E	44	PHE	3.4
1	K	278	ALA	3.4
1	F	382	GLY	3.4
1	D	262	LEU	3.4
1	K	248	LEU	3.4
1	K	353	ILE	3.4
1	C	212	ALA	3.4
1	J	269	GLY	3.4
1	N	241	ALA	3.4
1	N	383	ALA	3.4
1	J	281	PHE	3.4
1	M	281	PHE	3.4
1	C	284	ARG	3.4
1	E	221	LEU	3.4
1	E	295	LEU	3.4
1	F	187	LEU	3.4
1	J	289	LEU	3.4
1	M	215	LEU	3.4
1	E	339	GLU	3.4
1	J	177	VAL	3.4
1	K	273	VAL	3.4
1	F	159	GLY	3.4
1	K	335	GLY	3.4
1	H	243	ALA	3.4
1	K	223	ALA	3.4
1	K	356	ALA	3.4
1	F	317	LEU	3.4
1	N	44	PHE	3.4
1	N	526	LYS	3.4
1	B	387	VAL	3.4
1	E	273	VAL	3.4
1	K	376	VAL	3.4
1	N	264	VAL	3.4
1	N	369	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	218	PRO	3.4
1	G	269	GLY	3.4
1	A	243	ALA	3.4
1	G	227	ILE	3.4
1	H	220	ILE	3.4
1	I	239	ALA	3.4
1	I	325	ILE	3.4
1	E	237	LEU	3.4
1	K	314	LEU	3.4
1	N	200	LEU	3.4
1	K	44	PHE	3.4
1	B	224	ASP	3.3
1	K	334	ASP	3.3
1	F	182	GLY	3.3
1	G	228	SER	3.3
1	G	525	PRO	3.3
1	K	324	VAL	3.3
1	B	258	ALA	3.3
1	D	383	ALA	3.3
1	F	205	ILE	3.3
1	F	325	ILE	3.3
1	I	243	ALA	3.3
1	K	301	ILE	3.3
1	L	333	ILE	3.3
1	N	301	ILE	3.3
1	F	183	LEU	3.3
1	M	289	LEU	3.3
1	D	281	PHE	3.3
1	F	219	PHE	3.3
1	M	265	ASN	3.3
1	K	160	LYS	3.3
1	C	376	VAL	3.3
1	I	271	VAL	3.3
1	J	323	VAL	3.3
1	L	174	VAL	3.3
1	F	243	ALA	3.3
1	F	377	ALA	3.3
1	L	152	ALA	3.3
1	A	215	LEU	3.3
1	B	372	LEU	3.3
1	C	365	LEU	3.3
1	I	314	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	161	LEU	3.3
1	N	317	LEU	3.3
1	C	233	MET	3.3
1	K	288	MET	3.3
1	A	176	THR	3.3
1	C	299	THR	3.3
1	K	151	SER	3.3
1	C	182	GLY	3.3
1	I	202	PRO	3.3
1	E	341	ALA	3.3
1	J	243	ALA	3.3
1	F	342	ILE	3.3
1	H	301	ILE	3.3
1	B	234	LEU	3.3
1	L	309	LEU	3.3
1	M	187	LEU	3.3
1	L	233	MET	3.3
1	M	193	MET	3.3
1	K	313	THR	3.2
1	G	382	GLY	3.2
1	I	173	GLY	3.2
1	B	213	VAL	3.2
1	B	300	VAL	3.2
1	F	213	VAL	3.2
1	M	240	VAL	3.2
1	N	300	VAL	3.2
1	G	203	TYR	3.2
1	K	347	ALA	3.2
1	D	205	ILE	3.2
1	K	325	ILE	3.2
1	F	262	LEU	3.2
1	G	200	LEU	3.2
1	K	262	LEU	3.2
1	M	200	LEU	3.2
1	A	204	PHE	3.2
1	B	331	THR	3.2
1	C	210	THR	3.2
1	K	176	THR	3.2
1	C	375	GLY	3.2
1	M	256	GLY	3.2
1	H	273	VAL	3.2
1	I	240	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	240	VAL	3.2
1	L	376	VAL	3.2
1	N	263	VAL	3.2
1	D	243	ALA	3.2
1	M	239	ALA	3.2
1	M	272	LYS	3.2
1	B	248	LEU	3.2
1	C	325	ILE	3.2
1	C	353	ILE	3.2
1	D	314	LEU	3.2
1	I	230	ILE	3.2
1	K	221	LEU	3.2
1	L	215	LEU	3.2
1	L	270	ILE	3.2
1	G	182	GLY	3.2
1	I	526	LYS	3.2
1	C	158	VAL	3.2
1	D	273	VAL	3.2
1	J	254	VAL	3.2
1	K	240	VAL	3.2
1	B	260	ALA	3.2
1	C	251	ALA	3.2
1	E	356	ALA	3.2
1	M	384	ALA	3.2
1	A	200	LEU	3.2
1	B	317	LEU	3.2
1	C	309	LEU	3.2
1	E	250	ILE	3.2
1	F	372	LEU	3.2
1	G	259	LEU	3.2
1	I	317	LEU	3.2
1	J	332	ILE	3.2
1	L	222	LEU	3.2
1	L	332	ILE	3.2
1	B	182	GLY	3.2
1	E	182	GLY	3.2
1	I	159	GLY	3.2
1	K	210	THR	3.2
1	M	331	THR	3.2
1	A	236	VAL	3.1
1	B	273	VAL	3.1
1	B	370	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	190	VAL	3.1
1	E	215	LEU	3.1
1	E	234	LEU	3.1
1	F	292	ILE	3.1
1	H	259	LEU	3.1
1	J	295	LEU	3.1
1	J	301	ILE	3.1
1	C	219	PHE	3.1
1	F	204	PHE	3.1
1	L	44	PHE	3.1
1	A	266	THR	3.1
1	F	266	THR	3.1
1	C	279	PRO	3.1
1	B	320	ALA	3.1
1	C	240	VAL	3.1
1	D	254	VAL	3.1
1	I	383	ALA	3.1
1	B	249	ILE	3.1
1	C	234	LEU	3.1
1	D	309	LEU	3.1
1	N	262	LEU	3.1
1	N	305	ILE	3.1
1	I	203	TYR	3.1
1	I	233	MET	3.1
1	K	233	MET	3.1
1	B	244	GLY	3.1
1	F	180	GLY	3.1
1	H	297	GLY	3.1
1	E	240	VAL	3.1
1	F	190	VAL	3.1
1	F	260	ALA	3.1
1	F	340	ALA	3.1
1	F	369	VAL	3.1
1	K	213	VAL	3.1
1	N	384	ALA	3.1
1	B	221	LEU	3.1
1	K	234	LEU	3.1
1	M	365	LEU	3.1
1	G	230	ILE	3.1
1	K	292	ILE	3.1
1	M	292	ILE	3.1
1	K	360	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLY	3.1
1	F	176	THR	3.1
1	M	181	THR	3.1
1	K	219	PHE	3.1
1	C	246	PRO	3.1
1	A	188	ASP	3.1
1	L	258	ALA	3.1
1	A	381	VAL	3.1
1	I	177	VAL	3.1
1	I	300	VAL	3.1
1	J	189	VAL	3.1
1	A	372	LEU	3.1
1	C	259	LEU	3.1
1	I	372	LEU	3.1
1	B	353	ILE	3.1
1	F	249	ILE	3.1
1	G	233	MET	3.1
1	K	333	ILE	3.1
1	M	379	ILE	3.1
1	B	203	TYR	3.0
1	I	192	GLY	3.0
1	G	219	PHE	3.0
1	L	219	PHE	3.0
1	A	245	LYS	3.0
1	K	526	LYS	3.0
1	L	171	LYS	3.0
1	M	526	LYS	3.0
1	F	384	ALA	3.0
1	I	320	ALA	3.0
1	B	376	VAL	3.0
1	E	193	MET	3.0
1	C	183	LEU	3.0
1	E	323	VAL	3.0
1	G	236	VAL	3.0
1	N	254	VAL	3.0
1	L	141	SER	3.0
1	D	182	GLY	3.0
1	F	269	GLY	3.0
1	C	266	THR	3.0
1	B	199	TYR	3.0
1	C	203	TYR	3.0
1	D	525	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	279	PRO	3.0
1	M	204	PHE	3.0
1	A	260	ALA	3.0
1	F	383	ALA	3.0
1	K	152	ALA	3.0
1	K	258	ALA	3.0
1	B	309	LEU	3.0
1	E	262	LEU	3.0
1	F	248	LEU	3.0
1	G	263	VAL	3.0
1	I	273	VAL	3.0
1	I	289	LEU	3.0
1	I	376	VAL	3.0
1	J	240	VAL	3.0
1	D	301	ILE	3.0
1	J	205	ILE	3.0
1	L	205	ILE	3.0
1	M	220	ILE	3.0
1	G	282	GLY	3.0
1	K	265	ASN	3.0
1	C	176	THR	3.0
1	F	296	THR	3.0
1	E	360	TYR	3.0
1	G	283	ASP	3.0
1	D	526	LYS	3.0
1	M	168	LYS	3.0
1	G	204	PHE	3.0
1	C	228	SER	3.0
1	E	251	ALA	3.0
1	F	239	ALA	3.0
1	J	152	ALA	3.0
1	A	190	VAL	3.0
1	B	215	LEU	3.0
1	C	215	LEU	3.0
1	C	381	VAL	3.0
1	F	221	LEU	3.0
1	G	221	LEU	3.0
1	H	264	VAL	3.0
1	H	387	VAL	3.0
1	I	365	LEU	3.0
1	J	263	VAL	3.0
1	N	365	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	3.0
1	D	305	ILE	3.0
1	F	220	ILE	3.0
1	F	313	THR	3.0
1	M	299	THR	3.0
1	J	219	PHE	3.0
1	D	284	ARG	2.9
1	A	383	ALA	2.9
1	E	78	ALA	2.9
1	K	373	ALA	2.9
1	A	317	LEU	2.9
1	G	295	LEU	2.9
1	L	206	ASN	2.9
1	L	262	LEU	2.9
1	A	273	VAL	2.9
1	D	240	VAL	2.9
1	I	189	VAL	2.9
1	M	158	VAL	2.9
1	A	297	GLY	2.9
1	M	375	GLY	2.9
1	I	220	ILE	2.9
1	L	220	ILE	2.9
1	E	299	THR	2.9
1	F	331	THR	2.9
1	E	288	MET	2.9
1	M	44	PHE	2.9
1	F	178	GLU	2.9
1	B	383	ALA	2.9
1	H	356	ALA	2.9
1	J	340	ALA	2.9
1	A	221	LEU	2.9
1	A	222	LEU	2.9
1	I	222	LEU	2.9
1	I	262	LEU	2.9
1	L	272	LYS	2.9
1	N	259	LEU	2.9
1	C	236	VAL	2.9
1	D	263	VAL	2.9
1	L	264	VAL	2.9
1	A	325	ILE	2.9
1	C	162	ILE	2.9
1	C	379	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	333	ILE	2.9
1	I	301	ILE	2.9
1	I	342	ILE	2.9
1	K	401	HIS	2.9
1	L	359	ASP	2.9
1	B	176	THR	2.9
1	D	266	THR	2.9
1	H	266	THR	2.9
1	M	176	THR	2.9
1	G	202	PRO	2.9
1	M	288	MET	2.9
1	H	265	ASN	2.9
1	B	171	LYS	2.9
1	C	239	ALA	2.9
1	I	163	ALA	2.9
1	J	377	ALA	2.9
1	K	163	ALA	2.9
1	M	274	ALA	2.9
1	N	312	ALA	2.9
1	K	215	LEU	2.9
1	L	247	LEU	2.9
1	M	295	LEU	2.9
1	N	183	LEU	2.9
1	G	264	VAL	2.9
1	H	253	ASP	2.9
1	H	346	VAL	2.9
1	K	236	VAL	2.9
1	L	196	ASP	2.9
1	M	188	ASP	2.9
1	A	227	ILE	2.9
1	A	284	ARG	2.9
1	B	284	ARG	2.9
1	H	299	THR	2.9
1	K	205	ILE	2.9
1	A	281	PHE	2.9
1	E	203	TYR	2.9
1	I	272	LYS	2.9
1	E	383	ALA	2.9
1	G	312	ALA	2.9
1	K	384	ALA	2.9
1	K	180	GLY	2.9
1	C	231	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	193	MET	2.8
1	K	295	LEU	2.8
1	L	259	LEU	2.8
1	B	336	VAL	2.8
1	C	396	VAL	2.8
1	J	346	VAL	2.8
1	E	210	THR	2.8
1	H	357	THR	2.8
1	A	220	ILE	2.8
1	B	175	ILE	2.8
1	B	333	ILE	2.8
1	E	342	ILE	2.8
1	F	305	ILE	2.8
1	L	150	ILE	2.8
1	L	204	PHE	2.8
1	I	352	GLN	2.8
1	E	384	ALA	2.8
1	F	288	MET	2.8
1	M	383	ALA	2.8
1	B	183	LEU	2.8
1	F	161	LEU	2.8
1	I	259	LEU	2.8
1	I	309	LEU	2.8
1	J	221	LEU	2.8
1	K	200	LEU	2.8
1	B	77	VAL	2.8
1	C	276	VAL	2.8
1	E	176	THR	2.8
1	H	254	VAL	2.8
1	I	299	THR	2.8
1	I	381	VAL	2.8
1	J	369	VAL	2.8
1	L	331	THR	2.8
1	D	227	ILE	2.8
1	E	332	ILE	2.8
1	H	325	ILE	2.8
1	L	349	ILE	2.8
1	F	245	LYS	2.8
1	E	334	ASP	2.8
1	E	318	GLY	2.8
1	H	382	GLY	2.8
1	A	312	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	340	ALA	2.8
1	C	340	ALA	2.8
1	G	251	ALA	2.8
1	J	383	ALA	2.8
1	M	241	ALA	2.8
1	M	356	ALA	2.8
1	N	239	ALA	2.8
1	H	247	LEU	2.8
1	J	161	LEU	2.8
1	K	161	LEU	2.8
1	L	187	LEU	2.8
1	E	296	THR	2.8
1	M	210	THR	2.8
1	B	236	VAL	2.8
1	I	349	ILE	2.8
1	L	342	ILE	2.8
1	L	379	ILE	2.8
1	N	342	ILE	2.8
1	G	229	ASN	2.8
1	C	204	PHE	2.8
1	F	256	GLY	2.8
1	M	297	GLY	2.8
1	C	312	ALA	2.8
1	D	203	TYR	2.8
1	E	274	ALA	2.8
1	H	312	ALA	2.8
1	I	251	ALA	2.8
1	J	320	ALA	2.8
1	M	278	ALA	2.8
1	M	370	ALA	2.8
1	A	309	LEU	2.8
1	D	183	LEU	2.8
1	E	372	LEU	2.8
1	L	234	LEU	2.8
1	D	202	PRO	2.8
1	B	323	VAL	2.8
1	D	336	VAL	2.8
1	A	342	ILE	2.8
1	E	325	ILE	2.8
1	G	249	ILE	2.8
1	I	227	ILE	2.8
1	I	332	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	230	ILE	2.8
1	M	301	ILE	2.8
1	N	230	ILE	2.8
1	J	319	GLN	2.7
1	C	288	MET	2.7
1	K	283	ASP	2.7
1	H	298	GLY	2.7
