



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:05 AM UTC

PDB ID : 1SX3 / pdb_00001sx3
Title : GroEL14-(ATPgammaS)14
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-30
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:

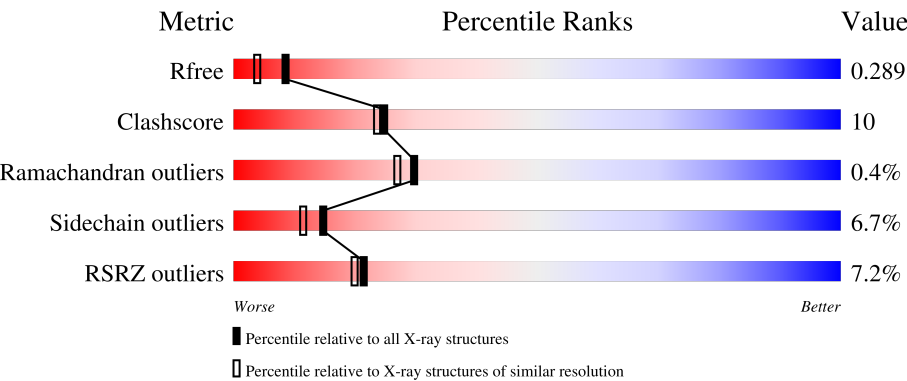
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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.



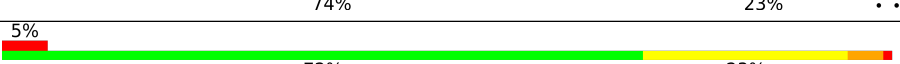
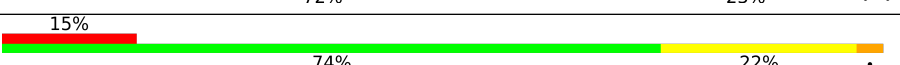
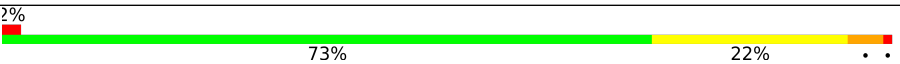
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	525	6% 73%23%.
1	B	525	9% 69%26%..
1	C	525	12% 75%20%..
1	D	525	4% 71%24%..
1	E	525	7% 66%28%6%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	525	
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
1	N	525	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55380 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 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	engineered mutation	UNP P0A6F5

Continued on next page...

Continued from previous page...

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0
2	N	1	Total 1	Mg 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

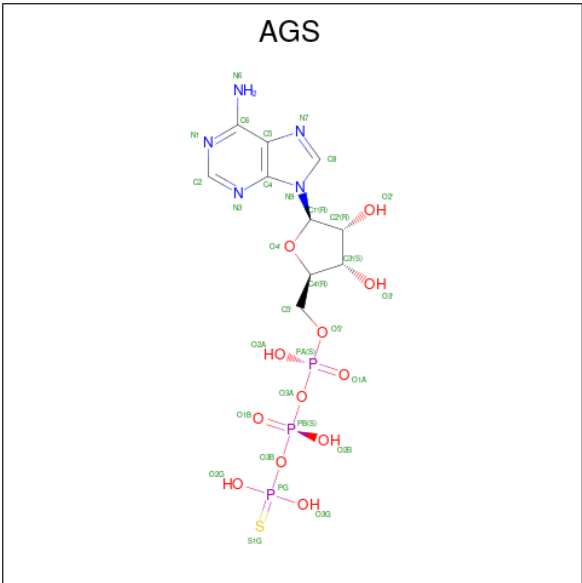
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	D	2	Total 2	K 2	0	0
3	E	2	Total 2	K 2	0	0
3	F	1	Total 1	K 1	0	0
3	G	1	Total 1	K 1	0	0
3	H	1	Total 1	K 1	0	0
3	I	1	Total 1	K 1	0	0
3	J	1	Total 1	K 1	0	0
3	K	1	Total 1	K 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total 62	O 62	0	0
5	B	83	Total 83	O 83	0	0
5	C	57	Total 57	O 57	0	0
5	D	91	Total 91	O 91	0	0
5	E	92	Total 92	O 92	0	0
5	F	71	Total 71	O 71	0	0
5	G	83	Total 83	O 83	0	0
5	H	77	Total 77	O 77	0	0
5	I	60	Total 60	O 60	0	0
5	J	50	Total 50	O 50	0	0
5	K	47	Total 47	O 47	0	0
5	L	61	Total 61	O 61	0	0
5	M	53	Total 53	O 53	0	0

Continued on next page...

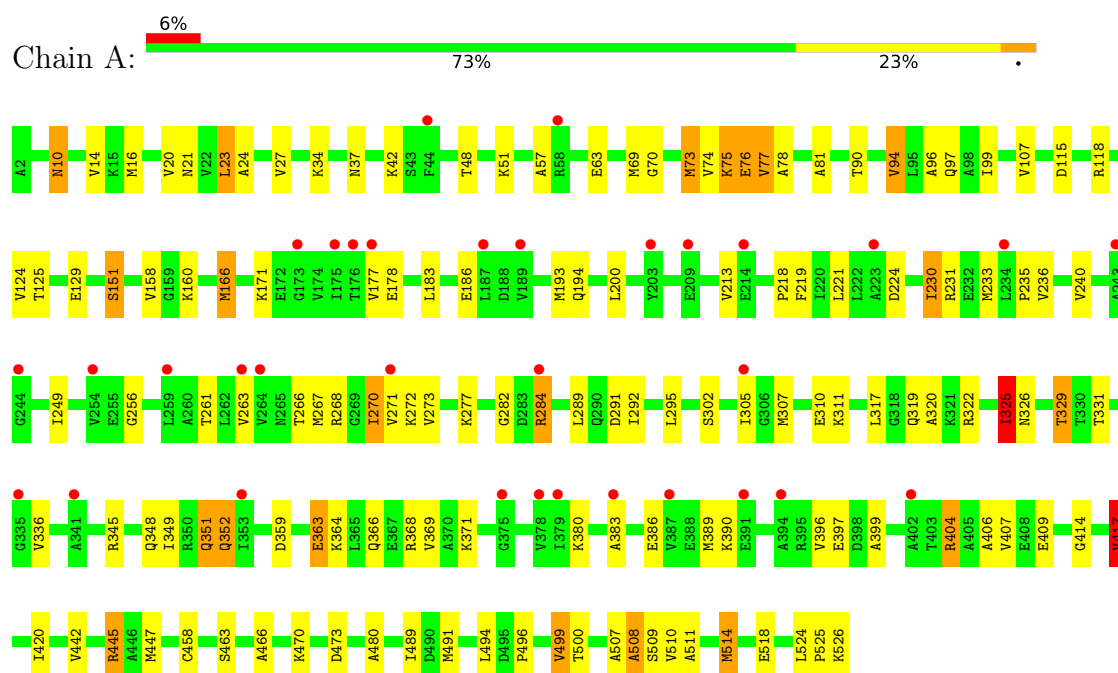
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	59	Total	O	0	0
			59	59		

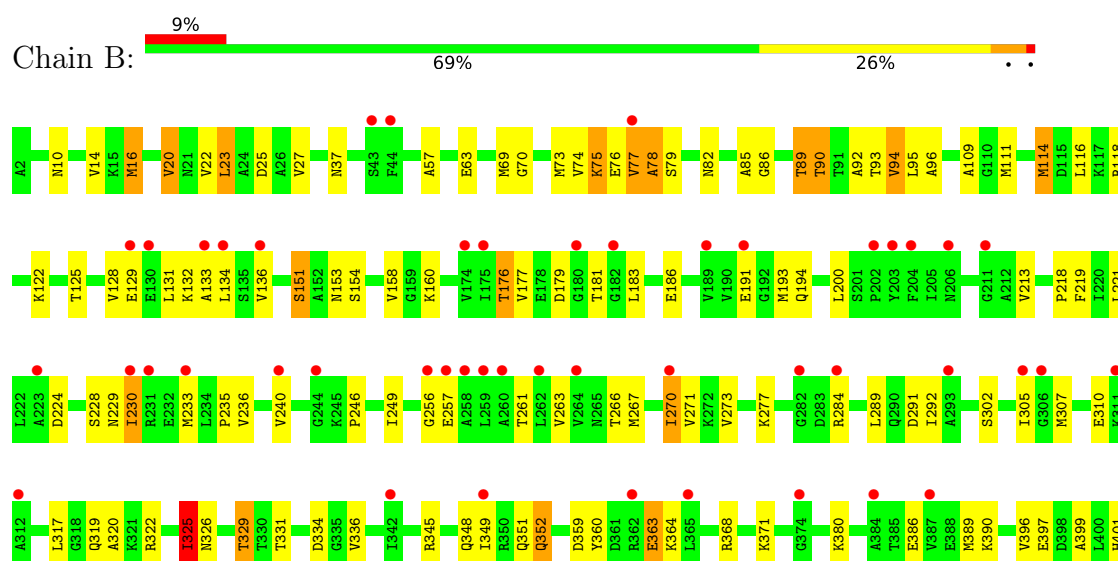
3 Residue-property plots [i](#)

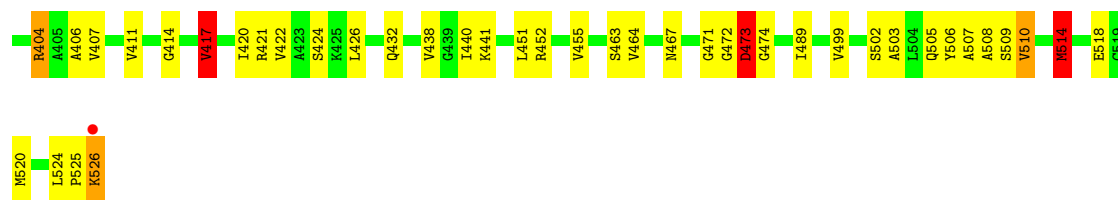
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

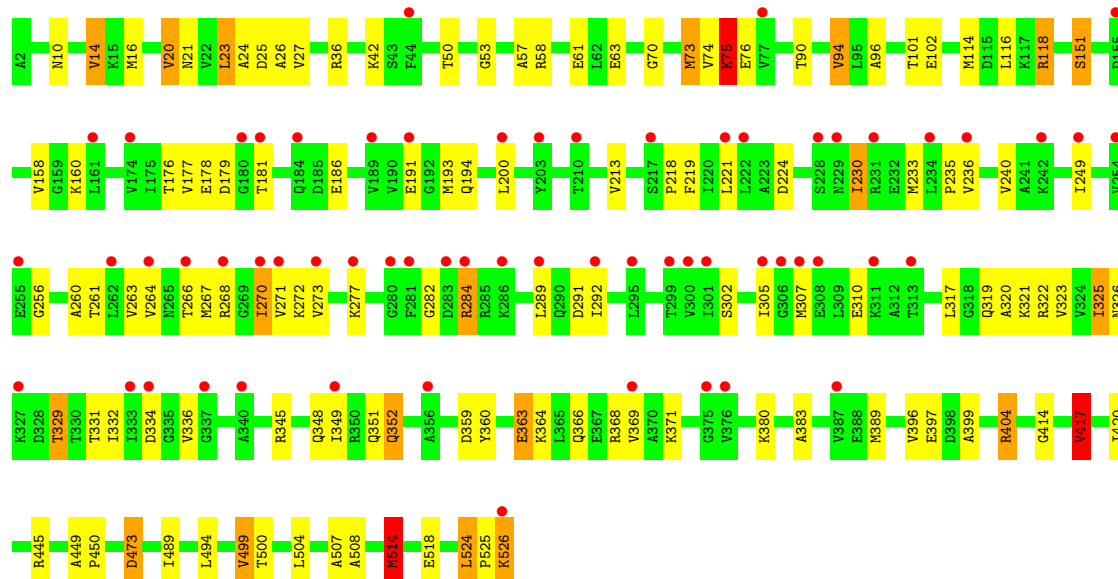
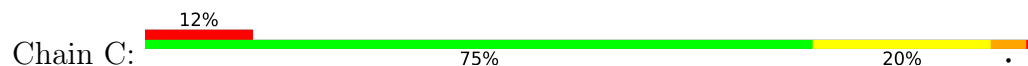