1	N	281	PHE	2.7
1	N	223	ALA	2.7
1	A	203	TYR	2.7
1	B	187	LEU	2.7
1	H	360	TYR	2.7
1	K	183	LEU	2.7
1	L	237	LEU	2.7
1	C	181	THR	2.7
1	A	376	VAL	2.7
1	H	323	VAL	2.7
1	I	346	VAL	2.7
1	L	254	VAL	2.7
1	A	205	ILE	2.7
1	I	292	ILE	2.7
1	K	138	CYS	2.7
1	C	193	MET	2.7
1	K	224	ASP	2.7
1	C	244	GLY	2.7
1	E	382	GLY	2.7
1	G	272	LYS	2.7
1	A	384	ALA	2.7
1	B	251	ALA	2.7
1	F	281	PHE	2.7
1	I	258	ALA	2.7
1	I	373	ALA	2.7
1	K	274	ALA	2.7
1	L	239	ALA	2.7
1	M	341	ALA	2.7
1	B	200	LEU	2.7
1	J	299	THR	2.7
1	K	289	LEU	2.7
1	M	247	LEU	2.7
1	N	181	THR	2.7
1	I	218	PRO	2.7
1	E	381	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	174	VAL	2.7
1	M	264	VAL	2.7
1	M	369	VAL	2.7
1	M	378	VAL	2.7
1	A	349	ILE	2.7
1	K	379	ILE	2.7
1	L	301	ILE	2.7
1	D	272	LYS	2.7
1	K	374	GLY	2.7
1	B	322	ARG	2.7
1	B	312	ALA	2.7
1	C	260	ALA	2.7
1	C	384	ALA	2.7
1	E	219	PHE	2.7
1	I	384	ALA	2.7
1	K	287	ALA	2.7
1	L	281	PHE	2.7
1	L	347	ALA	2.7
1	M	165	ALA	2.7
1	D	181	THR	2.7
1	E	317	LEU	2.7
1	F	299	THR	2.7
1	I	221	LEU	2.7
1	L	357	THR	2.7
1	N	313	THR	2.7
1	B	246	PRO	2.7
1	N	203	TYR	2.7
1	B	276	VAL	2.7
1	E	201	SER	2.7
1	E	254	VAL	2.7
1	F	396	VAL	2.7
1	H	305	ILE	2.7
1	K	230	ILE	2.7
1	M	227	ILE	2.7
1	C	245	LYS	2.7
1	K	350	ARG	2.7
1	L	244	GLY	2.7
1	L	269	GLY	2.7
1	A	209	GLU	2.6
1	B	347	ALA	2.6
1	G	384	ALA	2.6
1	H	152	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	260	ALA	2.6
1	I	312	ALA	2.6
1	K	312	ALA	2.6
1	B	281	PHE	2.6
1	B	296	THR	2.6
1	D	215	LEU	2.6
1	G	265	ASN	2.6
1	H	134	LEU	2.6
1	H	262	LEU	2.6
1	L	134	LEU	2.6
1	M	329	THR	2.6
1	B	208	PRO	2.6
1	J	235	PRO	2.6
1	B	360	TYR	2.6
1	F	141	SER	2.6
1	F	188	ASP	2.6
1	J	141	SER	2.6
1	K	139	SER	2.6
1	L	203	TYR	2.6
1	B	324	VAL	2.6
1	K	272	LYS	2.6
1	C	175	ILE	2.6
1	F	379	ILE	2.6
1	J	325	ILE	2.6
1	L	236	VAL	2.6
1	L	273	VAL	2.6
1	N	381	VAL	2.6
1	K	88	GLY	2.6
1	C	275	ALA	2.6
1	E	181	THR	2.6
1	F	210	THR	2.6
1	H	229	ASN	2.6
1	L	243	ALA	2.6
1	L	373	ALA	2.6
1	A	248	LEU	2.6
1	E	259	LEU	2.6
1	M	183	LEU	2.6
1	M	246	PRO	2.6
1	E	217	SER	2.6
1	F	151	SER	2.6
1	C	324	VAL	2.6
1	H	332	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	353	ILE	2.6
1	L	369	VAL	2.6
1	M	276	VAL	2.6
1	C	159	GLY	2.6
1	C	319	GLN	2.6
1	K	386	GLU	2.6
1	K	326	ASN	2.6
1	A	275	ALA	2.6
1	A	377	ALA	2.6
1	B	356	ALA	2.6
1	C	313	THR	2.6
1	D	329	THR	2.6
1	M	152	ALA	2.6
1	B	286	LYS	2.6
1	C	526	LYS	2.6
1	G	248	LEU	2.6
1	I	334	ASP	2.6
1	K	247	LEU	2.6
1	K	279	PRO	2.6
1	L	289	LEU	2.6
1	M	224	ASP	2.6
1	N	283	ASP	2.6
1	C	141	SER	2.6
1	M	284	ARG	2.6
1	A	332	ILE	2.6
1	C	77	VAL	2.6
1	C	150	ILE	2.6
1	C	213	VAL	2.6
1	E	190	VAL	2.6
1	E	369	VAL	2.6
1	F	158	VAL	2.6
1	F	254	VAL	2.6
1	H	353	ILE	2.6
1	I	174	VAL	2.6
1	D	214	GLU	2.6
1	F	214	GLU	2.6
1	B	256	GLY	2.6
1	K	244	GLY	2.6
1	B	288	MET	2.6
1	I	288	MET	2.6
1	F	371	LYS	2.6
1	D	384	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	157	THR	2.6
1	H	320	ALA	2.6
1	H	385	THR	2.6
1	I	241	ALA	2.6
1	J	241	ALA	2.6
1	J	331	THR	2.6
1	J	347	ALA	2.6
1	N	356	ALA	2.6
1	E	202	PRO	2.6
1	K	188	ASP	2.6
1	J	187	LEU	2.6
1	K	204	PHE	2.5
1	D	264	VAL	2.5
1	F	324	VAL	2.5
1	G	213	VAL	2.5
1	I	387	VAL	2.5
1	K	77	VAL	2.5
1	K	190	VAL	2.5
1	L	250	ILE	2.5
1	L	336	VAL	2.5
1	M	213	VAL	2.5
1	H	244	GLY	2.5
1	J	256	GLY	2.5
1	M	389	MET	2.5
1	N	192	GLY	2.5
1	N	193	MET	2.5
1	B	401	HIS	2.5
1	A	326	ASN	2.5
1	B	229	ASN	2.5
1	E	526	LYS	2.5
1	J	284	ARG	2.5
1	B	241	ALA	2.5
1	C	356	ALA	2.5
1	E	287	ALA	2.5
1	E	340	ALA	2.5
1	G	210	THR	2.5
1	I	212	ALA	2.5
1	J	356	ALA	2.5
1	K	165	ALA	2.5
1	L	176	THR	2.5
1	L	223	ALA	2.5
1	N	246	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	289	LEU	2.5
1	E	247	LEU	2.5
1	F	295	LEU	2.5
1	G	237	LEU	2.5
1	J	494	LEU	2.5
1	N	204	PHE	2.5
1	C	307	MET	2.5
1	B	264	VAL	2.5
1	B	346	VAL	2.5
1	C	378	VAL	2.5
1	D	244	GLY	2.5
1	E	305	ILE	2.5
1	E	375	GLY	2.5
1	F	175	ILE	2.5
1	K	220	ILE	2.5
1	K	300	VAL	2.5
1	L	324	VAL	2.5
1	L	387	VAL	2.5
1	M	175	ILE	2.5
1	M	342	ILE	2.5
1	N	158	VAL	2.5
1	F	392	LYS	2.5
1	E	265	ASN	2.5
1	G	188	ASP	2.5
1	D	331	THR	2.5
1	G	181	THR	2.5
1	A	320	ALA	2.5
1	C	243	ALA	2.5
1	A	262	LEU	2.5
1	B	400	LEU	2.5
1	D	234	LEU	2.5
1	J	259	LEU	2.5
1	N	309	LEU	2.5
1	B	318	GLY	2.5
1	E	335	GLY	2.5
1	G	256	GLY	2.5
1	I	180	GLY	2.5
1	K	306	GLY	2.5
1	K	318	GLY	2.5
1	N	382	GLY	2.5
1	A	158	VAL	2.5
1	B	292	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	333	ILE	2.5
1	D	285	ARG	2.5
1	F	284	ARG	2.5
1	F	301	ILE	2.5
1	G	250	ILE	2.5
1	G	305	ILE	2.5
1	J	77	VAL	2.5
1	N	336	VAL	2.5
1	G	224	ASP	2.5
1	C	296	THR	2.5
1	F	294	THR	2.5
1	F	329	THR	2.5
1	I	141	SER	2.5
1	I	181	THR	2.5
1	M	357	THR	2.5
1	M	212	ALA	2.5
1	A	183	LEU	2.5
1	A	289	LEU	2.5
1	A	295	LEU	2.5
1	E	289	LEU	2.5
1	F	247	LEU	2.5
1	G	215	LEU	2.5
1	G	317	LEU	2.5
1	H	215	LEU	2.5
1	H	237	LEU	2.5
1	N	295	LEU	2.5
1	B	526	LYS	2.5
1	F	242	LYS	2.5
1	K	371	LYS	2.5
1	H	231	ARG	2.5
1	I	284	ARG	2.5
1	A	244	GLY	2.5
1	A	335	GLY	2.5
1	I	269	GLY	2.5
1	J	229	ASN	2.5
1	E	177	VAL	2.4
1	F	333	ILE	2.5
1	H	336	VAL	2.4
1	J	273	VAL	2.4
1	K	150	ILE	2.5
1	K	177	VAL	2.4
1	L	175	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	189	VAL	2.4
1	L	300	VAL	2.4
1	C	334	ASP	2.4
1	F	224	ASP	2.4
1	L	224	ASP	2.4
1	N	360	TYR	2.4
1	G	313	THR	2.4
1	M	261	THR	2.4
1	F	246	PRO	2.4
1	F	223	ALA	2.4
1	F	394	ALA	2.4
1	G	239	ALA	2.4
1	M	340	ALA	2.4
1	N	251	ALA	2.4
1	A	207	LYS	2.4
1	H	526	LYS	2.4
1	I	237	LEU	2.4
1	J	272	LYS	2.4
1	N	207	LYS	2.4
1	E	322	ARG	2.4
1	N	368	ARG	2.4
1	F	297	GLY	2.4
1	H	281	PHE	2.4
1	M	159	GLY	2.4
1	A	229	ASN	2.4
1	A	300	VAL	2.4
1	A	333	ILE	2.4
1	B	325	ILE	2.4
1	C	391	GLU	2.4
1	F	386	GLU	2.4
1	J	338	GLU	2.4
1	J	324	VAL	2.4
1	K	249	ILE	2.4
1	M	319	GLN	2.4
1	D	473	ASP	2.4
1	L	185	ASP	2.4
1	M	174	VAL	2.4
1	M	300	VAL	2.4
1	N	250	ILE	2.4
1	C	217	SER	2.4
1	J	201	SER	2.4
1	J	203	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	141	SER	2.4
1	M	203	TYR	2.4
1	D	313	THR	2.4
1	H	210	THR	2.4
1	J	357	THR	2.4
1	L	313	THR	2.4
1	N	329	THR	2.4
1	A	341	ALA	2.4
1	G	207	LYS	2.4
1	J	384	ALA	2.4
1	M	260	ALA	2.4
1	M	322	ARG	2.4
1	I	187	LEU	2.4
1	I	215	LEU	2.4
1	C	344	GLY	2.4
1	I	224	ASP	2.4
1	C	144	ILE	2.4
1	E	236	VAL	2.4
1	E	376	VAL	2.4
1	F	323	VAL	2.4
1	H	292	ILE	2.4
1	I	236	VAL	2.4
1	J	387	VAL	2.4
1	K	162	ILE	2.4
1	N	189	VAL	2.4
1	A	288	MET	2.4
1	B	307	MET	2.4
1	G	307	MET	2.4
1	K	228	SER	2.4
1	M	267	MET	2.4
1	B	385	THR	2.4
1	C	385	THR	2.4
1	G	266	THR	2.4
1	K	242	LYS	2.4
1	H	246	PRO	2.4
1	B	287	ALA	2.4
1	E	212	ALA	2.4
1	E	373	ALA	2.4
1	F	251	ALA	2.4
1	H	384	ALA	2.4
1	J	278	ALA	2.4
1	L	212	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	163	ALA	2.4
1	G	262	LEU	2.4
1	G	289	LEU	2.4
1	G	309	LEU	2.4
1	M	400	LEU	2.4
1	A	319	GLN	2.4
1	G	280	GLY	2.4
1	K	269	GLY	2.4
1	G	281	PHE	2.4
1	N	219	PHE	2.4
1	A	177	VAL	2.4
1	D	381	VAL	2.4
1	E	249	ILE	2.4
1	I	213	VAL	2.4
1	I	264	VAL	2.4
1	J	220	ILE	2.4
1	A	193	MET	2.4
1	B	207	LYS	2.4
1	C	267	MET	2.4
1	D	233	MET	2.4
1	G	284	ARG	2.4
1	J	231	ARG	2.4
1	K	263	VAL	2.4
1	A	385	THR	2.4
1	E	313	THR	2.4
1	F	261	THR	2.4
1	G	329	THR	2.4
1	M	296	THR	2.4
1	J	208	PRO	2.4
1	B	384	ALA	2.3
1	D	312	ALA	2.3
1	E	241	ALA	2.3
1	E	275	ALA	2.3
1	F	163	ALA	2.3
1	F	287	ALA	2.3
1	F	320	ALA	2.3
1	L	320	ALA	2.3
1	N	243	ALA	2.3
1	H	221	LEU	2.3
1	I	234	LEU	2.3
1	I	295	LEU	2.3
1	K	365	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	318	GLY	2.3
1	J	382	GLY	2.3
1	M	170	GLY	2.3
1	E	224	ASP	2.3
1	B	193	MET	2.3
1	J	204	PHE	2.3
1	N	233	MET	2.3
1	B	270	ILE	2.3
1	H	250	ILE	2.3
1	H	349	ILE	2.3
1	B	381	VAL	2.3
1	F	177	VAL	2.3
1	H	240	VAL	2.3
1	I	323	VAL	2.3
1	J	174	VAL	2.3
1	L	201	SER	2.3
1	M	381	VAL	2.3
1	A	246	PRO	2.3
1	B	279	PRO	2.3
1	D	210	THR	2.3
1	G	385	THR	2.3
1	H	313	THR	2.3
1	K	181	THR	2.3
1	L	216	GLU	2.3
1	N	186	GLU	2.3
1	N	338	GLU	2.3
1	C	146	GLN	2.3
1	A	239	ALA	2.3
1	C	241	ALA	2.3
1	F	152	ALA	2.3
1	F	212	ALA	2.3
1	N	340	ALA	2.3
1	M	229	ASN	2.3
1	A	234	LEU	2.3
1	A	318	GLY	2.3
1	B	192	GLY	2.3
1	E	200	LEU	2.3
1	F	192	GLY	2.3
1	F	244	GLY	2.3
1	L	221	LEU	2.3
1	J	350	ARG	2.3
1	A	160	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	245	LYS	2.3
1	K	226	LYS	2.3
1	L	225	LYS	2.3
1	N	364	LYS	2.3
1	C	139	SER	2.3
1	B	205	ILE	2.3
1	E	227	ILE	2.3
1	M	325	ILE	2.3
1	B	263	VAL	2.3
1	D	213	VAL	2.3
1	D	339	GLU	2.3
1	F	236	VAL	2.3
1	H	214	GLU	2.3
1	J	276	VAL	2.3
1	N	190	VAL	2.3
1	A	181	THR	2.3
1	B	525	PRO	2.3
1	F	184	GLN	2.3
1	G	184	GLN	2.3
1	G	235	PRO	2.3
1	J	202	PRO	2.3
1	M	208	PRO	2.3
1	C	138	CYS	2.3
1	C	370	ALA	2.3
1	E	239	ALA	2.3
1	E	278	ALA	2.3
1	I	356	ALA	2.3
1	K	260	ALA	2.3
1	L	377	ALA	2.3
1	C	224	ASP	2.3
1	C	374	GLY	2.3
1	E	298	GLY	2.3
1	H	200	LEU	2.3
1	I	268	ARG	2.3
1	J	318	GLY	2.3
1	M	368	ARG	2.3
1	F	160	LYS	2.3
1	E	216	GLU	2.3
1	F	186	GLU	2.3
1	F	228	SER	2.3
1	M	228	SER	2.3
1	I	204	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	195	PHE	2.3
1	J	184	GLN	2.3
1	C	254	VAL	2.3
1	C	336	VAL	2.3
1	G	323	VAL	2.3
1	I	254	VAL	2.3
1	I	336	VAL	2.3
1	J	236	VAL	2.3
1	M	236	VAL	2.3
1	B	218	PRO	2.3
1	E	331	THR	2.3
1	G	246	PRO	2.3
1	I	210	THR	2.3
1	K	329	THR	2.3
1	K	385	THR	2.3
1	N	326	ASN	2.3
1	E	345	ARG	2.3
1	A	212	ALA	2.3
1	A	340	ALA	2.3
1	B	274	ALA	2.3
1	C	152	ALA	2.3
1	C	242	LYS	2.3
1	E	171	LYS	2.3
1	G	320	ALA	2.3
1	I	473	ASP	2.3
1	F	335	GLY	2.3
1	G	306	GLY	2.3
1	L	372	LEU	2.3
1	M	199	TYR	2.3
1	B	339	GLU	2.2
1	C	164	GLU	2.2
1	K	154	SER	2.2
1	B	204	PHE	2.2
1	N	332	ILE	2.2
1	A	210	THR	2.2
1	A	213	VAL	2.2
1	A	329	THR	2.2
1	B	261	THR	2.2
1	B	299	THR	2.2
1	G	357	THR	2.2
1	J	279	PRO	2.2
1	L	378	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	396	VAL	2.2
1	A	322	ARG	2.2
1	I	265	ASN	2.2
1	N	284	ARG	2.2
1	N	171	LYS	2.2
1	A	253	ASP	2.2
1	C	291	ASP	2.2
1	D	188	ASP	2.2
1	G	473	ASP	2.2
1	D	269	GLY	2.2
1	I	170	GLY	2.2
1	J	280	GLY	2.2
1	K	256	GLY	2.2
1	G	234	LEU	2.2
1	G	247	LEU	2.2
1	B	191	GLU	2.2
1	G	255	GLU	2.2
1	G	391	GLU	2.2
1	H	201	SER	2.2
1	E	231	ARG	2.2
1	E	281	PHE	2.2
1	L	350	ARG	2.2
1	B	206	ASN	2.2
1	B	265	ASN	2.2
1	A	189	VAL	2.2
1	E	208	PRO	2.2
1	E	272	LYS	2.2
1	E	279	PRO	2.2
1	H	333	ILE	2.2
1	J	292	ILE	2.2
1	K	147	VAL	2.2
1	K	245	LYS	2.2
1	N	249	ILE	2.2
1	N	333	ILE	2.2
1	G	267	MET	2.2
1	A	256	GLY	2.2
1	J	244	GLY	2.2
1	N	269	GLY	2.2
1	C	143	ALA	2.2
1	C	165	ALA	2.2
1	C	278	ALA	2.2
1	C	373	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	78	ALA	2.2
1	I	377	ALA	2.2
1	J	402	ALA	2.2
1	K	402	ALA	2.2
1	L	260	ALA	2.2
1	L	312	ALA	2.2
1	M	191	GLU	2.2
1	M	275	ALA	2.2
1	E	183	LEU	2.2
1	I	183	LEU	2.2
1	L	183	LEU	2.2
1	L	200	LEU	2.2
1	N	161	LEU	2.2
1	K	168	LYS	2.2
1	A	219	PHE	2.2
1	A	249	ILE	2.2
1	A	331	THR	2.2
1	B	235	PRO	2.2
1	B	294	THR	2.2
1	D	219	PHE	2.2
1	B	283	ASP	2.2
1	D	230	ILE	2.2
1	F	150	ILE	2.2
1	F	162	ILE	2.2
1	L	266	THR	2.2
1	L	385	THR	2.2
1	N	266	THR	2.2
1	A	336	VAL	2.2
1	C	323	VAL	2.2
1	D	177	VAL	2.2
1	E	336	VAL	2.2
1	L	263	VAL	2.2
1	N	213	VAL	2.2
1	C	306	GLY	2.2
1	D	363	GLU	2.2
1	E	280	GLY	2.2
1	G	172	GLU	2.2
1	I	306	GLY	2.2
1	J	216	GLU	2.2
1	B	341	ALA	2.2
1	C	290	GLN	2.2
1	F	341	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	347	ALA	2.2
1	N	258	ALA	2.2
1	C	200	LEU	2.2
1	I	248	LEU	2.2
1	L	286	LYS	2.2
1	M	286	LYS	2.2
1	D	326	ASN	2.2
1	F	265	ASN	2.2
1	G	206	ASN	2.2
1	D	288	MET	2.2
1	B	329	THR	2.2
1	E	188	ASP	2.2
1	I	246	PRO	2.1
1	K	83	ASP	2.2
1	M	137	PRO	2.1
1	M	385	THR	2.2
1	H	219	PHE	2.1
1	I	205	ILE	2.1
1	J	195	PHE	2.1
1	M	144	ILE	2.1
1	M	162	ILE	2.1
1	N	391	GLU	2.1
1	N	397	GLU	2.1
1	H	324	VAL	2.1
1	H	369	VAL	2.1
1	C	192	GLY	2.1
1	E	374	GLY	2.1
1	I	318	GLY	2.1
1	N	319	GLN	2.1
1	G	278	ALA	2.1
1	B	404	ARG	2.1
1	C	134	LEU	2.1
1	C	400	LEU	2.1
1	E	248	LEU	2.1
1	I	247	LEU	2.1
1	M	404	ARG	2.1
1	H	302	SER	2.1
1	J	151	SER	2.1
1	A	226	LYS	2.1
1	C	371	LYS	2.1
1	G	286	LYS	2.1
1	L	389	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	361	ASP	2.1
1	C	191	GLU	2.1
1	E	214	GLU	2.1
1	H	172	GLU	2.1
1	L	361	ASP	2.1
1	I	296	THR	2.1
1	J	525	PRO	2.1
1	M	313	THR	2.1
1	N	176	THR	2.1
1	H	319	GLN	2.1
1	A	182	GLY	2.1
1	C	256	GLY	2.1
1	H	190	VAL	2.1
1	L	396	VAL	2.1
1	M	244	GLY	2.1
1	N	180	GLY	2.1
1	J	395	ARG	2.1
1	B	152	ALA	2.1
1	G	274	ALA	2.1
1	H	239	ALA	2.1
1	I	165	ALA	2.1
1	I	347	ALA	2.1
1	A	247	LEU	2.1
1	C	392	LYS	2.1
1	H	171	LYS	2.1
1	J	200	LEU	2.1
1	M	392	LYS	2.1
1	E	229	ASN	2.1
1	G	389	MET	2.1
1	J	265	ASN	2.1
1	M	232	GLU	2.1
1	H	203	TYR	2.1
1	C	157	THR	2.1
1	E	246	PRO	2.1
1	F	208	PRO	2.1
1	I	313	THR	2.1
1	K	432	GLN	2.1
1	L	146	GLN	2.1
1	L	202	PRO	2.1
1	N	299	THR	2.1
1	A	382	GLY	2.1
1	I	162	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	175	ILE	2.1
1	L	284	ARG	2.1
1	M	211	GLY	2.1
1	M	282	GLY	2.1
1	N	318	GLY	2.1
1	K	195	PHE	2.1
1	E	189	VAL	2.1
1	E	276	VAL	2.1
1	F	174	VAL	2.1
1	I	369	VAL	2.1
1	L	346	VAL	2.1
1	N	311	LYS	2.1
1	D	223	ALA	2.1
1	E	347	ALA	2.1
1	F	347	ALA	2.1
1	L	293	ALA	2.1
1	L	402	ALA	2.1
1	N	287	ALA	2.1
1	G	222	LEU	2.1
1	H	183	LEU	2.1
1	H	372	LEU	2.1
1	A	257	GLU	2.1
1	F	307	MET	2.1
1	J	483	GLU	2.1
1	M	326	ASN	2.1
1	A	224	ASP	2.1
1	M	432	GLN	2.1
1	A	357	THR	2.1
1	B	313	THR	2.1
1	E	525	PRO	2.1
1	F	181	THR	2.1
1	H	322	ARG	2.1
1	H	525	PRO	2.1
1	J	322	ARG	2.1
1	J	385	THR	2.1
1	L	294	THR	2.1
1	M	330	THR	2.1
1	E	180	GLY	2.1
1	E	192	GLY	2.1
1	H	192	GLY	2.1
1	H	280	GLY	2.1
1	J	306	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	272	LYS	2.1
1	F	168	LYS	2.1
1	A	264	VAL	2.1
1	B	195	PHE	2.1
1	J	300	VAL	2.1
1	L	169	VAL	2.1
1	A	139	SER	2.1
1	C	163	ALA	2.1
1	E	186	GLU	2.0
1	G	341	ALA	2.1
1	H	139	SER	2.1
1	I	201	SER	2.1
1	J	275	ALA	2.1
1	K	212	ALA	2.1
1	L	274	ALA	2.1
1	M	287	ALA	2.1
1	N	43	SER	2.1
1	N	212	ALA	2.1
1	N	347	ALA	2.1
1	H	295	LEU	2.0
1	L	161	LEU	2.0
1	C	229	ASN	2.0
1	L	326	ASN	2.0
1	C	155	ASP	2.0
1	I	194	GLN	2.0
1	L	366	GLN	2.0
1	M	290	GLN	2.0
1	N	83	ASP	2.0
1	N	224	ASP	2.0
1	N	366	GLN	2.0
1	H	284	ARG	2.0
1	M	350	ARG	2.0
1	E	294	THR	2.0
1	H	329	THR	2.0
1	J	296	THR	2.0
1	J	313	THR	2.0
1	L	279	PRO	2.0
1	F	321	LYS	2.0
1	F	390	LYS	2.0
1	I	199	TYR	2.0
1	L	207	LYS	2.0
1	C	298	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	318	GLY	2.0
1	K	148	GLY	2.0
1	K	182	GLY	2.0
1	K	282	GLY	2.0
1	M	344	GLY	2.0
1	N	280	GLY	2.0
1	H	227	ILE	2.0
1	L	162	ILE	2.0
1	B	172	GLU	2.0
1	B	232	GLU	2.0
1	E	172	GLU	2.0
1	L	232	GLU	2.0
1	M	177	VAL	2.0
1	L	193	MET	2.0
1	B	278	ALA	2.0
1	H	340	ALA	2.0
1	M	373	ALA	2.0
1	M	402	ALA	2.0
1	B	153	ASN	2.0
1	A	352	GLN	2.0
1	H	188	ASP	2.0
1	K	253	ASP	2.0
1	B	350	ARG	2.0
1	B	395	ARG	2.0
1	J	181	THR	2.0
1	L	210	THR	2.0
1	N	279	PRO	2.0
1	E	269	GLY	2.0
1	J	180	GLY	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 oligosaccharides 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	C	4012	5/5	0.64	0.20	141,141,141,142	0
2	SO4	H	4018	5/5	0.66	0.23	125,125,126,126	0
2	SO4	K	4022	5/5	0.71	0.20	145,146,146,146	0
2	SO4	N	4016	5/5	0.71	0.17	137,137,137,138	0
2	SO4	M	4014	5/5	0.72	0.17	142,142,143,143	0
2	SO4	J	4020	5/5	0.77	0.20	160,160,160,160	0
2	SO4	H	4017	5/5	0.78	0.24	145,146,146,146	0
2	SO4	M	4013	5/5	0.78	0.21	126,126,127,127	0
2	SO4	A	4008	5/5	0.79	0.18	150,150,150,150	0
2	SO4	E	4006	5/5	0.81	0.18	118,119,119,120	0
2	SO4	B	4010	5/5	0.82	0.19	137,137,137,138	0
2	SO4	N	4015	5/5	0.82	0.22	132,133,133,133	0
2	SO4	K	4021	5/5	0.82	0.24	137,138,139,139	0
2	SO4	F	4004	5/5	0.83	0.20	137,138,138,138	0
2	SO4	A	4007	5/5	0.85	0.20	128,129,129,129	0
2	SO4	L	4003	5/5	0.85	0.16	130,131,132,132	0
2	SO4	C	4011	5/5	0.86	0.20	137,137,137,138	0
2	SO4	B	4009	5/5	0.86	0.18	118,119,119,120	0
2	SO4	G	4002	5/5	0.88	0.21	128,128,129,129	0
2	SO4	E	4005	5/5	0.89	0.22	140,141,141,141	0
2	SO4	J	4019	5/5	0.90	0.18	123,124,124,124	0
2	SO4	A	4001	5/5	0.91	0.17	119,120,120,120	0
5	AGS	D	551	31/31	0.94	0.07	25,31,39,41	0
5	AGS	G	1	31/31	0.94	0.07	25,32,40,41	0
5	AGS	J	1	31/31	0.94	0.08	39,42,53,54	0
5	AGS	K	1	31/31	0.94	0.07	37,40,51,54	0
5	AGS	M	1	31/31	0.94	0.07	38,42,50,52	0
5	AGS	I	1	31/31	0.95	0.07	37,41,48,51	0
5	AGS	E	1	31/31	0.95	0.06	27,30,34,37	0
5	AGS	F	1	31/31	0.95	0.07	34,37,44,45	0
5	AGS	L	1	31/31	0.95	0.07	34,37,45,48	0
5	AGS	C	1	31/31	0.95	0.07	37,41,49,52	0
5	AGS	N	1	31/31	0.95	0.07	35,39,47,48	0
5	AGS	B	1	31/31	0.96	0.07	31,37,48,50	0
5	AGS	A	1	31/31	0.96	0.06	35,38,42,44	0
5	AGS	H	1	31/31	0.96	0.06	30,34,38,42	0
4	K	D	549	1/1	0.97	0.04	34,34,34,34	0