• Molecule 1: groEL protein

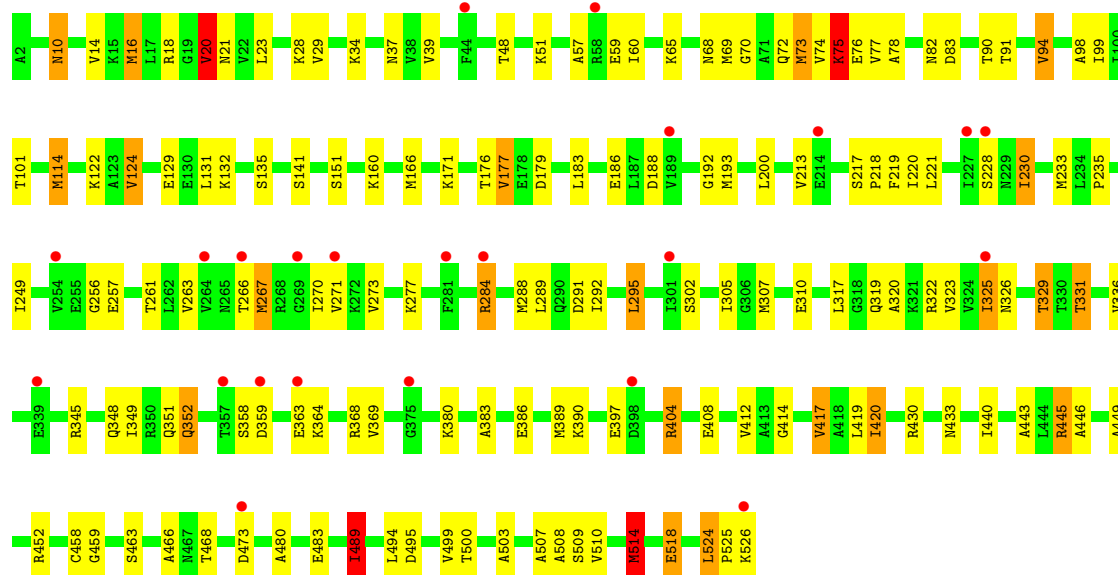




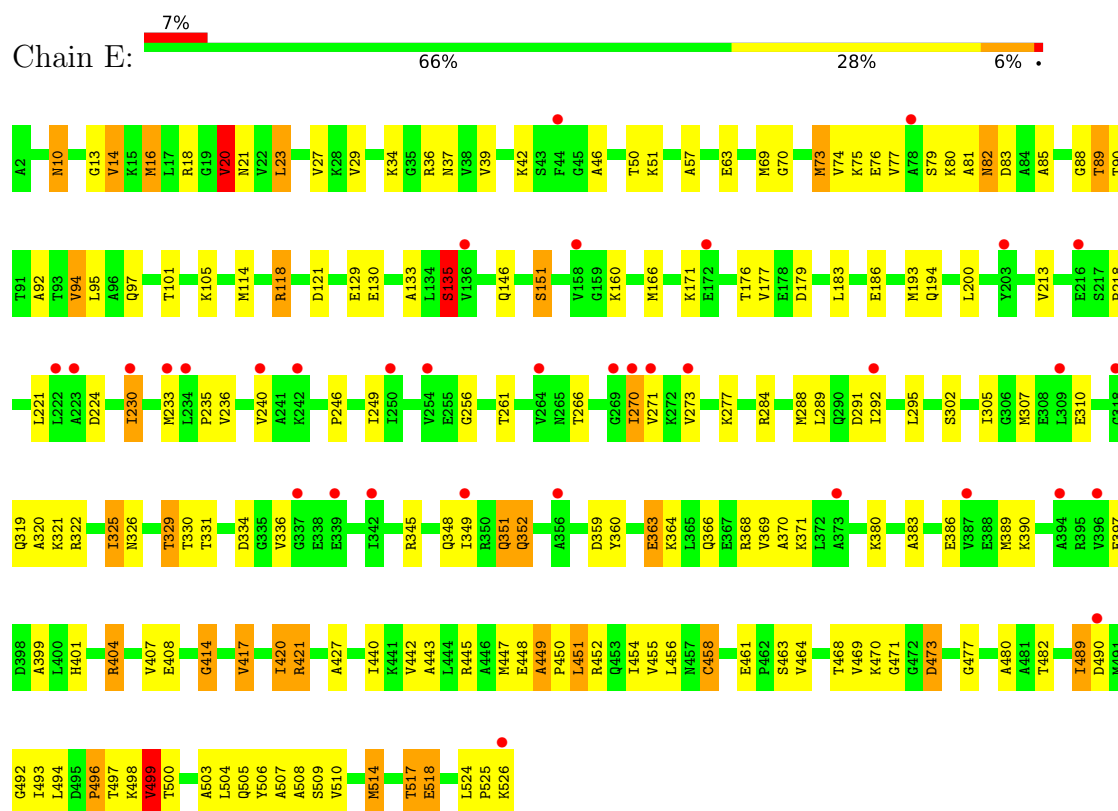
- Molecule 1: groEL protein



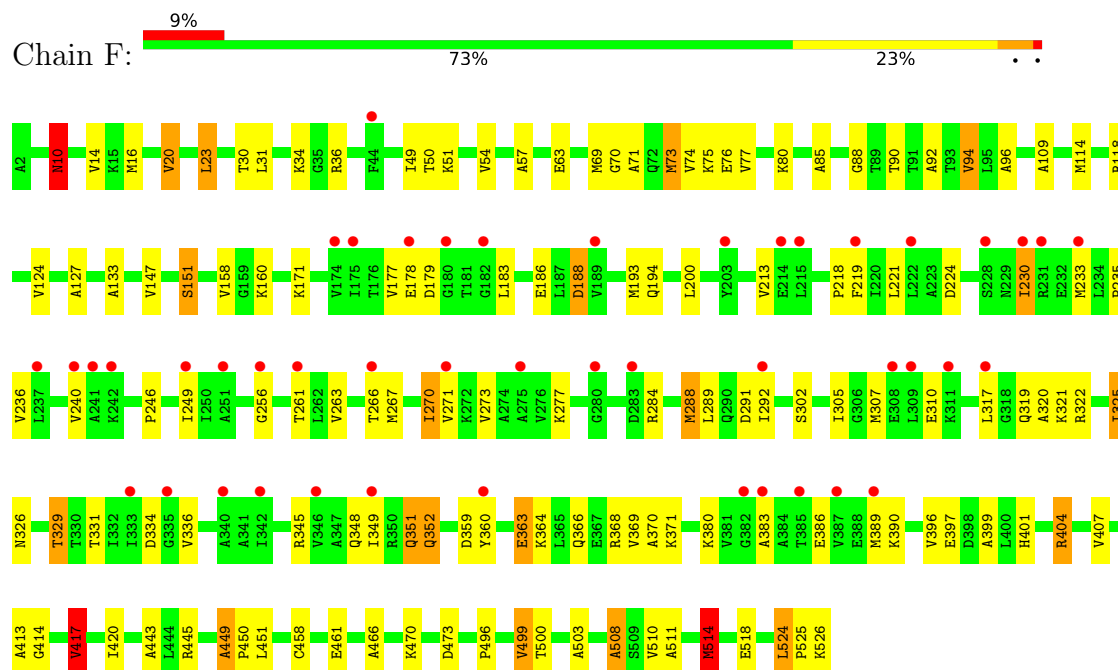
- Molecule 1: groEL protein



- Molecule 1: groEL protein

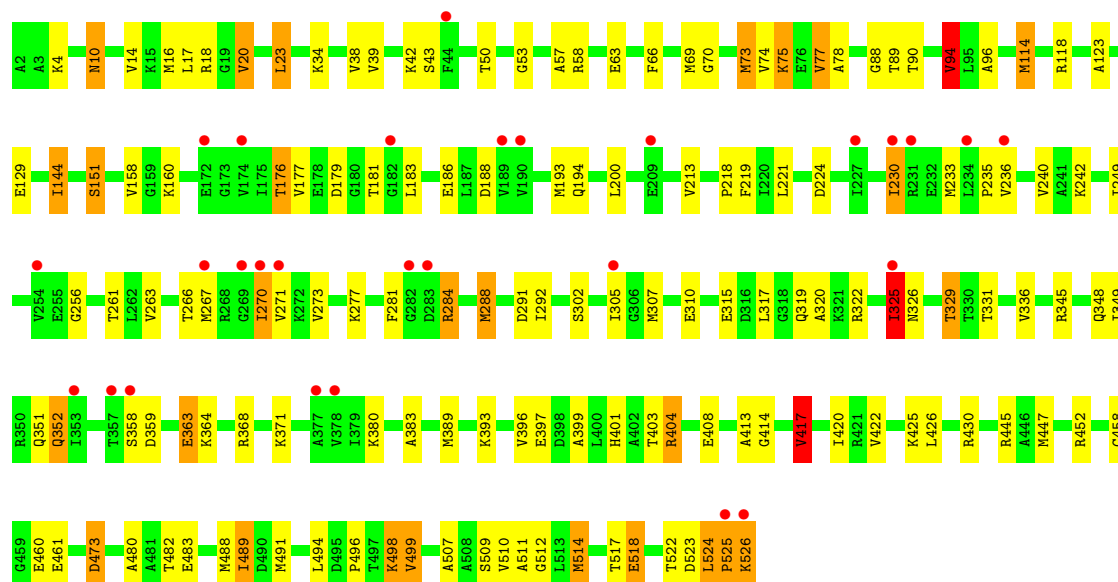


- Molecule 1: groEL protein

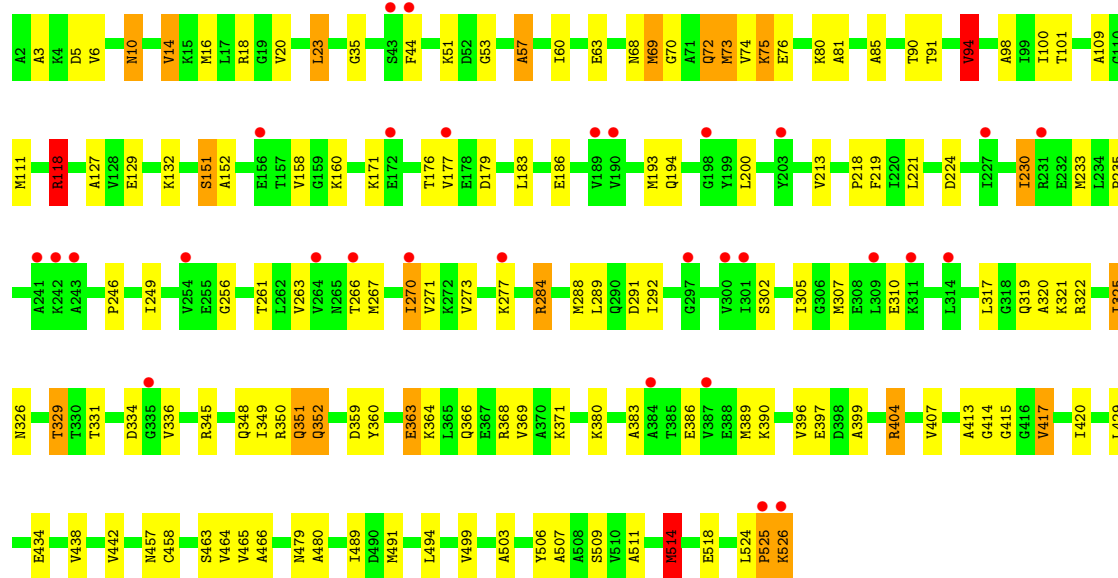


- Molecule 1: groEL protein

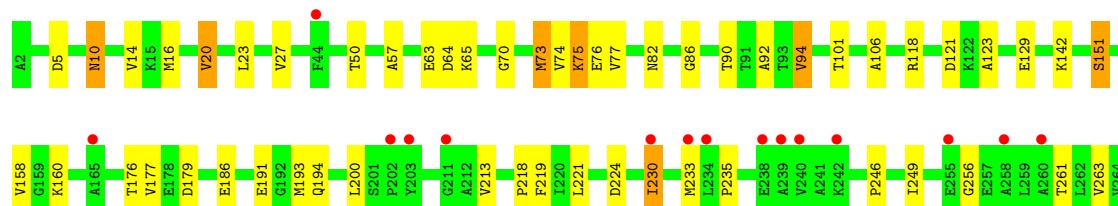


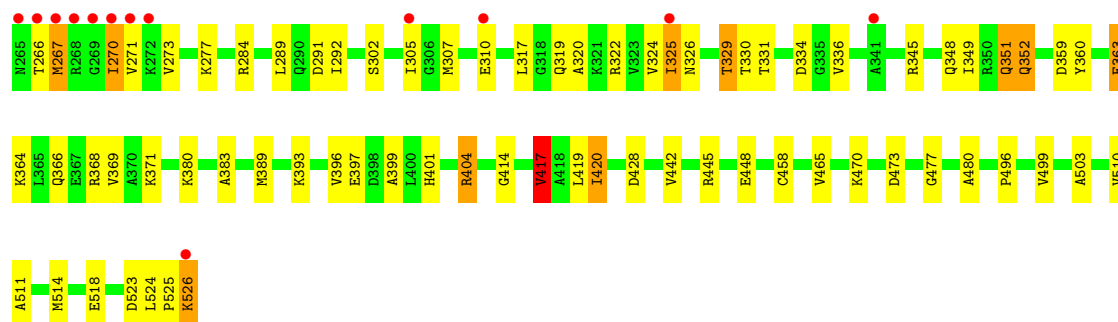


• Molecule 1: groEL protein

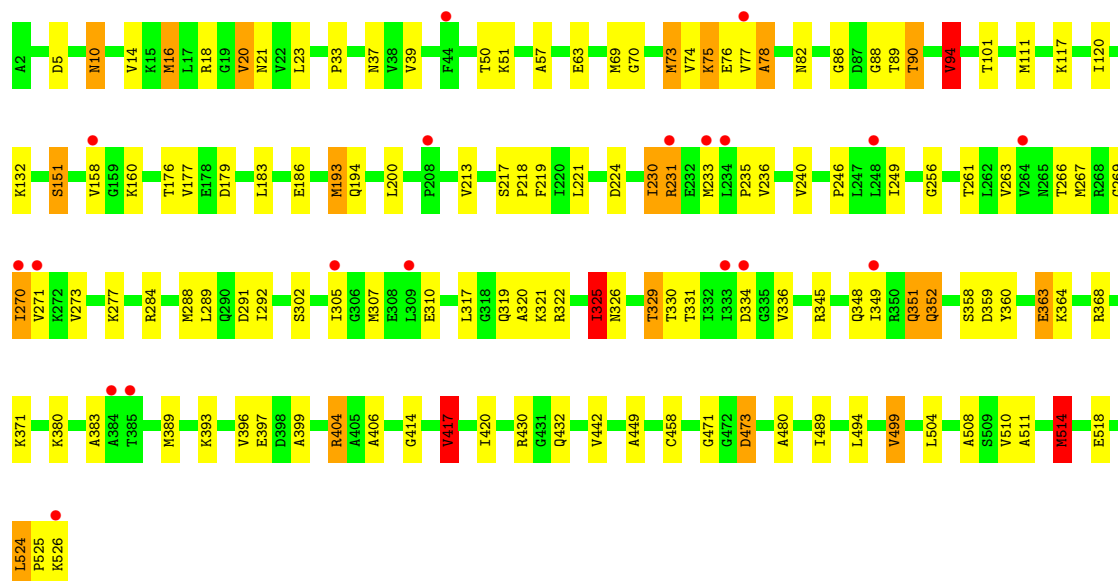
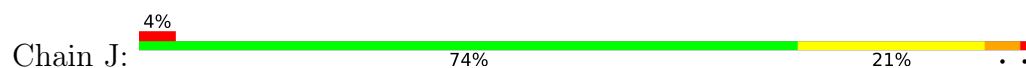


• Molecule 1: groEL protein

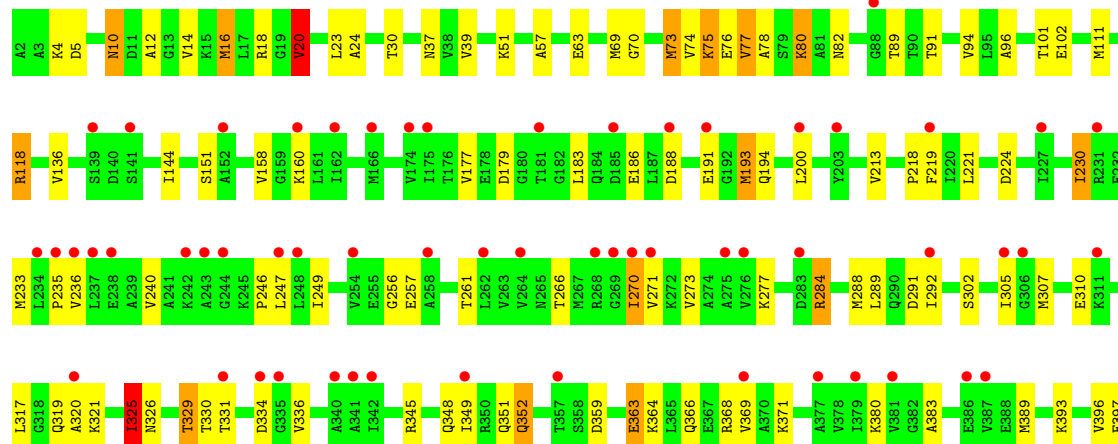
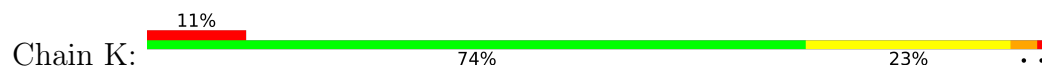