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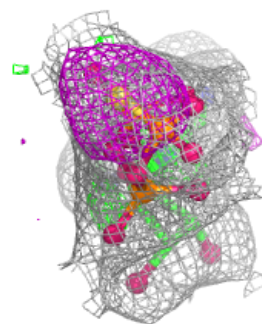
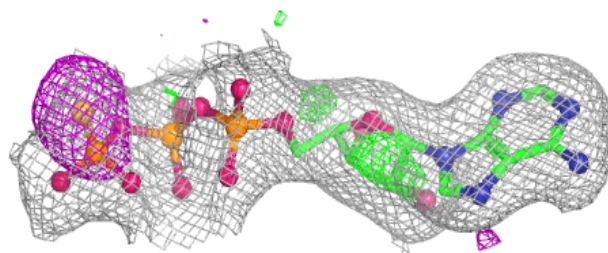
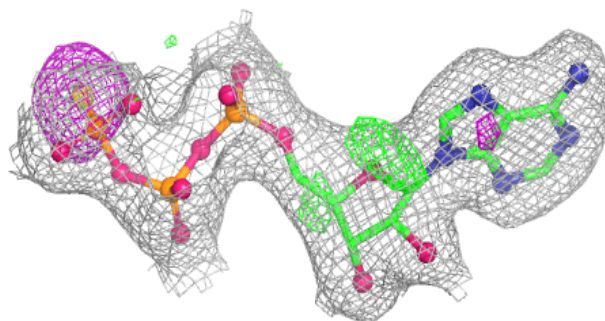
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	D	1	1/1	0.98	0.04	30,30,30,30	0
3	MG	G	550	1/1	0.98	0.05	29,29,29,29	0
4	K	E	549	1/1	0.98	0.06	31,31,31,31	0
4	K	E	4007	1/1	0.98	0.03	36,36,36,36	0
4	K	G	549	1/1	0.98	0.04	39,39,39,39	0
4	K	H	549	1/1	0.98	0.03	41,41,41,41	0
4	K	L	549	1/1	0.98	0.04	39,39,39,39	0
4	K	N	549	1/1	0.98	0.04	41,41,41,41	0
3	MG	L	550	1/1	0.98	0.03	31,31,31,31	0
4	K	B	549	1/1	0.98	0.04	38,38,38,38	0
4	K	C	549	1/1	0.98	0.03	45,45,45,45	0
4	K	M	549	1/1	0.99	0.02	45,45,45,45	0
3	MG	N	550	1/1	0.99	0.06	34,34,34,34	0
4	K	A	549	1/1	0.99	0.03	40,40,40,40	0
3	MG	C	550	1/1	0.99	0.02	36,36,36,36	0
3	MG	D	550	1/1	0.99	0.04	29,29,29,29	0
3	MG	E	550	1/1	0.99	0.02	24,24,24,24	0
3	MG	F	550	1/1	0.99	0.02	30,30,30,30	0
3	MG	A	550	1/1	0.99	0.06	31,31,31,31	0
3	MG	I	550	1/1	0.99	0.04	34,34,34,34	0
4	K	F	549	1/1	0.99	0.03	41,41,41,41	0
3	MG	J	550	1/1	0.99	0.03	37,37,37,37	0
3	MG	K	550	1/1	0.99	0.02	35,35,35,35	0
4	K	I	549	1/1	0.99	0.04	43,43,43,43	0
4	K	J	549	1/1	0.99	0.03	47,47,47,47	0
4	K	K	549	1/1	0.99	0.03	46,46,46,46	0
3	MG	B	550	1/1	0.99	0.04	31,31,31,31	0
3	MG	M	550	1/1	1.00	0.06	38,38,38,38	0
3	MG	H	550	1/1	1.00	0.04	26,26,26,26	0

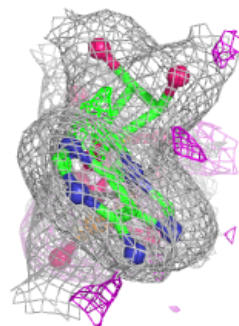
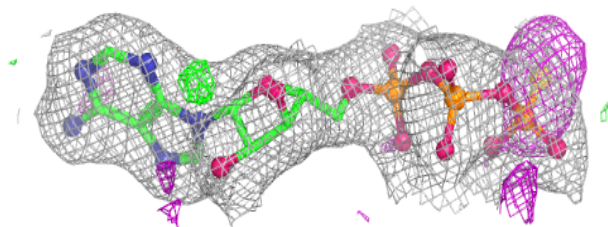
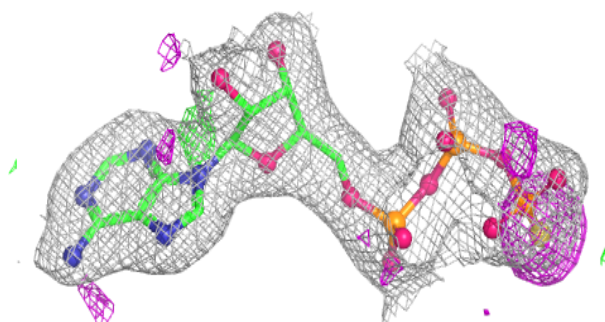
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