• Molecule 1: groEL protein

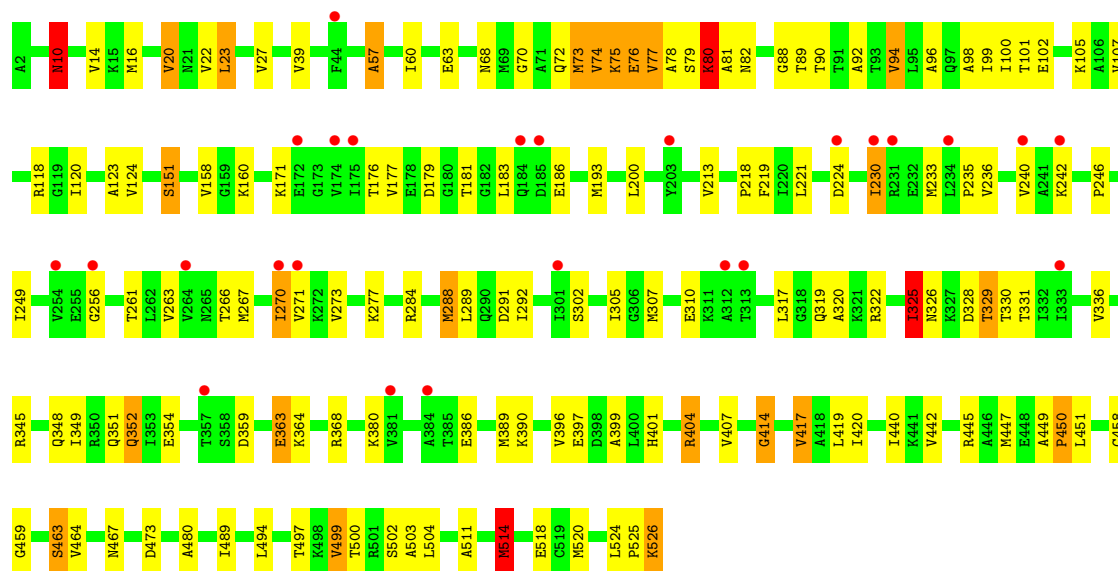


• Molecule 1: groEL protein

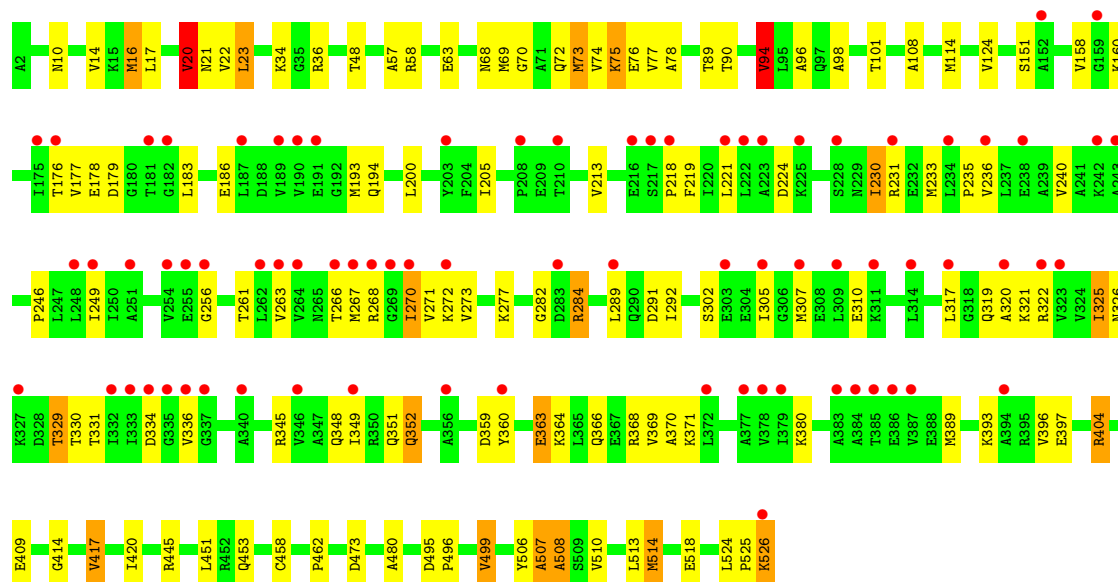
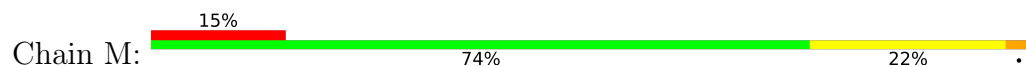




• Molecule 1: groEL protein

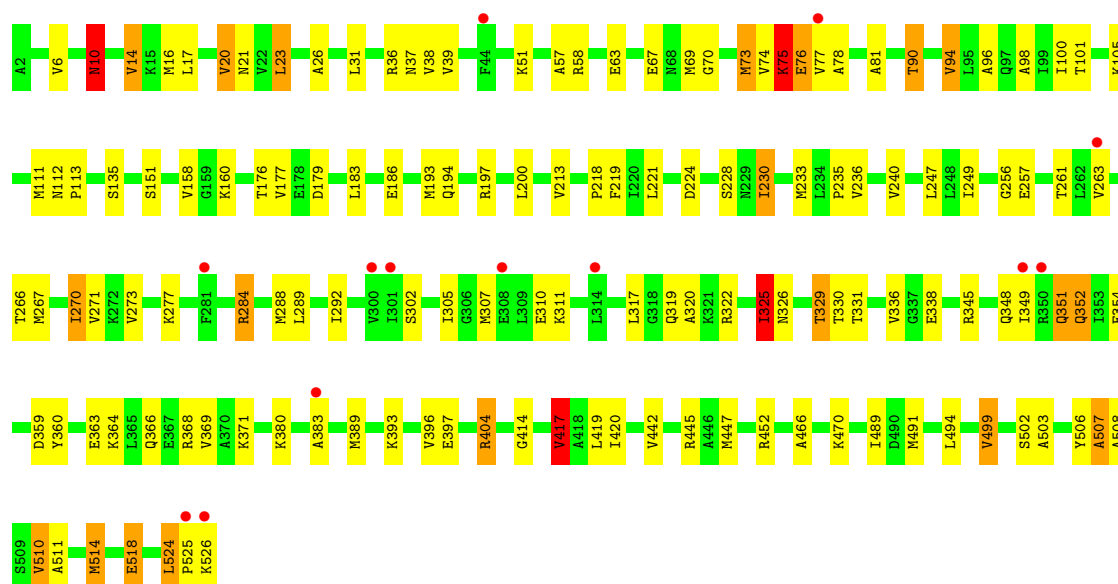


• Molecule 1: groEL protein



• 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)	39.84 – 2.00 39.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.84-2.00) 79.0 (39.84-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
R, R_{free}	0.245 , 0.265 0.274 , 0.289	Depositor DCC
R_{free} test set	12780 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.2	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	0.93	EDS
Total number of atoms	55380	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: K, AGS, MG

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	1.42	33/3883 (0.8%)	1.26	8/5243 (0.2%)
1	B	1.55	37/3883 (1.0%)	1.36	33/5243 (0.6%)
1	C	1.30	22/3883 (0.6%)	1.19	9/5243 (0.2%)
1	D	1.60	40/3883 (1.0%)	1.35	12/5243 (0.2%)
1	E	1.68	68/3883 (1.8%)	1.44	45/5243 (0.9%)
1	F	1.39	26/3883 (0.7%)	1.25	9/5243 (0.2%)
1	G	1.57	38/3883 (1.0%)	1.33	14/5243 (0.3%)
1	H	1.53	39/3883 (1.0%)	1.31	10/5243 (0.2%)
1	I	1.34	20/3883 (0.5%)	1.23	8/5243 (0.2%)
1	J	1.38	28/3883 (0.7%)	1.25	12/5243 (0.2%)
1	K	1.32	29/3883 (0.7%)	1.19	8/5243 (0.2%)
1	L	1.48	46/3883 (1.2%)	1.31	16/5243 (0.3%)
1	M	1.30	21/3883 (0.5%)	1.24	9/5243 (0.2%)
1	N	1.47	40/3883 (1.0%)	1.28	14/5243 (0.3%)
All	All	1.46	487/54362 (0.9%)	1.29	207/73402 (0.3%)