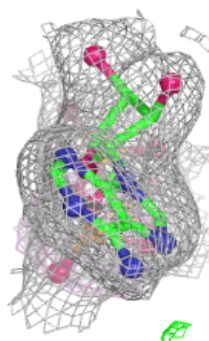
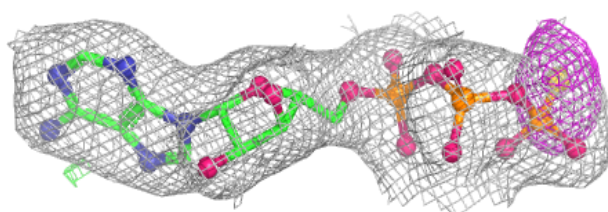
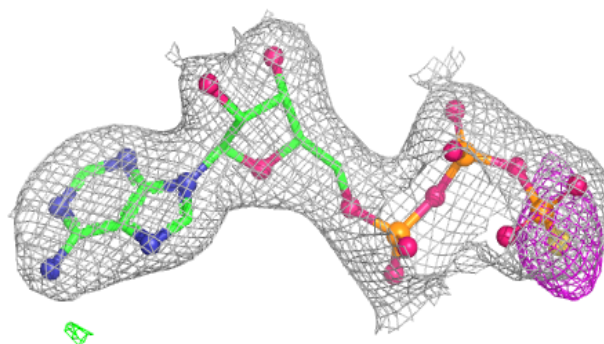
**Electron density around AGS G 1:**

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

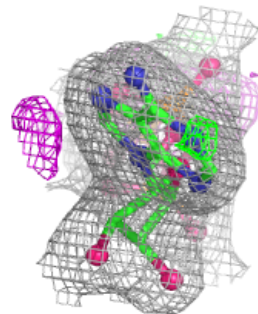
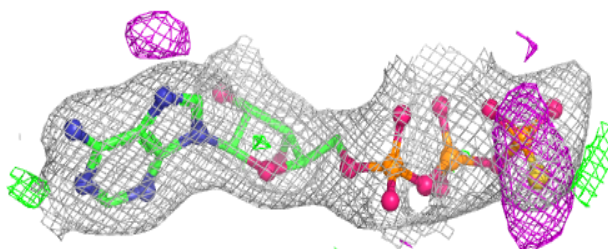
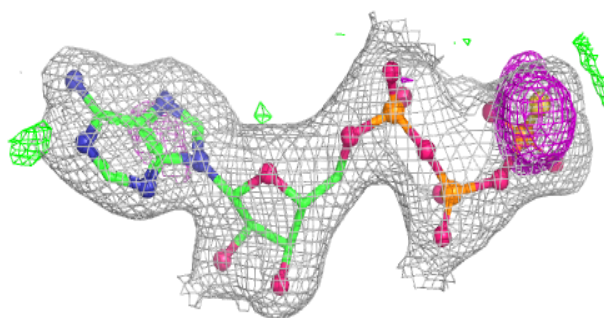


Electron density around AGS J 1:

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

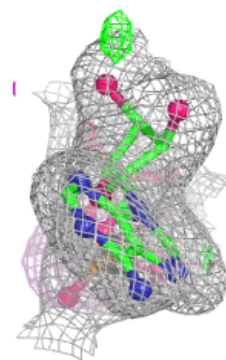
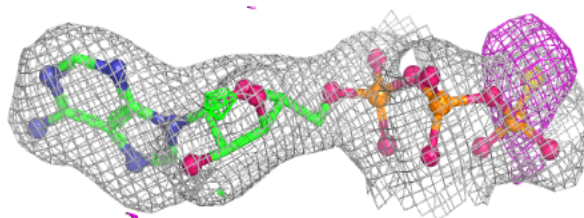
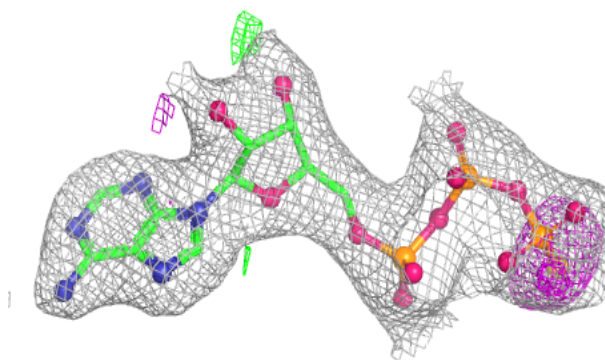
**Electron density around AGS K 1:**

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

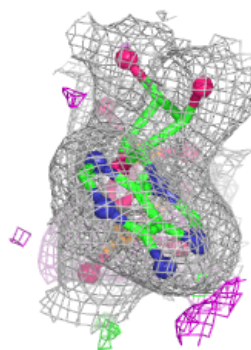
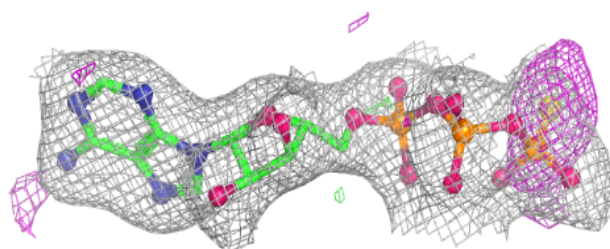
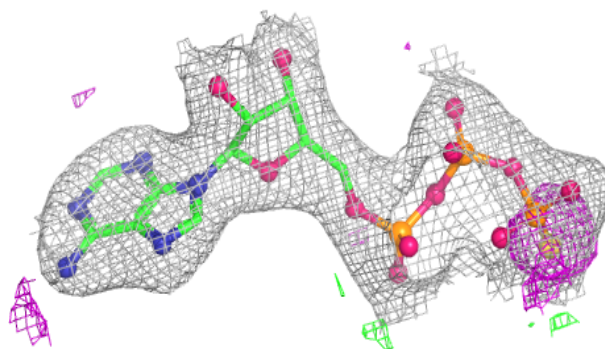


Electron density around AGS M 1:

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

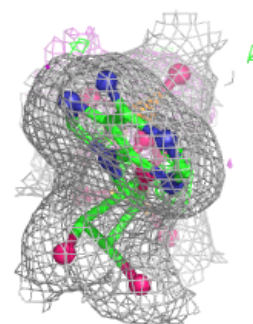
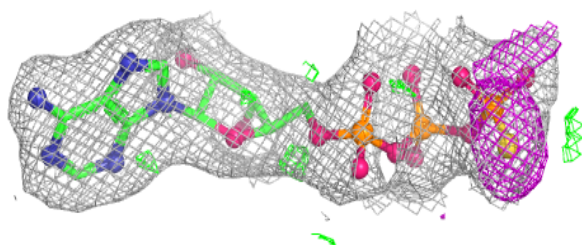
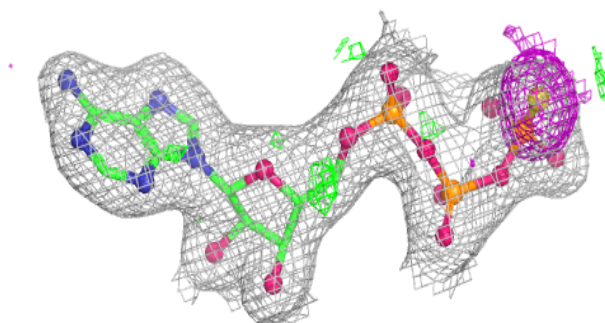
**Electron density around AGS I 1:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

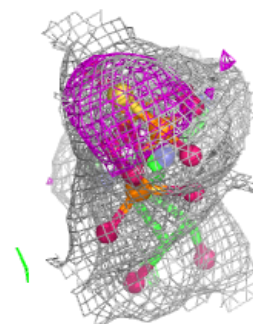
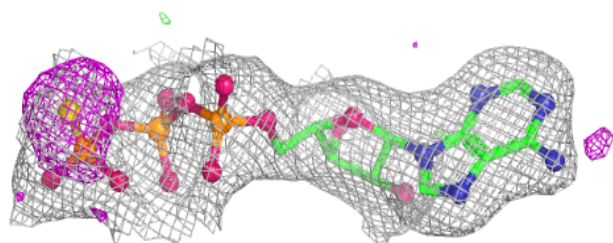
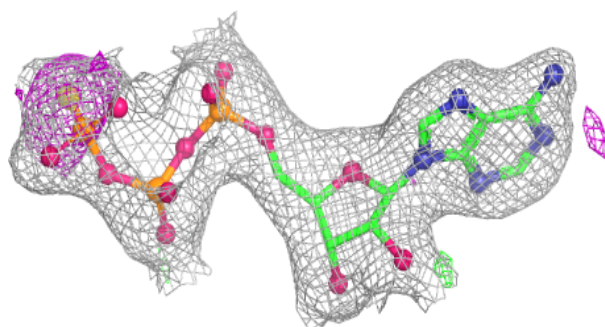


Electron density around AGS E 1:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