All (487) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	73	MET	SD-CE	-16.75	1.37	1.79
1	J	16	MET	SD-CE	14.58	2.16	1.79
1	E	73	MET	SD-CE	-14.22	1.44	1.79
1	N	98	ALA	C-O	-12.06	1.09	1.24
1	A	73	MET	SD-CE	-12.03	1.49	1.79
1	M	16	MET	SD-CE	11.86	2.09	1.79
1	D	73	MET	SD-CE	-11.45	1.50	1.79
1	M	73	MET	SD-CE	-11.15	1.51	1.79
1	B	90	THR	C-O	11.02	1.37	1.24
1	N	96	ALA	CA-CB	-10.99	1.36	1.53
1	N	507	ALA	CA-CB	-10.94	1.36	1.53
1	L	511	ALA	CA-CB	-10.80	1.36	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	MET	SD-CE	-10.76	1.52	1.79
1	B	114	MET	SD-CE	10.72	2.06	1.79
1	E	94	VAL	C-O	-10.69	1.11	1.24
1	L	92	ALA	CA-CB	10.34	1.69	1.53
1	A	81	ALA	CA-CB	-10.19	1.37	1.53
1	H	73	MET	SD-CE	-10.08	1.54	1.79
1	L	88	GLY	C-O	10.07	1.37	1.24
1	L	514	MET	SD-CE	9.87	2.04	1.79
1	D	449	ALA	CA-CB	9.83	1.65	1.53
1	E	490	ASP	CB-CG	-9.79	1.27	1.52
1	B	16	MET	SD-CE	9.62	2.03	1.79
1	E	16	MET	SD-CE	9.60	2.03	1.79
1	N	510	VAL	CB-CG2	9.51	1.83	1.52
1	K	101	THR	C-O	-9.34	1.13	1.24
1	G	20	VAL	CA-CB	9.34	1.66	1.54
1	B	509	SER	N-CA	-9.30	1.35	1.46
1	D	114	MET	CG-SD	9.27	2.04	1.80
1	G	114	MET	SD-CE	9.17	2.02	1.79
1	A	511	ALA	CA-CB	-9.13	1.38	1.53
1	E	507	ALA	CA-CB	-9.10	1.39	1.53
1	E	414	GLY	C-O	9.04	1.32	1.24
1	F	92	ALA	C-O	9.04	1.34	1.24
1	D	114	MET	SD-CE	8.98	2.02	1.79
1	K	16	MET	SD-CE	8.68	2.01	1.79
1	B	520	MET	SD-CE	-8.59	1.58	1.79
1	A	77	VAL	CA-CB	8.57	1.64	1.54
1	L	96	ALA	CA-CB	-8.49	1.40	1.53
1	K	507	ALA	CA-CB	-8.43	1.40	1.53
1	E	101	THR	C-O	-8.40	1.14	1.24
1	H	491	MET	SD-CE	8.38	2.00	1.79
1	L	80	LYS	CG-CD	8.36	1.77	1.52
1	L	288	MET	SD-CE	8.31	2.00	1.79
1	D	445	ARG	NE-CZ	8.30	1.42	1.33
1	K	514	MET	SD-CE	8.24	2.00	1.79
1	C	114	MET	CG-SD	8.21	2.01	1.80
1	F	445	ARG	NE-CZ	8.17	1.42	1.33
1	K	96	ALA	CA-CB	-8.12	1.40	1.53
1	G	123	ALA	CA-CB	-8.12	1.40	1.53
1	H	415	GLY	C-O	8.11	1.34	1.24
1	J	193	MET	SD-CE	8.09	1.99	1.79
1	F	73	MET	SD-CE	-8.07	1.59	1.79
1	N	76	GLU	N-CA	8.07	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	MET	SD-CE	8.03	1.99	1.79
1	B	510	VAL	CB-CG2	8.02	1.79	1.52
1	E	105	LYS	N-CA	7.88	1.56	1.46
1	C	73	MET	SD-CE	-7.88	1.59	1.79
1	I	101	THR	C-O	-7.87	1.15	1.24
1	N	452	ARG	C-O	-7.86	1.15	1.24
1	M	101	THR	C-O	-7.80	1.15	1.24
1	L	105	LYS	C-O	7.77	1.33	1.24
1	B	129	GLU	CD-OE2	7.77	1.40	1.25
1	A	16	MET	SD-CE	7.73	1.98	1.79
1	E	448	GLU	CA-CB	7.70	1.66	1.53
1	G	114	MET	CG-SD	7.70	2.00	1.80
1	F	449	ALA	C-O	-7.67	1.17	1.24
1	D	452	ARG	N-CA	7.64	1.56	1.46
1	A	507	ALA	CA-CB	-7.62	1.41	1.53
1	N	81	ALA	CA-CB	7.60	1.65	1.53
1	K	24	ALA	CA-CB	7.58	1.65	1.53
1	K	504	LEU	C-O	-7.56	1.15	1.24
1	E	288	MET	SD-CE	7.55	1.98	1.79
1	M	98	ALA	C-O	-7.50	1.15	1.24
1	H	434	GLU	CA-CB	7.47	1.65	1.53
1	F	16	MET	SD-CE	7.45	1.98	1.79
1	F	511	ALA	C-O	-7.43	1.15	1.24
1	D	507	ALA	N-CA	7.42	1.55	1.46
1	N	288	MET	SD-CE	7.41	1.98	1.79
1	I	77	VAL	CA-CB	7.38	1.62	1.54
1	H	3	ALA	CA-CB	-7.37	1.41	1.53
1	I	267	MET	SD-CE	7.33	1.97	1.79
1	F	127	ALA	CA-CB	7.32	1.64	1.53
1	D	509	SER	N-CA	-7.32	1.37	1.46
1	F	71	ALA	CA-CB	7.29	1.64	1.53
1	A	447	MET	SD-CE	7.26	1.97	1.79
1	D	514	MET	SD-CE	7.25	1.97	1.79
1	E	464	VAL	CA-C	7.24	1.61	1.52
1	B	132	LYS	CD-CE	7.24	1.74	1.52
1	L	94	VAL	N-CA	-7.22	1.38	1.46
1	H	288	MET	SD-CE	7.21	1.97	1.79
1	B	417	VAL	C-O	-7.17	1.15	1.24
1	E	89	THR	CA-CB	-7.17	1.41	1.53
1	E	490	ASP	CG-OD1	7.16	1.39	1.25
1	I	73	MET	SD-CE	-7.16	1.61	1.79
1	G	417	VAL	CA-CB	7.15	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	490	ASP	CA-CB	-7.14	1.41	1.53
1	H	5	ASP	CA-C	7.13	1.61	1.52
1	K	76	GLU	C-O	-7.08	1.14	1.24
1	A	509	SER	N-CA	-7.08	1.37	1.46
1	L	98	ALA	CA-CB	7.06	1.64	1.53
1	C	500	THR	C-O	-7.04	1.16	1.24
1	L	16	MET	SD-CE	6.99	1.97	1.79
1	L	82	ASN	N-CA	-6.99	1.38	1.46
1	L	440	ILE	CA-CB	6.98	1.62	1.54
1	D	443	ALA	CA-C	6.98	1.61	1.52
1	E	88	GLY	C-O	6.98	1.33	1.23
1	E	81	ALA	CA-C	6.96	1.62	1.52
1	N	445	ARG	NE-CZ	6.95	1.40	1.33
1	J	111	MET	SD-CE	6.95	1.97	1.79
1	N	69	MET	SD-CE	-6.94	1.62	1.79
1	N	507	ALA	N-CA	6.94	1.54	1.46
1	J	94	VAL	CA-CB	6.93	1.63	1.54
1	B	441	LYS	CA-CB	6.92	1.64	1.53
1	B	114	MET	CG-SD	6.91	1.98	1.80
1	C	14	VAL	CA-CB	6.91	1.64	1.54
1	F	96	ALA	CA-CB	-6.89	1.42	1.53
1	L	76	GLU	N-CA	6.89	1.55	1.46
1	E	85	ALA	CA-CB	6.87	1.64	1.54
1	N	511	ALA	N-CA	6.87	1.54	1.46
1	E	509	SER	N-CA	-6.86	1.38	1.46
1	M	495	ASP	CA-C	-6.85	1.46	1.52
1	B	129	GLU	CG-CD	6.84	1.69	1.52
1	E	471	GLY	C-O	-6.84	1.16	1.24
1	C	499	VAL	CA-CB	6.84	1.63	1.54
1	A	99	ILE	C-O	6.83	1.31	1.24
1	D	76	GLU	C-O	-6.82	1.15	1.24
1	E	80	LYS	CG-CD	6.80	1.72	1.52
1	M	34	LYS	N-CA	-6.79	1.38	1.46
1	G	517	THR	C-O	-6.79	1.15	1.24
1	A	491	MET	SD-CE	6.78	1.96	1.79
1	K	136	VAL	CA-C	6.78	1.58	1.52
1	K	12	ALA	CA-CB	-6.77	1.42	1.53
1	L	107	VAL	CA-C	6.76	1.61	1.52
1	C	96	ALA	CA-CB	-6.76	1.42	1.53
1	L	99	ILE	CA-CB	6.74	1.63	1.54
1	J	511	ALA	CA-CB	-6.74	1.42	1.53
1	H	57	ALA	CA-CB	6.74	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	424	SER	C-O	-6.72	1.15	1.24
1	I	5	ASP	CA-C	6.72	1.61	1.52
1	K	508	ALA	C-O	-6.70	1.16	1.24
1	L	73	MET	SD-CE	-6.70	1.62	1.79
1	H	466	ALA	C-O	-6.70	1.16	1.24
1	E	490	ASP	CA-C	-6.69	1.43	1.52
1	B	432	GLN	CG-CD	6.68	1.68	1.52
1	N	98	ALA	N-CA	6.67	1.54	1.46
1	M	96	ALA	CA-CB	-6.65	1.43	1.53
1	E	92	ALA	C-O	6.64	1.31	1.24
1	N	58	ARG	NE-CZ	6.63	1.40	1.33
1	I	123	ALA	CA-CB	-6.58	1.43	1.53
1	B	89	THR	CA-CB	-6.57	1.42	1.53
1	N	21	ASN	N-CA	-6.56	1.38	1.46
1	F	16	MET	C-O	-6.56	1.16	1.24
1	B	114	MET	CB-CG	6.55	1.72	1.52
1	B	22	VAL	CA-CB	6.53	1.62	1.54
1	H	509	SER	N-CA	-6.52	1.38	1.46
1	L	57	ALA	C-O	-6.52	1.16	1.24
1	A	500	THR	C-O	-6.50	1.16	1.24
1	G	16	MET	SD-CE	6.50	1.95	1.79
1	L	520	MET	SD-CE	6.50	1.95	1.79
1	N	75	LYS	N-CA	6.48	1.54	1.46
1	E	497	THR	C-N	-6.48	1.25	1.34
1	E	83	ASP	N-CA	6.48	1.54	1.46
1	J	101	THR	C-O	-6.47	1.16	1.24
1	C	514	MET	SD-CE	6.46	1.95	1.79
1	E	469	VAL	CA-C	6.44	1.60	1.52
1	L	94	VAL	CA-CB	6.44	1.62	1.54
1	B	93	THR	C-O	6.43	1.31	1.24
1	M	453	GLN	N-CA	-6.43	1.38	1.46
1	I	420	ILE	C-O	-6.42	1.16	1.24
1	K	510	VAL	CB-CG2	6.42	1.73	1.52
1	L	101	THR	C-O	-6.42	1.16	1.24
1	J	120	ILE	CA-CB	6.41	1.61	1.54
1	K	73	MET	SD-CE	-6.41	1.63	1.79
1	J	508	ALA	C-O	-6.40	1.16	1.24
1	H	127	ALA	C-N	-6.39	1.25	1.33
1	E	443	ALA	CA-C	6.37	1.61	1.52
1	F	508	ALA	CA-CB	6.37	1.63	1.53
1	F	503	ALA	N-CA	-6.37	1.38	1.46
1	D	60	ILE	CA-C	6.36	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	GLU	CD-OE1	6.36	1.37	1.25
1	G	23	LEU	CA-C	6.35	1.60	1.52
1	H	132	LYS	C-O	-6.35	1.16	1.24
1	M	507	ALA	CA-CB	-6.34	1.43	1.53
1	J	514	MET	CG-SD	6.32	1.96	1.80
1	N	90	THR	C-O	-6.29	1.16	1.24
1	N	94	VAL	CA-CB	6.29	1.62	1.54
1	G	10	ASN	N-CA	-6.28	1.38	1.46
1	G	88	GLY	C-O	6.27	1.32	1.24
1	D	98	ALA	C-O	-6.26	1.16	1.24
1	J	510	VAL	CB-CG2	6.26	1.73	1.52
1	F	510	VAL	CB-CG2	6.23	1.73	1.52
1	B	406	ALA	CA-CB	-6.22	1.43	1.53
1	A	417	VAL	CA-CB	6.21	1.61	1.54
1	L	105	LYS	N-CA	6.21	1.53	1.46
1	C	58	ARG	NE-CZ	6.21	1.39	1.33
1	E	90	THR	C-O	6.21	1.31	1.24
1	C	24	ALA	C-O	-6.20	1.16	1.24
1	A	76	GLU	N-CA	6.19	1.54	1.46
1	M	114	MET	CG-SD	6.18	1.96	1.80
1	A	514	MET	SD-CE	6.17	1.95	1.79
1	E	69	MET	SD-CE	-6.16	1.64	1.79
1	B	474	GLY	C-O	6.16	1.32	1.24
1	H	81	ALA	CA-CB	-6.14	1.43	1.53
1	J	33	PRO	C-O	-6.14	1.16	1.24
1	K	111	MET	SD-CE	6.14	1.95	1.79
1	N	511	ALA	CA-CB	-6.14	1.43	1.53
1	E	449	ALA	CA-CB	6.14	1.62	1.53
1	K	118	ARG	C-O	-6.13	1.16	1.24
1	K	445	ARG	NE-CZ	6.13	1.39	1.33
1	E	455	VAL	CA-CB	-6.12	1.47	1.54
1	H	526	LYS	CB-CG	6.11	1.70	1.52
1	I	419	LEU	C-O	-6.11	1.16	1.24
1	D	459	GLY	C-O	-6.11	1.16	1.24
1	D	16	MET	SD-CE	6.10	1.94	1.79
1	J	88	GLY	C-O	6.09	1.32	1.23
1	C	514	MET	CG-SD	6.08	1.96	1.80
1	D	124	VAL	CA-CB	6.08	1.62	1.54
1	J	406	ALA	CA-CB	-6.08	1.43	1.53
1	J	504	LEU	C-O	-6.06	1.16	1.24
1	N	17	LEU	N-CA	-6.05	1.39	1.46
1	H	94	VAL	CA-CB	6.04	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	447	MET	SD-CE	6.04	1.94	1.79
1	G	488	MET	N-CA	-6.02	1.39	1.46
1	J	442	VAL	CA-C	-6.02	1.45	1.52
1	A	94	VAL	CA-CB	6.02	1.62	1.54
1	G	511	ALA	CA-CB	-6.01	1.44	1.53
1	E	510	VAL	CB-CG2	6.00	1.72	1.52
1	E	498	LYS	N-CA	-6.00	1.38	1.46
1	N	101	THR	C-O	-6.00	1.17	1.24
1	J	73	MET	SD-CE	-5.99	1.64	1.79
1	A	511	ALA	N-CA	5.97	1.53	1.46
1	E	449	ALA	C-O	-5.96	1.19	1.24
1	E	508	ALA	C-O	-5.96	1.16	1.24
1	H	111	MET	SD-CE	5.95	1.94	1.79
1	H	514	MET	CG-SD	5.94	1.95	1.80
1	H	6	VAL	C-O	-5.93	1.17	1.24
1	D	500	THR	C-O	-5.93	1.17	1.24
1	N	39	VAL	CA-CB	5.91	1.61	1.54
1	N	75	LYS	CA-C	-5.89	1.44	1.52
1	D	412	VAL	CA-C	-5.89	1.46	1.52
1	E	79	SER	C-O	5.89	1.31	1.24
1	N	499	VAL	C-O	5.88	1.31	1.24
1	E	504	LEU	C-O	-5.88	1.17	1.24
1	H	442	VAL	N-CA	-5.87	1.39	1.46
1	D	468	THR	C-O	-5.87	1.17	1.24
1	H	100	ILE	C-O	-5.86	1.17	1.24
1	E	121	ASP	C-O	-5.86	1.17	1.24
1	E	464	VAL	CA-CB	-5.86	1.47	1.54
1	A	48	THR	C-O	-5.85	1.16	1.23
1	A	445	ARG	NE-CZ	5.85	1.39	1.33
1	D	449	ALA	C-O	-5.85	1.18	1.24
1	N	508	ALA	C-O	-5.83	1.16	1.24
1	E	114	MET	CG-SD	5.82	1.95	1.80
1	A	96	ALA	CA-CB	-5.82	1.44	1.53
1	K	514	MET	CG-SD	5.82	1.95	1.80
1	D	369	VAL	CA-CB	5.82	1.61	1.54
1	E	81	ALA	CA-CB	-5.81	1.44	1.53
1	M	108	ALA	CA-CB	5.80	1.62	1.53
1	A	508	ALA	C-O	-5.80	1.16	1.24
1	N	20	VAL	CA-CB	5.80	1.61	1.54
1	B	111	MET	SD-CE	5.80	1.94	1.79
1	A	409	GLU	CA-C	-5.79	1.45	1.52
1	L	503	ALA	N-CA	-5.78	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	491	MET	SD-CE	5.78	1.94	1.79
1	H	72	GLN	N-CA	5.78	1.53	1.46
1	A	21	ASN	N-CA	-5.78	1.39	1.46
1	F	30	THR	C-O	5.77	1.31	1.24
1	N	16	MET	SD-CE	5.77	1.94	1.79
1	F	288	MET	SD-CE	5.76	1.94	1.79
1	N	135	SER	C-O	-5.76	1.17	1.23
1	J	449	ALA	CA-CB	5.76	1.61	1.53
1	L	497	THR	C-O	-5.75	1.17	1.24
1	G	426	LEU	C-O	-5.74	1.16	1.24
1	M	94	VAL	CA-CB	5.74	1.61	1.54
1	B	506	TYR	CA-CB	-5.72	1.44	1.53
1	E	493	ILE	CA-CB	-5.72	1.45	1.53
1	E	442	VAL	N-CA	-5.72	1.39	1.46
1	L	120	ILE	CA-CB	5.72	1.61	1.54
1	E	420	ILE	CA-CB	-5.71	1.47	1.54
1	F	514	MET	CG-SD	5.71	1.95	1.80
1	A	97	GLN	CA-C	-5.71	1.45	1.52
1	G	58	ARG	NE-CZ	5.71	1.39	1.33
1	G	96	ALA	C-O	-5.71	1.17	1.24
1	G	129	GLU	CD-OE2	5.70	1.36	1.25
1	I	445	ARG	NE-CZ	5.69	1.39	1.33
1	J	471	GLY	C-O	-5.68	1.17	1.23
1	E	506	TYR	CD2-CE2	5.68	1.55	1.38
1	A	406	ALA	CA-CB	-5.68	1.44	1.53
1	G	473	ASP	CA-C	-5.67	1.45	1.52
1	K	91	THR	C-O	-5.67	1.17	1.24
1	L	118	ARG	NE-CZ	5.66	1.39	1.33
1	J	90	THR	C-O	-5.64	1.17	1.24
1	M	21	ASN	N-CA	-5.64	1.39	1.46
1	H	118	ARG	C-O	-5.63	1.17	1.24
1	G	445	ARG	NE-CZ	5.63	1.39	1.33
1	E	90	THR	N-CA	5.63	1.53	1.46
1	B	77	VAL	CA-CB	5.62	1.60	1.54
1	K	449	ALA	CA-C	5.62	1.59	1.52
1	D	101	THR	C-O	-5.62	1.17	1.24
1	J	20	VAL	C-O	-5.61	1.17	1.24
1	E	473	ASP	CA-C	-5.60	1.45	1.52
1	G	512	GLY	C-O	-5.60	1.17	1.23
1	E	90	THR	CA-C	-5.59	1.45	1.52
1	E	514	MET	CG-SD	5.59	1.94	1.80
1	K	288	MET	SD-CE	5.58	1.93	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	21	ASN	N-CA	-5.58	1.39	1.46
1	N	491	MET	SD-CE	5.58	1.93	1.79
1	E	101	THR	CB-CG2	5.57	1.71	1.52
1	B	95	LEU	C-O	5.57	1.30	1.24
1	B	440	ILE	CA-CB	5.57	1.61	1.54
1	I	526	LYS	CD-CE	5.57	1.69	1.52
1	E	34	LYS	CA-C	5.56	1.61	1.52
1	H	152	ALA	CA-CB	-5.56	1.45	1.53
1	B	440	ILE	C-O	-5.56	1.17	1.24
1	G	10	ASN	CA-CB	-5.56	1.44	1.53
1	G	509	SER	N-CA	-5.55	1.39	1.46
1	I	465	VAL	CA-CB	-5.54	1.47	1.54
1	H	69	MET	SD-CE	-5.54	1.65	1.79
1	L	76	GLU	CA-C	5.54	1.60	1.52
1	F	88	GLY	C-O	5.54	1.31	1.24
1	E	492	GLY	C-O	-5.53	1.16	1.24
1	L	459	GLY	C-O	-5.53	1.16	1.24
1	B	92	ALA	C-O	5.52	1.30	1.24
1	C	504	LEU	C-O	-5.52	1.17	1.24
1	G	425	LYS	N-CA	-5.52	1.38	1.46
1	A	496	PRO	CA-C	5.52	1.59	1.52
1	I	526	LYS	CB-CG	5.52	1.69	1.52
1	A	24	ALA	CA-CB	-5.51	1.44	1.53
1	B	502	SER	CA-C	5.51	1.60	1.52
1	G	4	LYS	C-O	-5.51	1.17	1.23
1	H	44	PHE	CA-CB	5.51	1.63	1.53
1	I	511	ALA	C-O	-5.49	1.17	1.24
1	M	20	VAL	CA-CB	5.49	1.62	1.54
1	J	21	ASN	N-CA	-5.48	1.39	1.46
1	K	39	VAL	C-O	-5.47	1.17	1.24
1	H	457	ASN	N-CA	-5.47	1.39	1.46
1	L	74	VAL	CA-CB	-5.46	1.46	1.54
1	A	94	VAL	C-O	-5.46	1.17	1.24
1	L	81	ALA	CA-CB	5.45	1.61	1.53
1	I	523	ASP	C-O	-5.44	1.17	1.23
1	K	517	THR	C-O	-5.44	1.17	1.24
1	H	14	VAL	CA-CB	5.44	1.61	1.54
1	L	77	VAL	CA-CB	5.44	1.60	1.54
1	K	4	LYS	C-O	-5.44	1.17	1.23
1	E	97	GLN	CA-C	-5.43	1.45	1.52
1	E	461	GLU	CA-C	5.43	1.59	1.52
1	B	96	ALA	CA-CB	-5.43	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	498	LYS	CE-NZ	5.43	1.65	1.49
1	G	430	ARG	NE-CZ	5.42	1.39	1.33
1	J	430	ARG	NE-CZ	5.42	1.39	1.33
1	D	10	ASN	N-CA	-5.42	1.39	1.46
1	L	60	ILE	CA-CB	-5.42	1.47	1.53
1	N	75	LYS	C-O	5.40	1.30	1.24
1	G	526	LYS	CB-CG	5.40	1.68	1.52
1	H	16	MET	SD-CE	5.39	1.93	1.79
1	N	111	MET	SD-CE	5.39	1.93	1.79
1	J	499	VAL	CA-CB	5.38	1.61	1.54
1	E	464	VAL	C-N	-5.38	1.27	1.33
1	A	166	MET	SD-CE	5.38	1.93	1.79
1	F	114	MET	CB-CG	5.38	1.68	1.52
1	L	124	VAL	CA-CB	5.38	1.61	1.54
1	M	58	ARG	NE-CZ	5.38	1.39	1.33
1	L	100	ILE	CA-CB	-5.37	1.47	1.54
1	G	77	VAL	CA-CB	5.37	1.60	1.54
1	D	408	GLU	C-O	-5.36	1.17	1.24
1	D	220	ILE	CA-CB	5.36	1.60	1.54
1	N	514	MET	CG-SD	5.36	1.94	1.80
1	D	440	ILE	C-O	-5.36	1.18	1.24
1	G	408	GLU	C-O	-5.36	1.17	1.24
1	L	502	SER	CA-C	5.36	1.59	1.52
1	F	80	LYS	C-O	5.35	1.30	1.24
1	F	31	LEU	C-O	-5.35	1.17	1.24
1	C	508	ALA	C-O	-5.34	1.17	1.24
1	B	505	GLN	CA-C	5.34	1.59	1.52
1	D	48	THR	C-O	-5.34	1.17	1.24
1	G	69	MET	SD-CE	-5.34	1.66	1.79
1	J	69	MET	SD-CE	-5.34	1.66	1.79
1	F	118	ARG	NE-CZ	5.34	1.39	1.33
1	G	507	ALA	CA-CB	-5.33	1.45	1.53
1	I	92	ALA	CA-CB	5.33	1.61	1.53
1	I	106	ALA	CA-CB	5.33	1.61	1.53
1	N	10	ASN	N-CA	-5.32	1.40	1.46
1	B	508	ALA	C-O	-5.32	1.17	1.24
1	K	193	MET	SD-CE	5.32	1.92	1.79
1	G	38	VAL	C-O	-5.32	1.18	1.24
1	M	445	ARG	NE-CZ	5.32	1.38	1.33
1	G	288	MET	SD-CE	5.31	1.92	1.79
1	L	79	SER	C-O	5.31	1.30	1.24
1	K	30	THR	CA-C	5.31	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	GLU	C-O	-5.31	1.17	1.24
1	G	460	GLU	CD-OE1	5.30	1.35	1.25
1	D	69	MET	C-O	-5.30	1.18	1.24
1	D	466	ALA	CA-CB	5.30	1.61	1.53
1	L	123	ALA	CA-CB	-5.30	1.44	1.53
1	K	102	GLU	C-O	-5.30	1.17	1.24
1	F	49	ILE	N-CA	-5.29	1.39	1.46
1	L	504	LEU	C-O	-5.29	1.18	1.24
1	E	21	ASN	N-CA	-5.28	1.40	1.46
1	L	98	ALA	C-O	-5.28	1.18	1.24
1	H	60	ILE	N-CA	5.28	1.52	1.46
1	L	445	ARG	NE-CZ	5.28	1.38	1.33
1	F	54	VAL	CA-CB	5.28	1.61	1.54
1	N	6	VAL	C-O	-5.27	1.18	1.24
1	H	506	TYR	CZ-OH	5.27	1.49	1.38
1	C	61	GLU	CA-C	5.27	1.59	1.52
1	E	27	VAL	CA-C	5.27	1.59	1.52
1	N	67	GLU	C-O	-5.26	1.18	1.24
1	M	17	LEU	CA-C	5.26	1.59	1.52
1	E	408	GLU	C-O	-5.25	1.17	1.24
1	E	92	ALA	CA-C	5.25	1.59	1.52
1	L	445	ARG	CA-CB	-5.25	1.45	1.53
1	N	31	LEU	C-O	-5.25	1.17	1.24
1	M	508	ALA	C-O	-5.24	1.17	1.24
1	N	14	VAL	N-CA	-5.24	1.40	1.46
1	A	499	VAL	CA-CB	5.24	1.61	1.54
1	F	133	ALA	C-O	-5.24	1.17	1.24
1	C	118	ARG	NE-CZ	5.24	1.38	1.33
1	D	91	THR	C-O	-5.24	1.18	1.24
1	I	324	VAL	CA-CB	5.23	1.60	1.54
1	D	430	ARG	NE-CZ	5.22	1.38	1.33
1	G	498	LYS	N-CA	-5.22	1.40	1.46
1	B	455	VAL	CA-CB	-5.22	1.47	1.54
1	L	118	ARG	C-O	-5.22	1.18	1.24
1	F	443	ALA	CA-CB	-5.21	1.44	1.53
1	D	288	MET	SD-CE	5.21	1.92	1.79
1	G	498	LYS	CE-NZ	5.20	1.65	1.49
1	H	80	LYS	C-O	-5.20	1.18	1.24
1	D	510	VAL	CB-CG2	5.20	1.69	1.52
1	C	417	VAL	C-O	-5.19	1.17	1.24
1	D	75	LYS	CE-NZ	-5.19	1.33	1.49
1	B	411	VAL	CA-C	-5.18	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	447	MET	SD-CE	5.18	1.92	1.79
1	D	28	LYS	C-O	-5.17	1.17	1.24
1	M	76	GLU	N-CA	5.17	1.53	1.46
1	J	117	LYS	C-O	-5.16	1.18	1.24
1	I	496	PRO	C-O	-5.16	1.18	1.23
1	C	116	LEU	CA-C	-5.16	1.46	1.52
1	J	21	ASN	C-O	-5.15	1.18	1.24
1	H	44	PHE	CD2-CE2	5.13	1.54	1.38
1	E	445	ARG	NE-CZ	5.13	1.38	1.33
1	E	46	ALA	CA-C	-5.13	1.47	1.53
1	C	102	GLU	C-O	-5.13	1.17	1.24
1	G	523	ASP	C-O	-5.11	1.17	1.23
1	H	91	THR	CA-CB	5.11	1.61	1.53
1	H	98	ALA	N-CA	5.11	1.52	1.46
1	D	129	GLU	CD-OE2	5.10	1.35	1.25
1	F	51	LYS	CA-C	-5.10	1.46	1.52
1	B	118	ARG	NE-CZ	5.09	1.38	1.33
1	J	5	ASP	C-O	-5.09	1.17	1.24
1	H	525	PRO	C-O	5.09	1.30	1.24
1	E	440	ILE	CA-CB	5.09	1.60	1.54
1	H	511	ALA	CA-CB	-5.08	1.45	1.53
1	J	432	GLN	C-O	-5.08	1.17	1.24
1	E	454	ILE	CA-CB	-5.08	1.48	1.54
1	L	499	VAL	N-CA	-5.08	1.40	1.46
1	L	502	SER	CA-CB	-5.07	1.45	1.53
1	E	517	THR	C-O	-5.07	1.17	1.24
1	C	21	ASN	CA-CB	5.07	1.61	1.53
1	D	141	SER	CB-OG	-5.07	1.32	1.42
1	H	465	VAL	CA-CB	-5.06	1.48	1.54
1	N	105	LYS	N-CA	5.06	1.52	1.46
1	K	456	LEU	C-O	-5.06	1.18	1.24
1	E	456	LEU	C-O	-5.06	1.18	1.24
1	I	510	VAL	CB-CG2	5.06	1.69	1.52
1	A	442	VAL	C-O	-5.05	1.18	1.24
1	I	118	ARG	NE-CZ	5.05	1.38	1.33
1	B	69	MET	SD-CE	-5.05	1.67	1.79
1	M	48	THR	C-O	-5.05	1.17	1.24
1	D	420	ILE	CA-C	5.05	1.59	1.52
1	B	438	VAL	CA-CB	-5.04	1.47	1.54
1	C	75	LYS	CD-CE	-5.04	1.37	1.52
1	M	510	VAL	CB-CG2	5.04	1.69	1.52
1	C	53	GLY	C-N	-5.03	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	505	GLN	C-O	-5.03	1.18	1.24
1	H	429	LEU	CA-C	5.02	1.59	1.52
1	L	450	PRO	CG-CD	5.02	1.67	1.50
1	K	447	MET	SD-CE	5.02	1.92	1.79
1	A	129	GLU	CD-OE1	5.02	1.34	1.25
1	E	500	THR	N-CA	5.02	1.52	1.46
1	D	433	ASN	C-O	-5.01	1.18	1.23
1	H	438	VAL	CB-CG2	5.01	1.69	1.52
1	L	100	ILE	CB-CG1	5.01	1.63	1.53
1	C	445	ARG	NE-CZ	5.00	1.38	1.33
1	A	107	VAL	CA-CB	-5.00	1.48	1.54
1	K	5	ASP	CA-C	5.00	1.58	1.52
1	N	38	VAL	N-CA	-5.00	1.40	1.46

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	284	ARG	NE-CZ-NH2	13.16	131.04	119.20
1	B	132	LYS	N-CA-C	-12.79	97.00	111.71
1	J	231	ARG	NE-CZ-NH2	12.28	130.25	119.20
1	M	284	ARG	NE-CZ-NH1	-11.30	110.20	121.50
1	E	464	VAL	N-CA-C	-11.08	100.11	110.53
1	A	417	VAL	N-CA-C	11.05	121.03	110.42
1	J	231	ARG	NE-CZ-NH1	-10.66	110.84	121.50
1	N	368	ARG	NE-CZ-NH2	10.14	128.32	119.20
1	M	284	ARG	CD-NE-CZ	9.84	138.18	124.40
1	N	368	ARG	NE-CZ-NH1	-8.85	112.65	121.50
1	J	231	ARG	CD-NE-CZ	8.74	136.63	124.40
1	I	417	VAL	N-CA-C	8.51	119.31	110.72
1	E	468	THR	N-CA-C	-7.96	101.91	111.69
1	D	99	ILE	N-CA-C	7.79	117.90	110.42
1	E	452	ARG	N-CA-C	-7.74	102.47	112.23
1	E	77	VAL	CB-CA-C	-7.31	102.44	111.87
1	N	76	GLU	N-CA-C	-7.31	103.82	112.89
1	B	133	ALA	N-CA-C	-7.25	103.90	112.89
1	M	513	LEU	N-CA-C	7.25	119.81	111.11
1	N	368	ARG	CD-NE-CZ	7.22	134.50	124.40
1	I	94	VAL	N-CA-CB	7.21	118.98	110.55
1	L	464	VAL	N-CA-C	-7.19	103.84	110.82
1	I	442	VAL	N-CA-C	-7.19	103.52	110.42
1	J	78	ALA	CA-C-N	-7.11	110.19	120.29
1	J	78	ALA	C-N-CA	-7.11	110.19	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	ASN	N-CA-C	7.06	119.59	111.11
1	E	82	ASN	N-CA-C	-7.05	103.52	111.14
1	J	77	VAL	CB-CA-C	-7.02	102.82	111.87
1	E	445	ARG	N-CA-C	-7.01	103.39	112.23
1	K	442	VAL	N-CA-C	-6.95	103.53	110.62
1	F	417	VAL	N-CA-C	6.94	117.73	110.72
1	L	76	GLU	N-CA-C	-6.88	104.36	112.89
1	E	18	ARG	N-CA-C	-6.77	103.98	111.36
1	E	101	THR	OG1-CB-CG2	-6.74	95.81	109.30
1	E	29	VAL	N-CA-C	-6.73	103.14	112.50
1	H	85	ALA	N-CA-C	-6.72	106.28	114.75
1	L	447	MET	N-CA-C	-6.66	104.64	112.89
1	G	20	VAL	N-CA-CB	6.60	119.52	110.54
1	B	77	VAL	CB-CA-C	-6.60	103.35	111.87
1	N	20	VAL	N-CA-CB	6.60	119.52	110.54
1	D	489	ILE	N-CA-C	-6.60	103.81	111.00
1	E	95	LEU	N-CA-C	-6.58	104.19	111.36
1	L	94	VAL	N-CA-CB	6.56	119.47	110.54
1	D	483	GLU	N-CA-C	6.53	120.40	111.39
1	F	10	ASN	N-CA-C	6.51	119.21	111.33
1	E	490	ASP	N-CA-C	6.49	119.35	111.82
1	K	20	VAL	N-CA-CB	6.45	120.26	110.58
1	E	490	ASP	CB-CA-C	-6.42	98.35	110.67
1	B	472	GLY	N-CA-C	-6.40	103.45	112.60
1	B	116	LEU	N-CA-C	-6.33	104.46	111.36
1	G	325	ILE	N-CA-C	6.32	117.22	108.12
1	K	417	VAL	N-CA-C	6.27	117.05	110.72
1	E	496	PRO	CA-C-O	-6.26	114.54	121.23
1	E	500	THR	N-CA-C	-6.25	104.01	111.69
1	B	132	LYS	CD-CE-NZ	6.21	131.77	111.90
1	E	482	THR	N-CA-C	-6.21	104.98	113.30
1	D	503	ALA	N-CA-C	-6.20	104.43	111.07
1	J	473	ASP	N-CA-C	6.18	117.27	108.74
1	F	77	VAL	CB-CA-C	-6.18	103.90	111.87
1	C	507	ALA	CA-C-N	6.16	128.54	120.28
1	C	507	ALA	C-N-CA	6.16	128.54	120.28
1	E	129	GLU	N-CA-C	-6.13	103.91	111.33
1	E	133	ALA	N-CA-C	-6.13	104.71	111.82
1	D	20	VAL	N-CA-CB	6.12	118.87	110.54
1	A	509	SER	CA-CB-OG	-6.10	98.89	111.10
1	L	463	SER	CA-CB-OG	-6.09	98.92	111.10
1	N	100	ILE	N-CA-C	-6.07	104.58	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	VAL	N-CA-C	-6.07	103.30	111.44
1	D	82	ASN	N-CA-C	6.07	117.58	110.97
1	G	94	VAL	N-CA-C	6.06	116.80	110.62
1	M	94	VAL	N-CA-CB	6.02	117.60	110.55
1	L	503	ALA	N-CA-C	-6.01	104.64	111.07
1	B	510	VAL	N-CA-C	-6.01	103.39	111.44
1	H	10	ASN	N-CA-C	6.00	118.59	111.33
1	I	473	ASP	N-CA-C	6.00	117.01	108.74
1	B	132	LYS	CB-CG-CD	5.99	125.07	111.30
1	K	80	LYS	N-CA-C	-5.96	104.35	111.69
1	B	132	LYS	CA-C-O	5.96	126.84	120.10
1	G	50	THR	OG1-CB-CG2	-5.93	97.44	109.30
1	B	133	ALA	O-C-N	-5.93	114.28	122.46
1	J	50	THR	OG1-CB-CG2	-5.90	97.50	109.30
1	E	421	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	133	ALA	CA-C-O	5.85	126.57	119.31
1	B	507	ALA	N-CA-C	-5.84	104.82	111.07
1	E	461	GLU	CA-C-O	5.84	123.09	119.29
1	F	20	VAL	N-CA-CB	5.84	119.34	110.58
1	A	125	THR	OG1-CB-CG2	-5.82	97.65	109.30
1	E	36	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	B	109	ALA	N-CA-C	-5.82	105.95	113.16
1	B	125	THR	N-CA-C	-5.81	105.03	111.36
1	K	10	ASN	N-CA-C	5.81	118.36	111.33
1	M	77	VAL	CB-CA-C	-5.81	104.41	112.02
1	E	451	LEU	CD1-CG-CD2	-5.77	98.10	110.80
1	L	325	ILE	N-CA-C	5.77	116.31	107.77
1	E	79	SER	N-CA-C	5.75	117.63	111.36
1	A	325	ILE	N-CA-C	5.74	116.26	107.77
1	I	50	THR	OG1-CB-CG2	-5.72	97.85	109.30
1	B	503	ALA	N-CA-C	-5.71	104.95	111.07
1	H	53	GLY	N-CA-C	5.71	119.58	112.73
1	G	422	VAL	N-CA-C	5.70	116.35	110.36
1	M	94	VAL	N-CA-C	5.69	115.88	110.42
1	B	464	VAL	N-CA-C	-5.68	104.82	110.62
1	M	22	VAL	N-CA-C	-5.68	104.99	110.72
1	B	78	ALA	CA-C-N	-5.67	112.24	120.29
1	B	78	ALA	C-N-CA	-5.67	112.24	120.29
1	E	42	LYS	CB-CG-CD	-5.67	98.26	111.30
1	E	135	SER	CA-CB-OG	-5.65	99.79	111.10
1	L	467	ASN	N-CA-C	-5.63	105.22	111.36
1	E	83	ASP	CB-CA-C	-5.63	101.45	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	427	ALA	N-CA-C	5.60	118.91	111.75
1	B	128	VAL	CB-CA-C	5.59	119.94	112.22
1	J	325	ILE	N-CA-C	5.59	116.17	108.12
1	E	401	HIS	N-CA-C	5.59	117.81	111.11
1	B	514	MET	N-CA-C	-5.58	104.82	111.69
1	D	83	ASP	N-CA-C	5.58	118.08	111.33
1	F	20	VAL	CG1-CB-CG2	5.57	123.05	110.80
1	N	325	ILE	N-CA-C	5.57	116.13	108.12
1	G	17	LEU	N-CA-C	-5.55	105.31	111.36
1	E	14	VAL	N-CA-CB	5.55	118.90	110.58
1	E	509	SER	CA-CB-OG	-5.54	100.01	111.10
1	H	503	ALA	N-CA-C	-5.54	105.14	111.07
1	H	525	PRO	N-CA-C	-5.54	101.06	112.47
1	C	26	ALA	N-CA-C	-5.54	104.88	111.69
1	G	144	ILE	N-CA-C	-5.53	105.14	110.72
1	N	445	ARG	N-CA-C	-5.53	104.89	111.69
1	B	122	LYS	N-CA-C	-5.51	105.35	111.36
1	K	510	VAL	N-CA-C	-5.50	104.07	111.44
1	E	470	LYS	N-CA-C	5.49	118.77	111.75
1	E	85	ALA	N-CA-C	-5.45	107.64	114.56
1	E	89	THR	N-CA-CB	5.45	118.22	110.16
1	L	414	GLY	CA-C-O	-5.43	116.60	122.47
1	H	464	VAL	N-CA-C	-5.43	105.43	110.53
1	L	22	VAL	N-CA-C	-5.42	105.25	110.72
1	F	50	THR	OG1-CB-CG2	-5.42	98.46	109.30
1	N	75	LYS	CA-C-O	5.42	126.00	119.61
1	C	20	VAL	N-CA-CB	5.41	117.89	110.54
1	A	10	ASN	N-CA-C	5.40	117.86	111.33
1	B	25	ASP	N-CA-C	5.39	117.15	111.28
1	G	483	GLU	N-CA-C	5.38	119.00	111.74
1	B	438	VAL	N-CA-C	-5.37	105.14	111.00
1	L	10	ASN	N-CA-C	5.37	117.83	111.33
1	B	134	LEU	CB-CA-C	-5.37	101.13	110.09
1	C	101	THR	OG1-CB-CG2	-5.37	98.57	109.30
1	D	59	GLU	N-CA-C	-5.37	106.58	113.23
1	D	495	ASP	N-CA-C	-5.37	102.04	110.14
1	C	473	ASP	N-CA-C	5.36	116.14	108.74
1	L	500	THR	N-CA-C	-5.36	105.52	111.36
1	K	503	ALA	N-CA-C	-5.33	105.37	111.07
1	N	26	ALA	N-CA-C	-5.33	105.14	111.69
1	M	76	GLU	N-CA-C	-5.32	106.29	112.89
1	N	417	VAL	N-CA-C	5.32	116.09	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ILE	N-CA-C	5.31	115.52	110.42
1	E	20	VAL	N-CA-CB	5.31	117.76	110.54
1	A	94	VAL	N-CA-CB	5.31	118.54	110.58
1	H	101	THR	OG1-CB-CG2	-5.30	98.71	109.30
1	I	129	GLU	N-CA-C	-5.30	105.51	111.28
1	C	50	THR	OG1-CB-CG2	-5.29	98.71	109.30
1	E	130	GLU	CA-C-O	5.29	126.12	120.24
1	J	417	VAL	N-CA-C	5.28	116.06	110.72
1	E	458	CYS	N-CA-C	-5.28	106.80	113.18
1	E	499	VAL	CG1-CB-CG2	5.27	122.40	110.80
1	G	43	SER	CA-CB-OG	-5.27	100.57	111.10
1	G	53	GLY	N-CA-C	5.26	119.04	112.73
1	F	500	THR	N-CA-C	-5.25	105.63	111.36
1	E	50	THR	OG1-CB-CG2	-5.24	98.81	109.30
1	G	482	THR	N-CA-C	-5.24	106.93	113.38
1	E	473	ASP	N-CA-C	5.24	115.97	108.74
1	E	20	VAL	CA-CB-CG2	5.24	119.30	110.40
1	E	499	VAL	N-CA-C	5.22	115.99	110.72
1	B	136	VAL	CA-C-O	-5.22	115.49	119.98
1	F	461	GLU	CA-C-N	5.20	124.65	119.24
1	F	461	GLU	C-N-CA	5.20	124.65	119.24
1	L	20	VAL	CG1-CB-CG2	5.20	122.24	110.80
1	L	20	VAL	N-CA-CB	5.20	118.38	110.58
1	J	10	ASN	N-CA-C	5.18	116.93	111.28
1	J	101	THR	CA-C-O	-5.17	115.57	120.90
1	B	129	GLU	CB-CG-CD	5.16	121.38	112.60
1	I	503	ALA	N-CA-C	-5.16	105.56	111.14
1	B	131	LEU	CA-C-O	-5.14	115.08	120.63
1	L	401	HIS	N-CA-C	5.13	117.27	111.11
1	C	42	LYS	CB-CG-CD	-5.13	99.50	111.30
1	K	325	ILE	N-CA-C	5.13	115.36	107.77
1	B	325	ILE	N-CA-C	5.12	115.35	107.77
1	D	131	LEU	N-CA-C	-5.12	105.88	111.82
1	G	401	HIS	N-CA-C	5.12	116.86	111.28
1	D	331	THR	CB-CA-C	5.12	118.65	110.16
1	G	42	LYS	CD-CE-NZ	-5.12	95.53	111.90
1	A	42	LYS	CB-CG-CD	-5.11	99.55	111.30
1	B	467	ASN	N-CA-C	-5.10	105.63	111.14
1	E	442	VAL	N-CA-C	-5.10	105.41	110.62
1	H	129	GLU	N-CA-C	-5.09	105.73	111.28
1	H	5	ASP	N-CA-C	-5.07	101.42	109.59
1	E	13	GLY	N-CA-C	-5.07	106.28	112.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	401	HIS	N-CA-C	5.07	117.19	111.11
1	N	510	VAL	N-CA-C	-5.06	105.61	110.72
1	B	471	GLY	N-CA-C	-5.05	108.39	114.66
1	E	503	ALA	CA-C-O	-5.05	115.51	120.82
1	G	525	PRO	N-CA-C	-5.04	102.08	112.47
1	N	442	VAL	N-CA-C	-5.04	105.58	110.42
1	N	447	MET	N-CA-C	-5.04	107.08	113.18
1	E	420	ILE	CA-C-O	-5.02	115.53	120.85
1	B	422	VAL	N-CA-C	-5.02	105.60	110.42
1	L	107	VAL	N-CA-C	5.02	115.63	110.36
1	B	473	ASP	N-CA-C	5.01	115.66	108.74
1	D	122	LYS	N-CA-C	-5.01	105.90	111.36
1	H	507	ALA	N-CA-C	-5.01	105.71	111.07
1	C	25	ASP	N-CA-C	5.00	116.73	111.28