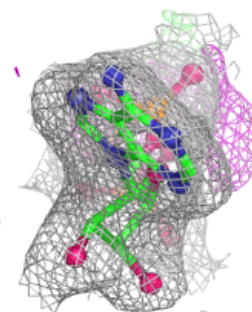
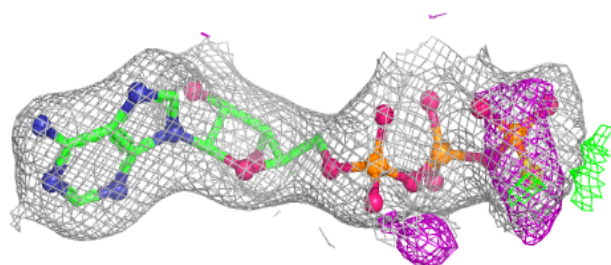
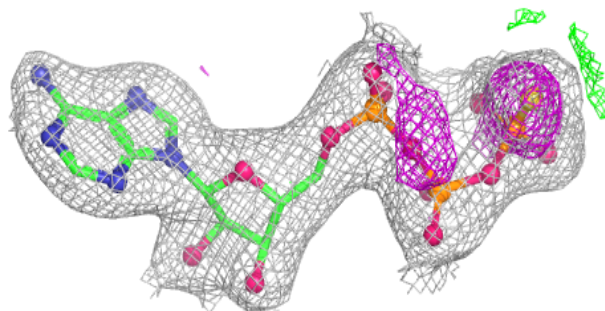
**Electron density around AGS F 1:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

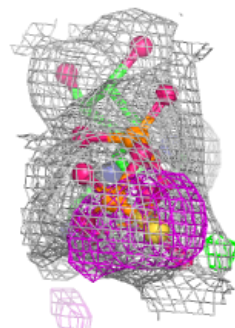
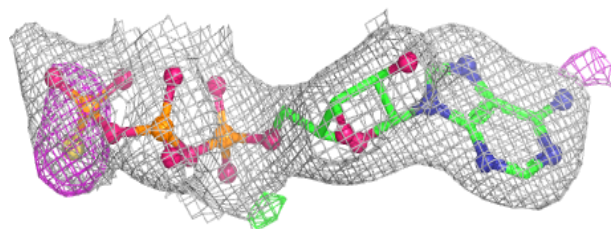
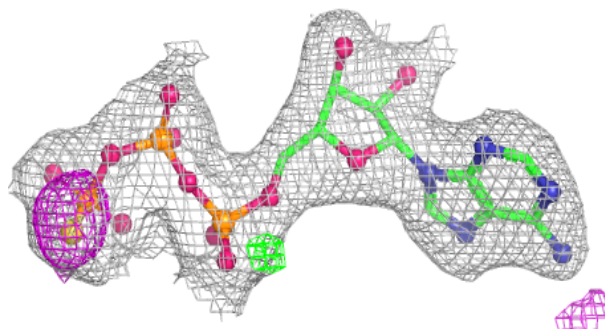


Electron density around AGS L 1:

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

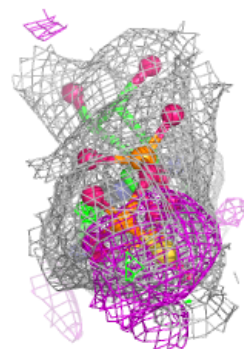
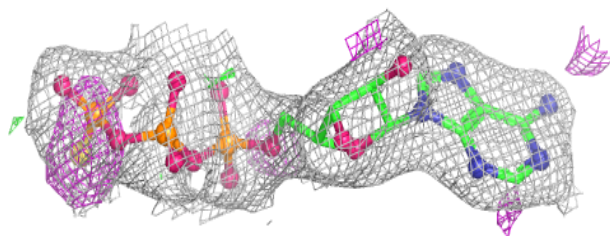
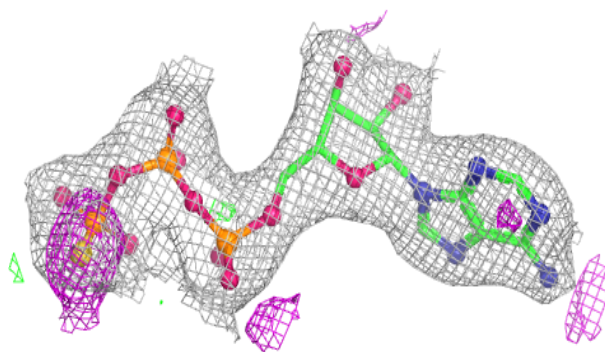
**Electron density around AGS C 1:**

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

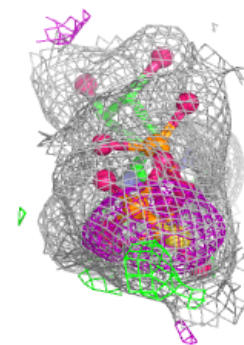
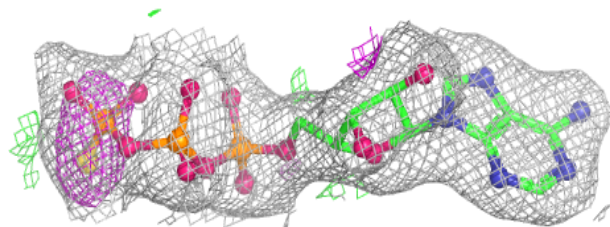
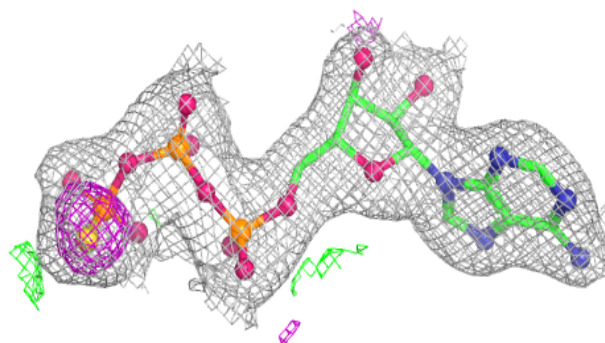


Electron density around AGS N 1:

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

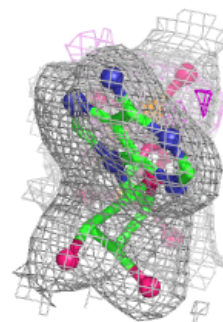
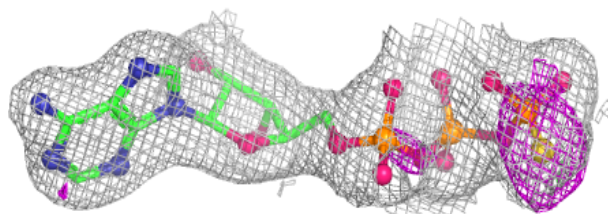
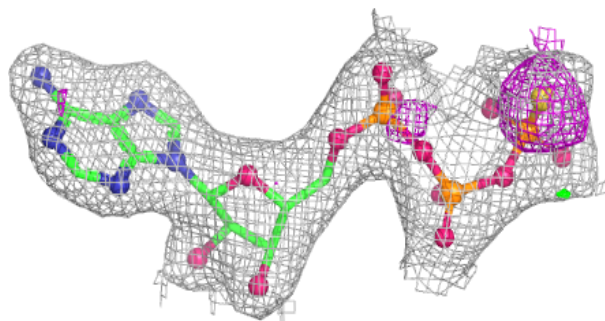
**Electron density around AGS B 1:**

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

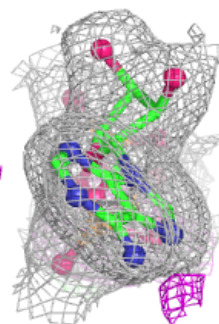
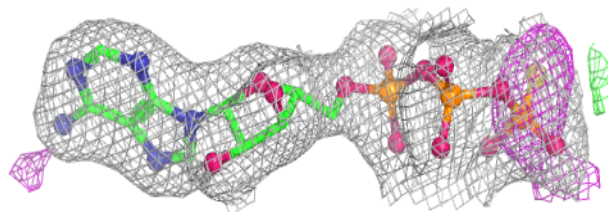
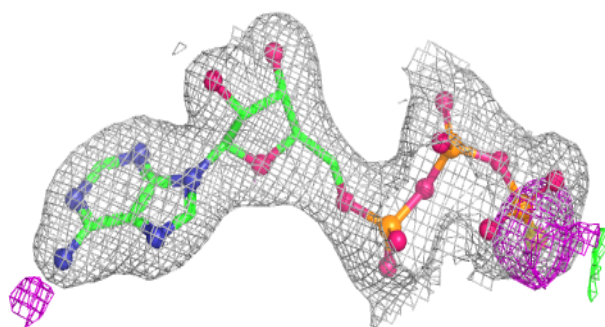


Electron density around AGS A 1:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.