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	3979	84	1
1	B	3855	0	3979	81	0
1	C	3855	0	3979	74	0
1	D	3855	0	3979	84	0
1	E	3855	0	3979	75	0
1	F	3855	0	3979	84	0
1	G	3855	0	3979	87	2
1	H	3855	0	3979	72	1
1	I	3855	0	3979	69	1
1	J	3855	0	3979	72	0
1	K	3855	0	3979	72	0
1	L	3855	0	3979	79	1
1	M	3855	0	3979	87	0
1	N	3855	0	3979	76	4
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	2	0	0	0	0
3	E	2	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	31	0	12	3	0
4	B	31	0	12	4	0
4	C	31	0	12	2	0
4	D	31	0	12	4	0
4	E	31	0	12	3	0
4	F	31	0	11	4	0
4	G	31	0	12	4	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	2	0
4	L	31	0	12	3	0
4	M	31	0	12	3	0
4	N	31	0	12	5	0
5	A	62	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	83	0	0	5	0
5	C	57	0	0	3	0
5	D	91	0	0	6	0
5	E	92	0	0	4	0
5	F	71	0	0	1	0
5	G	83	0	0	8	0
5	H	77	0	0	4	0
5	I	60	0	0	4	0
5	J	50	0	0	2	0
5	K	47	0	0	3	0
5	L	61	0	0	2	0
5	M	53	0	0	3	0
5	N	59	0	0	2	0
All	All	55380	0	55873	1081	5

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 10.

All (1081) 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)
1:L:80:LYS:CD	1:L:80:LYS:CG	1.77	1.62
1:B:510:VAL:CG2	1:B:510:VAL:CB	1.79	1.61
4:A:1:AGS:PG	4:A:1:AGS:S1G	1.53	1.52
1:N:510:VAL:CG2	1:N:510:VAL:CB	1.83	1.51
4:B:1:AGS:PG	4:B:1:AGS:S1G	1.52	1.51
4:J:1:AGS:PG	4:J:1:AGS:S1G	1.52	1.51
4:C:1:AGS:PG	4:C:1:AGS:S1G	1.51	1.51
4:H:1:AGS:PG	4:H:1:AGS:S1G	1.51	1.51
4:K:1:AGS:PG	4:K:1:AGS:S1G	1.51	1.50
4:F:1:AGS:PG	4:F:1:AGS:S1G	1.51	1.50
4:M:1:AGS:PG	4:M:1:AGS:S1G	1.51	1.49
4:I:1:AGS:PG	4:I:1:AGS:S1G	1.50	1.49
4:D:561:AGS:PG	4:D:561:AGS:S1G	1.48	1.47
4:L:1:AGS:PG	4:L:1:AGS:S1G	1.49	1.47
1:G:114:MET:SD	1:G:114:MET:CE	2.02	1.47
4:E:1:AGS:PG	4:E:1:AGS:S1G	1.47	1.46
4:N:1:AGS:PG	4:N:1:AGS:S1G	1.47	1.46
1:E:16:MET:SD	1:E:16:MET:CE	2.03	1.46
1:L:514:MET:SD	1:L:514:MET:CE	2.04	1.45
1:B:16:MET:SD	1:B:16:MET:CE	2.03	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:SD	1:B:114:MET:CE	2.06	1.44
1:D:114:MET:SD	1:D:114:MET:CG	2.03	1.44
4:G:1:AGS:PG	4:G:1:AGS:S1G	1.45	1.44
1:D:114:MET:SD	1:D:114:MET:CE	2.02	1.44
1:M:16:MET:CE	1:M:16:MET:SD	2.09	1.41
3:C:560:K:K	5:C:566:HOH:O	1.34	1.34
1:J:16:MET:SD	1:J:16:MET:CE	2.16	1.33
1:H:463:SER:HB2	5:H:583:HOH:O	1.34	1.24
1:A:463:SER:HB2	5:A:570:HOH:O	1.43	1.16
1:K:463:SER:HB2	5:K:572:HOH:O	1.43	1.12
1:B:404:ARG:NH1	5:B:586:HOH:O	1.93	1.02
1:C:63:GLU:OE2	1:D:526:LYS:HE2	1.62	0.99
1:M:268:ARG:O	1:N:257:GLU:HG3	1.63	0.99
1:I:10:ASN:ND2	5:I:600:HOH:O	1.97	0.95
1:A:282:GLY:HA3	1:G:181:THR:O	1.67	0.95
4:E:1:AGS:S1G	4:E:1:AGS:O3B	2.26	0.94
1:A:231:ARG:NH1	1:G:242:LYS:HA	1.81	0.93
1:E:63:GLU:OE2	1:F:526:LYS:HE2	1.70	0.91
1:F:10:ASN:ND2	5:F:630:HOH:O	2.03	0.91
1:G:404:ARG:NH1	5:G:576:HOH:O	2.05	0.90
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.56	0.88
1:E:193:MET:HE1	1:E:292:ILE:HG12	1.57	0.87
1:F:193:MET:HE1	1:F:292:ILE:HG12	1.58	0.86
1:A:63:GLU:OE2	1:B:526:LYS:HE2	1.75	0.85
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.58	0.85
1:B:193:MET:HE1	1:B:292:ILE:HG12	1.59	0.85
1:L:514:MET:HB3	1:L:514:MET:HE3	1.57	0.85
1:L:193:MET:HE1	1:L:292:ILE:HG12	1.59	0.85
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.58	0.84
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.59	0.84
1:N:10:ASN:ND2	5:N:598:HOH:O	2.09	0.84
1:K:193:MET:HE1	1:K:292:ILE:HG12	1.60	0.83
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.61	0.83
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.61	0.82
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.62	0.82
1:L:514:MET:CE	1:L:514:MET:HB3	2.10	0.82
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.62	0.81
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.62	0.81
1:A:193:MET:HE1	1:A:292:ILE:HG12	1.63	0.81
4:C:1:AGS:S1G	4:C:1:AGS:O3G	2.39	0.81
1:E:345:ARG:HA	1:E:348:GLN:HE21	1.46	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.63	0.80
1:L:10:ASN:ND2	5:L:586:HOH:O	2.14	0.80
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.63	0.80
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.64	0.80
1:L:514:MET:CE	1:L:514:MET:CB	2.60	0.80
1:L:80:LYS:CD	1:L:80:LYS:CB	2.60	0.79
1:M:193:MET:HE1	1:M:292:ILE:HG12	1.65	0.79
1:A:326:ASN:HD22	1:A:329:THR:HB	1.48	0.79
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.65	0.79
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.65	0.79
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.65	0.79
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.64	0.78
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.62	0.78
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.65	0.78
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.64	0.78
4:L:1:AGS:S1G	4:L:1:AGS:O3B	2.41	0.78
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.66	0.78
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.65	0.78
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.66	0.78
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.65	0.78
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.66	0.78
1:E:404:ARG:NH1	5:E:604:HOH:O	2.15	0.77
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.65	0.77
1:H:404:ARG:NH1	5:H:626:HOH:O	2.16	0.77
1:M:177:VAL:HG21	1:M:397:GLU:HG3	1.64	0.77
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.66	0.77
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.65	0.77
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.64	0.77
4:M:1:AGS:S1G	4:M:1:AGS:O2G	2.43	0.77
4:A:1:AGS:S1G	4:A:1:AGS:O3B	2.43	0.77
4:N:1:AGS:S1G	4:N:1:AGS:O3G	2.42	0.76
1:G:57:ALA:O	1:G:75:LYS:HE3	1.85	0.76
1:A:345:ARG:HA	1:A:348:GLN:HE21	1.51	0.76
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.67	0.76
4:H:1:AGS:S1G	4:H:1:AGS:O3B	2.44	0.76
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.66	0.76
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.66	0.76
4:F:1:AGS:S1G	4:F:1:AGS:O3G	2.43	0.76
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.67	0.75
1:K:326:ASN:HD22	1:K:329:THR:HB	1.49	0.75
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.69	0.75
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.52	0.75
4:G:1:AGS:S1G	4:G:1:AGS:O3B	2.44	0.75
1:J:63:GLU:OE2	1:K:526:LYS:HE2	1.87	0.75
4:B:1:AGS:S1G	4:B:1:AGS:O3B	2.44	0.75
1:C:326:ASN:HD22	1:C:329:THR:HB	1.52	0.75
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.69	0.75
1:I:63:GLU:OE2	1:J:526:LYS:HE2	1.87	0.75
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.51	0.74
1:N:73:MET:O	1:N:76:GLU:HB2	1.87	0.74
4:F:1:AGS:S1G	4:F:1:AGS:O3B	2.45	0.74
1:M:462:PRO:HD2	5:M:605:HOH:O	1.86	0.74
1:B:86:GLY:HA3	1:B:401:HIS:CE1	2.22	0.74
1:D:326:ASN:HD22	1:D:329:THR:HB	1.53	0.73
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.70	0.73
1:B:73:MET:O	1:B:76:GLU:HB2	1.88	0.73
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.70	0.73
1:J:345:ARG:HA	1:J:348:GLN:HE21	1.54	0.73
1:M:326:ASN:HD22	1:M:329:THR:HB	1.52	0.72
1:D:302:SER:H	1:D:307:MET:HE3	1.55	0.72
1:B:345:ARG:HA	1:B:348:GLN:HE21	1.53	0.72
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.55	0.72
1:B:510:VAL:CG2	1:B:510:VAL:CA	2.67	0.72
1:N:326:ASN:HD22	1:N:329:THR:HB	1.55	0.72
1:G:345:ARG:HA	1:G:348:GLN:HE21	1.55	0.71
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.72	0.71
1:A:57:ALA:O	1:A:75:LYS:HE3	1.90	0.71
1:A:268:ARG:O	1:B:257:GLU:HG3	1.90	0.71
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.72	0.71
4:J:1:AGS:S1G	4:J:1:AGS:O3B	2.49	0.71
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.73	0.71
1:J:359:ASP:O	1:J:363:GLU:HG2	1.90	0.71
4:D:561:AGS:S1G	4:D:561:AGS:O3B	2.48	0.71
4:D:561:AGS:S1G	4:D:561:AGS:O3G	2.47	0.71
1:G:359:ASP:O	1:G:363:GLU:HG2	1.91	0.71
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.71	0.71
1:K:345:ARG:HA	1:K:348:GLN:HE21	1.55	0.70
1:N:359:ASP:O	1:N:363:GLU:HG2	1.91	0.70
1:G:489:ILE:HD12	1:G:494:LEU:CD2	2.21	0.70
1:I:345:ARG:HA	1:I:348:GLN:HE21	1.56	0.70
1:B:510:VAL:CG2	1:B:510:VAL:CG1	2.68	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASP:O	1:B:363:GLU:HG2	1.91	0.70
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.74	0.70
1:H:345:ARG:HA	1:H:348:GLN:HE21	1.56	0.70
1:N:345:ARG:HA	1:N:348:GLN:HE21	1.57	0.70
1:L:326:ASN:HD22	1:L:329:THR:HB	1.57	0.70
1:B:63:GLU:OE2	1:C:526:LYS:HE2	1.91	0.69
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.74	0.69
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.74	0.69
1:K:359:ASP:O	1:K:363:GLU:HG2	1.92	0.69
4:K:1:AGS:S1G	4:K:1:AGS:O3B	2.47	0.69
1:L:63:GLU:OE2	1:M:526:LYS:HE2	1.91	0.69
1:I:73:MET:O	1:I:76:GLU:HB2	1.92	0.69
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.58	0.69
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.74	0.69
1:F:57:ALA:O	1:F:75:LYS:HE3	1.92	0.69
4:G:1:AGS:S1G	4:G:1:AGS:O3G	2.51	0.69
1:L:73:MET:O	1:L:76:GLU:HB2	1.92	0.69
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.75	0.69
1:C:291:ASP:OD2	1:C:368:ARG:HD2	1.93	0.68
4:G:1:AGS:S1G	4:G:1:AGS:O2G	2.48	0.68
1:F:326:ASN:HD22	1:F:329:THR:HB	1.58	0.68
4:H:1:AGS:S1G	4:H:1:AGS:O3G	2.49	0.68
1:I:525:PRO:O	1:I:526:LYS:HG2	1.94	0.68
1:L:181:THR:O	1:M:282:GLY:HA3	1.93	0.68
1:M:359:ASP:O	1:M:363:GLU:HG2	1.93	0.68
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.59	0.68
1:A:231:ARG:HH11	1:G:242:LYS:HA	1.56	0.68
1:H:57:ALA:O	1:H:75:LYS:HE3	1.93	0.68
1:A:23:LEU:HD22	1:A:74:VAL:HG13	1.75	0.67
1:L:291:ASP:OD2	1:L:368:ARG:HD2	1.95	0.67
4:M:1:AGS:S1G	4:M:1:AGS:O3G	2.47	0.67
1:H:359:ASP:O	1:H:363:GLU:HG2	1.95	0.67
4:J:1:AGS:S1G	4:J:1:AGS:O2G	2.50	0.67
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.77	0.67
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.59	0.67
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	0.67
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.76	0.67
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.77	0.67
1:J:291:ASP:OD2	1:J:368:ARG:HD2	1.96	0.66
1:N:510:VAL:CG2	1:N:510:VAL:CA	2.73	0.66
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:359:ASP:O	1:L:363:GLU:HG2	1.95	0.66
1:M:291:ASP:OD2	1:M:368:ARG:HD2	1.95	0.66
1:M:345:ARG:HA	1:M:348:GLN:HE21	1.60	0.66
1:E:359:ASP:O	1:E:363:GLU:HG2	1.96	0.66
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.61	0.66
4:B:1:AGS:S1G	4:B:1:AGS:O3G	2.51	0.66
1:L:23:LEU:HD22	1:L:74:VAL:HG13	1.79	0.65
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.76	0.65
1:G:193:MET:HE1	1:G:292:ILE:HG12	1.78	0.65
4:I:1:AGS:S1G	4:I:1:AGS:O3G	2.49	0.65
1:E:194:GLN:O	1:E:371:LYS:HE3	1.97	0.65
1:N:510:VAL:CG2	1:N:510:VAL:CG1	2.70	0.65
1:E:218:PRO:HD2	1:E:320:ALA:O	1.97	0.65
1:C:359:ASP:O	1:C:363:GLU:HG2	1.97	0.65
1:D:359:ASP:O	1:D:363:GLU:HG2	1.97	0.65
1:D:489:ILE:HD12	1:D:494:LEU:CD2	2.27	0.65
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.79	0.65
1:F:389:MET:HE3	1:G:281:PHE:CE2	2.32	0.64
1:M:63:GLU:OE2	1:N:526:LYS:HE2	1.95	0.64
1:L:80:LYS:CG	1:L:80:LYS:NZ	2.60	0.64
1:G:291:ASP:OD2	1:G:368:ARG:HD2	1.98	0.64
1:F:63:GLU:OE2	1:G:526:LYS:HE2	1.96	0.64
1:J:326:ASN:HD22	1:J:329:THR:HB	1.62	0.64
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.98	0.64
1:A:359:ASP:O	1:A:363:GLU:HG2	1.98	0.64
1:E:489:ILE:HD12	1:E:494:LEU:CD2	2.28	0.64
1:L:266:THR:HG21	1:L:273:VAL:O	1.98	0.64
1:M:194:GLN:O	1:M:371:LYS:HE3	1.98	0.64
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.80	0.63
1:B:326:ASN:HD22	1:B:329:THR:HB	1.62	0.63
1:F:359:ASP:O	1:F:363:GLU:HG2	1.98	0.63
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.62	0.63
1:G:326:ASN:HD22	1:G:329:THR:HB	1.64	0.63
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.63
1:H:266:THR:CG2	1:H:273:VAL:H	2.12	0.63
1:E:326:ASN:HD22	1:E:329:THR:HB	1.63	0.63
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.62	0.63
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.81	0.63
1:I:291:ASP:OD2	1:I:368:ARG:HD2	1.98	0.63
1:K:291:ASP:OD2	1:K:368:ARG:HD2	1.98	0.63
1:E:291:ASP:OD2	1:E:368:ARG:HD2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:PRO:HD2	1:G:320:ALA:O	1.99	0.62
4:A:1:AGS:S1G	4:A:1:AGS:O3G	2.51	0.62
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.99	0.62
1:H:302:SER:H	1:H:307:MET:HE3	1.63	0.62
1:I:326:ASN:HD22	1:I:329:THR:HB	1.65	0.62
1:N:266:THR:HG21	1:N:273:VAL:O	2.00	0.62
1:C:181:THR:N	5:C:615:HOH:O	2.29	0.62
1:M:272:LYS:NZ	1:N:228:SER:HB2	2.14	0.62
1:K:266:THR:HG21	1:K:273:VAL:O	2.00	0.62
1:L:345:ARG:HA	1:L:348:GLN:HE21	1.65	0.62
1:F:266:THR:HG21	1:F:273:VAL:O	1.99	0.61
1:G:114:MET:HB3	5:G:608:HOH:O	1.98	0.61
1:H:326:ASN:HD22	1:H:329:THR:HB	1.64	0.61
1:M:525:PRO:O	1:M:526:LYS:HG2	2.00	0.61
1:A:445:ARG:NH2	5:A:607:HOH:O	2.32	0.61
1:E:525:PRO:O	1:E:526:LYS:HG2	2.00	0.61
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.83	0.61
1:B:463:SER:HB2	5:B:601:HOH:O	1.99	0.61
4:N:1:AGS:S1G	4:N:1:AGS:O2G	2.51	0.61
1:E:414:GLY:O	1:E:417:VAL:HG13	2.01	0.61
1:B:78:ALA:HB1	1:B:89:THR:HB	1.83	0.61
1:B:218:PRO:HD2	1:B:320:ALA:O	2.00	0.61
4:I:1:AGS:S1G	4:I:1:AGS:O2G	2.55	0.61
1:G:498:LYS:NZ	5:G:586:HOH:O	1.97	0.61
1:F:73:MET:O	1:F:76:GLU:HB2	2.01	0.60
1:I:428:ASP:HB2	5:I:608:HOH:O	2.00	0.60
1:L:266:THR:CG2	1:L:273:VAL:H	2.14	0.60
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.82	0.60
1:B:266:THR:HG21	1:B:273:VAL:O	2.00	0.60
1:C:266:THR:CG2	1:C:273:VAL:H	2.14	0.60
1:F:233:MET:HE1	1:F:249:ILE:HD12	1.83	0.60
1:H:414:GLY:O	1:H:417:VAL:HG13	2.01	0.60
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.83	0.60
1:G:266:THR:HG21	1:G:273:VAL:O	2.01	0.60
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.67	0.60
1:D:266:THR:HG21	1:D:273:VAL:O	2.02	0.60
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.83	0.60
1:L:90:THR:OG1	4:L:1:AGS:S1G	2.59	0.60
1:M:496:PRO:HB2	1:M:499:VAL:HG13	1.83	0.60
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.82	0.60
1:D:284:ARG:HH11	1:D:364:LYS:HD2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ALA:O	1:E:75:LYS:HE3	2.02	0.59
4:N:1:AGS:S1G	4:N:1:AGS:O3B	2.57	0.59
4:E:1:AGS:S1G	4:E:1:AGS:O3G	2.53	0.59
1:G:266:THR:CG2	1:G:273:VAL:H	2.16	0.59
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.42	0.59
1:B:23:LEU:HD22	1:B:74:VAL:HG13	1.84	0.59
1:K:414:GLY:O	1:K:417:VAL:HG13	2.02	0.59
1:L:218:PRO:HD2	1:L:320:ALA:O	2.03	0.59
1:E:266:THR:CG2	1:E:273:VAL:H	2.15	0.59
1:F:74:VAL:HG22	1:F:74:VAL:O	2.02	0.59
1:A:266:THR:HG21	1:A:273:VAL:O	2.02	0.59
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.85	0.59
1:H:266:THR:HG21	1:H:273:VAL:O	2.02	0.59
1:I:525:PRO:O	1:I:526:LYS:CG	2.51	0.59
1:E:266:THR:HG21	1:E:273:VAL:O	2.01	0.58
1:J:266:THR:CG2	1:J:273:VAL:H	2.16	0.58
1:G:18:ARG:NE	5:G:595:HOH:O	2.22	0.58
1:I:359:ASP:O	1:I:363:GLU:HG2	2.03	0.58
1:J:266:THR:HG21	1:J:273:VAL:O	2.04	0.58
1:N:218:PRO:HD2	1:N:320:ALA:O	2.03	0.58
1:D:90:THR:OG1	4:D:561:AGS:S1G	2.58	0.58
1:F:266:THR:CG2	1:F:273:VAL:H	2.16	0.58
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.85	0.58
1:D:233:MET:HE1	1:D:249:ILE:HD12	1.86	0.58
1:B:525:PRO:O	1:B:526:LYS:HG2	2.04	0.58
1:C:194:GLN:O	1:C:371:LYS:HE3	2.02	0.58
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.86	0.58
1:K:218:PRO:HD2	1:K:320:ALA:O	2.03	0.58
1:G:302:SER:H	1:G:307:MET:HE3	1.68	0.57
1:J:176:THR:HG21	1:J:322:ARG:HH12	1.68	0.57
1:B:90:THR:O	1:B:94:VAL:HG13	2.03	0.57
1:L:233:MET:HE1	1:L:249:ILE:HD12	1.86	0.57
1:A:194:GLN:O	1:A:371:LYS:HE3	2.03	0.57
1:B:266:THR:CG2	1:B:273:VAL:H	2.17	0.57
1:L:57:ALA:O	1:L:75:LYS:HE3	2.05	0.57
1:I:194:GLN:O	1:I:371:LYS:HE3	2.05	0.57
1:E:302:SER:H	1:E:307:MET:HE3	1.69	0.57
1:M:266:THR:CG2	1:M:273:VAL:H	2.17	0.57
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.04	0.57
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.86	0.57
1:D:132:LYS:HE2	5:D:595:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:218:PRO:HD2	1:J:320:ALA:O	2.05	0.57
1:C:266:THR:HG22	1:C:273:VAL:H	1.70	0.56
1:H:526:LYS:HE2	1:N:63:GLU:OE2	2.05	0.56
1:I:266:THR:CG2	1:I:273:VAL:H	2.18	0.56
1:L:242:LYS:HA	1:M:231:ARG:NH1	2.20	0.56
1:A:266:THR:CG2	1:A:273:VAL:H	2.18	0.56
1:B:525:PRO:O	1:B:526:LYS:CG	2.53	0.56
1:C:218:PRO:HD2	1:C:320:ALA:O	2.04	0.56
1:C:266:THR:HG21	1:C:273:VAL:O	2.05	0.56
1:E:266:THR:HG22	1:E:273:VAL:H	1.71	0.56
1:I:266:THR:HG21	1:I:273:VAL:O	2.04	0.56
1:I:448:GLU:OE2	1:I:470:LYS:NZ	2.32	0.56
1:L:266:THR:HG22	1:L:273:VAL:H	1.69	0.56
1:L:514:MET:CE	1:L:514:MET:CG	2.83	0.56
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.88	0.56
1:J:23:LEU:CD2	1:J:74:VAL:HG13	2.35	0.56
1:M:233:MET:HE1	1:M:249:ILE:HD12	1.88	0.56
1:M:266:THR:HG21	1:M:273:VAL:O	2.05	0.56
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.86	0.56
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.87	0.56
1:K:266:THR:CG2	1:K:273:VAL:H	2.18	0.56
1:A:231:ARG:NH1	1:G:242:LYS:CA	2.64	0.56
1:H:525:PRO:O	1:H:526:LYS:CG	2.54	0.56
1:I:57:ALA:O	1:I:75:LYS:HE3	2.05	0.56
1:D:266:THR:CG2	1:D:273:VAL:H	2.19	0.56
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.87	0.56
1:I:266:THR:HG22	1:I:271:VAL:O	2.05	0.56
1:J:404:ARG:HG2	1:J:404:ARG:HH11	1.71	0.56
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.05	0.56
1:K:193:MET:HE1	1:K:292:ILE:CG1	2.33	0.56
1:N:302:SER:H	1:N:307:MET:HE3	1.71	0.56
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.88	0.55
1:I:65:LYS:NZ	5:I:618:HOH:O	2.39	0.55
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.06	0.55
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.88	0.55
1:D:218:PRO:HD2	1:D:320:ALA:O	2.05	0.55
1:G:525:PRO:O	1:G:526:LYS:CG	2.54	0.55
1:H:73:MET:O	1:H:76:GLU:HB2	2.06	0.55
1:B:85:ALA:O	1:B:401:HIS:HE1	1.89	0.55
1:B:302:SER:H	1:B:307:MET:HE3	1.71	0.55
1:C:233:MET:HE1	1:C:249:ILE:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.55
1:N:266:THR:CG2	1:N:273:VAL:H	2.20	0.55
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.72	0.55
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.88	0.55
1:G:525:PRO:O	1:G:526:LYS:HG2	2.06	0.55
1:F:178:GLU:OE2	1:F:322:ARG:HD3	2.06	0.55
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.87	0.55
1:J:18:ARG:NE	5:J:572:HOH:O	2.27	0.55
1:J:194:GLN:O	1:J:371:LYS:HE3	2.05	0.55
1:M:266:THR:HG22	1:M:273:VAL:H	1.72	0.55
1:D:18:ARG:NE	5:D:587:HOH:O	2.36	0.55
1:E:345:ARG:HA	1:E:348:GLN:NE2	2.21	0.55
1:G:266:THR:HG22	1:G:271:VAL:O	2.06	0.55
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.88	0.55
1:G:233:MET:HE1	1:G:249:ILE:HD12	1.89	0.55
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.88	0.54
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.88	0.54
1:L:80:LYS:CG	1:L:80:LYS:CE	2.79	0.54
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.06	0.54
1:A:231:ARG:HH12	1:G:242:LYS:CG	2.21	0.54
1:D:90:THR:O	1:D:94:VAL:HG13	2.07	0.54
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.72	0.54
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.90	0.54
1:C:302:SER:H	1:C:307:MET:HE3	1.73	0.54
1:F:266:THR:HG22	1:F:273:VAL:H	1.72	0.54
1:G:461:GLU:OE1	5:G:630:HOH:O	2.19	0.54
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.72	0.54
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.89	0.54
1:N:90:THR:OG1	4:N:1:AGS:S1G	2.63	0.54
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.89	0.54
1:C:305:ILE:HB	1:C:307:MET:HE2	1.90	0.54
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.73	0.54
1:A:218:PRO:HD2	1:A:320:ALA:O	2.08	0.54
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.89	0.54
1:J:193:MET:HE1	1:J:292:ILE:CG1	2.35	0.54
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.72	0.54
1:C:73:MET:O	1:C:76:GLU:HB2	2.08	0.54
1:G:404:ARG:HH11	1:G:404:ARG:HG2	1.72	0.54
1:H:266:THR:HG22	1:H:271:VAL:O	2.06	0.54
1:B:181:THR:O	1:C:282:GLY:HA3	2.08	0.54
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:525:PRO:O	1:L:526:LYS:HG2	2.08	0.54
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.89	0.54
1:H:218:PRO:HD2	1:H:320:ALA:O	2.08	0.54
1:I:233:MET:HE1	1:I:249:ILE:HD12	1.90	0.54
1:K:266:THR:HG22	1:K:273:VAL:H	1.73	0.54
1:L:80:LYS:CG	1:L:80:LYS:HZ3	2.20	0.54
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.89	0.54
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.91	0.53
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.37	0.53
1:F:414:GLY:O	1:F:417:VAL:HG13	2.08	0.53
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.89	0.53
1:F:345:ARG:HA	1:F:348:GLN:NE2	2.21	0.53
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.91	0.53
1:E:73:MET:O	1:E:76:GLU:HB2	2.08	0.53
1:E:525:PRO:O	1:E:526:LYS:CG	2.57	0.53
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.90	0.53
1:J:266:THR:HG22	1:J:273:VAL:H	1.71	0.53
1:M:218:PRO:HD2	1:M:320:ALA:O	2.08	0.53
1:N:77:VAL:O	1:N:78:ALA:C	2.51	0.53
1:F:302:SER:H	1:F:307:MET:HE3	1.72	0.53
1:G:266:THR:HG22	1:G:273:VAL:H	1.73	0.53
1:K:305:ILE:HB	1:K:307:MET:HE2	1.90	0.53
1:B:57:ALA:O	1:B:75:LYS:HE3	2.08	0.53
1:E:525:PRO:HD3	5:E:594:HOH:O	2.09	0.53
1:M:302:SER:H	1:M:307:MET:HE3	1.72	0.53
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.90	0.53
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.90	0.53
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.91	0.53
1:J:224:ASP:HB3	1:J:302:SER:HB3	1.91	0.53
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.90	0.53
1:A:270:ILE:HA	1:B:229:ASN:OD1	2.09	0.53
1:C:319:GLN:HB3	1:C:336:VAL:HG21	1.91	0.53
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.09	0.53
1:A:345:ARG:HA	1:A:348:GLN:NE2	2.22	0.53
1:B:90:THR:OG1	4:B:1:AGS:S1G	2.66	0.53
1:A:231:ARG:HH12	1:G:242:LYS:HG3	1.74	0.52
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.90	0.52
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.91	0.52
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.91	0.52
1:M:319:GLN:HB3	1:M:336:VAL:CG2	2.39	0.52
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLY:O	1:A:417:VAL:HG13	2.09	0.52
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.91	0.52
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.75	0.52
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.22	0.52
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.91	0.52
1:A:115:ASP:OD2	5:A:610:HOH:O	2.19	0.52
1:C:268:ARG:O	1:D:257:GLU:HG3	2.09	0.52
1:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.52
1:H:266:THR:HG22	1:H:273:VAL:H	1.74	0.52
1:J:179:ASP:HB3	1:J:389:MET:HE1	1.92	0.52
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.90	0.52
1:C:272:LYS:NZ	1:D:228:SER:CB	2.73	0.52
1:E:193:MET:HE1	1:E:292:ILE:CG1	2.35	0.52
1:I:179:ASP:HB3	1:I:389:MET:HE1	1.91	0.52
1:L:193:MET:HE1	1:L:292:ILE:CG1	2.36	0.52
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.25	0.52
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.50	0.52
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.91	0.52
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.91	0.52
1:L:414:GLY:O	1:L:417:VAL:HG13	2.09	0.52
1:A:525:PRO:O	1:A:526:LYS:HG2	2.09	0.52
1:B:16:MET:O	1:B:20:VAL:HG13	2.09	0.52
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.92	0.52
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.91	0.52
1:H:479:ASN:OD1	1:H:479:ASN:C	2.53	0.52
1:I:218:PRO:HD2	1:I:320:ALA:O	2.11	0.51
1:L:77:VAL:O	1:L:78:ALA:C	2.53	0.51
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.91	0.51
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.75	0.51
1:M:525:PRO:O	1:M:526:LYS:CG	2.58	0.51
1:M:525:PRO:HD3	5:M:596:HOH:O	2.10	0.51
1:A:272:LYS:NZ	1:B:228:SER:HB2	2.25	0.51
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.91	0.51
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.93	0.51
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.93	0.51
1:B:266:THR:HG22	1:B:273:VAL:H	1.74	0.51
1:B:414:GLY:O	1:B:417:VAL:HG13	2.11	0.51
1:F:404:ARG:HG2	1:F:404:ARG:HH11	1.75	0.51
1:K:179:ASP:HB3	1:K:389:MET:HE1	1.92	0.51
1:M:266:THR:HG22	1:M:271:VAL:O	2.10	0.51
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.93	0.51
1:H:176:THR:HG21	1:H:322:ARG:HH12	1.75	0.51
1:N:414:GLY:O	1:N:417:VAL:HG13	2.11	0.51
1:A:224:ASP:HB3	1:A:302:SER:HB3	1.92	0.51
1:B:194:GLN:O	1:B:371:LYS:HE3	2.11	0.51
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.92	0.51
1:J:233:MET:HE1	1:J:249:ILE:HD12	1.93	0.51
1:K:57:ALA:O	1:K:75:LYS:HE3	2.11	0.51
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.91	0.51
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.93	0.51
1:D:132:LYS:CE	5:D:595:HOH:O	2.58	0.51
1:G:345:ARG:HA	1:G:348:GLN:NE2	2.24	0.51
1:H:525:PRO:O	1:H:526:LYS:HG2	2.11	0.51
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.92	0.51
1:K:302:SER:H	1:K:307:MET:HE3	1.74	0.51
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.92	0.51
1:K:489:ILE:HD12	1:K:494:LEU:CD2	2.41	0.51
1:A:489:ILE:HD12	1:A:494:LEU:CD2	2.41	0.50
1:H:194:GLN:O	1:H:371:LYS:HE3	2.11	0.50
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.91	0.50
1:K:451:LEU:C	1:K:451:LEU:HD23	2.36	0.50
1:N:489:ILE:HD12	1:N:494:LEU:CD2	2.40	0.50
1:C:525:PRO:HD3	5:C:588:HOH:O	2.11	0.50
1:D:37:ASN:ND2	1:D:51:LYS:HE3	2.27	0.50
1:F:74:VAL:O	1:F:74:VAL:CG2	2.58	0.50
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.93	0.50
1:C:272:LYS:HZ1	1:D:228:SER:HB3	1.77	0.50
1:D:458:CYS:SG	1:D:480:ALA:HB1	2.52	0.50
1:F:218:PRO:HD2	1:F:320:ALA:O	2.11	0.50
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.94	0.50
1:D:345:ARG:HA	1:D:348:GLN:NE2	2.24	0.50
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.94	0.50
1:J:266:THR:HG22	1:J:271:VAL:O	2.12	0.50
1:J:414:GLY:O	1:J:417:VAL:HG13	2.12	0.50
1:A:266:THR:HG22	1:A:273:VAL:H	1.76	0.50
1:M:270:ILE:HG22	1:M:271:VAL:HG23	1.93	0.50
1:N:345:ARG:HA	1:N:348:GLN:NE2	2.24	0.50
1:B:452:ARG:HD3	5:B:594:HOH:O	2.11	0.50
1:G:176:THR:HG21	1:G:322:ARG:HH12	1.77	0.50
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.93	0.50
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:ILE:HB	1:I:307:MET:HE2	1.94	0.50
1:K:77:VAL:O	1:K:78:ALA:C	2.55	0.50
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.93	0.50
1:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.49
1:M:272:LYS:HZ3	1:N:228:SER:HB2	1.77	0.49
1:N:194:GLN:O	1:N:371:LYS:HE3	2.10	0.49
1:B:233:MET:HE1	1:B:249:ILE:HD12	1.94	0.49
1:D:525:PRO:O	1:D:526:LYS:HG2	2.11	0.49
1:E:266:THR:HG22	1:E:271:VAL:O	2.12	0.49
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.94	0.49
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.93	0.49
1:J:179:ASP:OD1	1:J:393:LYS:HE3	2.13	0.49
1:J:525:PRO:O	1:J:526:LYS:HG2	2.11	0.49
1:K:460:GLU:HB3	5:K:586:HOH:O	2.12	0.49
1:E:23:LEU:HD22	1:E:74:VAL:HG13	1.93	0.49
1:F:90:THR:O	1:F:94:VAL:HG13	2.13	0.49
1:F:224:ASP:HB3	1:F:302:SER:HB3	1.93	0.49
1:J:302:SER:H	1:J:307:MET:HE3	1.76	0.49
1:C:179:ASP:HB3	1:C:389:MET:HE1	1.95	0.49
1:C:404:ARG:HG2	1:C:404:ARG:NH1	2.25	0.49
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.93	0.49
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.95	0.49
1:E:366:GLN:O	1:E:369:VAL:HG22	2.13	0.49
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.95	0.49
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.95	0.49
1:B:266:THR:HG22	1:B:271:VAL:O	2.13	0.49
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.94	0.49
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.53	0.49
1:A:272:LYS:HZ1	1:B:228:SER:HB2	1.78	0.49
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.94	0.49
1:C:414:GLY:O	1:C:417:VAL:HG13	2.13	0.49
1:H:68:ASN:O	1:H:72:GLN:HG2	2.13	0.49
1:I:325:ILE:HG22	1:I:330:THR:HG23	1.95	0.49
1:K:266:THR:HG22	1:K:271:VAL:O	2.13	0.49
1:N:266:THR:HG22	1:N:271:VAL:O	2.12	0.49
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.95	0.48
1:L:451:LEU:HD23	1:L:451:LEU:C	2.38	0.48
1:C:36:ARG:HG3	1:D:518:GLU:HG2	1.95	0.48
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.94	0.48
1:D:192:GLY:HA2	1:D:295:LEU:HD11	1.93	0.48
1:D:266:THR:HG22	1:D:273:VAL:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:SER:HB2	1:F:399:ALA:HA	1.96	0.48
1:F:305:ILE:HB	1:F:307:MET:HE2	1.94	0.48
1:N:179:ASP:HB3	1:N:389:MET:HE1	1.95	0.48
1:B:74:VAL:O	1:B:77:VAL:HB	2.12	0.48
1:B:151:SER:HB2	1:B:399:ALA:HA	1.96	0.48
1:H:319:GLN:HB3	1:H:336:VAL:HG21	1.95	0.48
1:J:90:THR:OG1	4:J:1:AGS:S1G	2.68	0.48
1:I:266:THR:HG22	1:I:273:VAL:H	1.79	0.48
1:J:345:ARG:HA	1:J:348:GLN:NE2	2.26	0.48
1:D:177:VAL:CG2	1:D:397:GLU:HG3	2.41	0.48
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.95	0.48
1:M:90:THR:O	1:M:94:VAL:HG13	2.13	0.48
1:B:305:ILE:HB	1:B:307:MET:HE2	1.95	0.48
1:I:121:ASP:OD1	5:I:594:HOH:O	2.20	0.48
1:K:460:GLU:O	1:K:462:PRO:HD3	2.14	0.48
1:L:404:ARG:HH11	1:L:404:ARG:HG2	1.78	0.48
1:C:236:VAL:O	1:C:240:VAL:HG23	2.13	0.48
1:H:233:MET:HE1	1:H:249:ILE:HD12	1.95	0.48
1:K:233:MET:HE1	1:K:249:ILE:HD12	1.96	0.48
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.96	0.48
1:E:82:ASN:HB2	1:E:89:THR:HG21	1.95	0.48
1:E:325:ILE:HG22	1:E:330:THR:HG23	1.94	0.48
1:G:489:ILE:HD12	1:G:494:LEU:HD22	1.95	0.48
1:H:266:THR:HG21	1:H:273:VAL:H	1.78	0.48
1:M:404:ARG:HH11	1:M:404:ARG:CG	2.26	0.48
1:N:74:VAL:O	1:N:74:VAL:HG22	2.13	0.48
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.13	0.48
1:B:176:THR:HG22	1:B:177:VAL:H	1.78	0.48
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.48
1:I:345:ARG:HA	1:I:348:GLN:NE2	2.26	0.48
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.48
1:F:194:GLN:O	1:F:371:LYS:HE3	2.13	0.47
1:G:194:GLN:O	1:G:371:LYS:HE3	2.14	0.47
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.43	0.47
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.95	0.47
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.96	0.47
1:N:266:THR:HG22	1:N:273:VAL:H	1.78	0.47
1:G:90:THR:O	1:G:94:VAL:HG13	2.13	0.47
1:G:179:ASP:OD1	1:G:393:LYS:HE3	2.14	0.47
1:G:452:ARG:HD3	5:G:585:HOH:O	2.15	0.47
1:L:80:LYS:CD	1:L:80:LYS:HB2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLY:O	1:D:417:VAL:HG13	2.13	0.47
1:M:224:ASP:HB3	1:M:302:SER:HB3	1.95	0.47
1:N:233:MET:HE1	1:N:249:ILE:HD12	1.95	0.47
1:A:302:SER:H	1:A:307:MET:HE3	1.78	0.47
1:D:404:ARG:HH11	1:D:404:ARG:CG	2.25	0.47
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.96	0.47
1:F:63:GLU:HB2	1:G:524:LEU:CD2	2.45	0.47
1:J:236:VAL:O	1:J:240:VAL:HG23	2.14	0.47
1:M:78:ALA:HB1	1:M:89:THR:HB	1.97	0.47
1:F:85:ALA:O	1:F:401:HIS:HE1	1.98	0.47
1:F:525:PRO:O	1:F:526:LYS:HG2	2.14	0.47
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.54	0.47
1:L:514:MET:CB	1:L:514:MET:HE2	2.44	0.47
1:D:29:VAL:HG11	1:E:518:GLU:HG3	1.97	0.47
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.45	0.47
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.95	0.47
1:A:73:MET:O	1:A:76:GLU:HB2	2.15	0.47
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.95	0.47
1:H:345:ARG:HA	1:H:348:GLN:NE2	2.29	0.47
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.96	0.47
1:I:302:SER:H	1:I:307:MET:HE3	1.78	0.47
1:K:345:ARG:HA	1:K:348:GLN:NE2	2.26	0.47
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.96	0.47
1:D:263:VAL:O	1:D:267:MET:HB2	2.14	0.47
1:E:319:GLN:HB3	1:E:336:VAL:CG2	2.44	0.47
1:E:489:ILE:HD12	1:E:494:LEU:HD22	1.97	0.47
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.96	0.47
1:D:166:MET:HE2	1:D:171:LYS:O	2.15	0.47
1:D:305:ILE:HB	1:D:307:MET:HE2	1.97	0.47
1:G:236:VAL:O	1:G:240:VAL:HG23	2.13	0.47
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.97	0.47
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.97	0.47
1:A:74:VAL:HG22	1:A:74:VAL:O	2.14	0.47
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.97	0.46
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.96	0.46
1:G:18:ARG:NH2	5:G:595:HOH:O	2.41	0.46
1:J:132:LYS:NZ	5:J:603:HOH:O	2.44	0.46
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.96	0.46
1:K:194:GLN:O	1:K:371:LYS:HE3	2.15	0.46
1:N:525:PRO:O	1:N:526:LYS:HG2	2.14	0.46
1:G:263:VAL:O	1:G:267:MET:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:236:VAL:O	1:K:240:VAL:HG23	2.15	0.46
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.97	0.46
1:C:319:GLN:HB3	1:C:336:VAL:CG2	2.45	0.46
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.98	0.46
1:I:177:VAL:CG2	1:I:397:GLU:HG3	2.40	0.46
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.98	0.46
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.97	0.46
1:N:348:GLN:O	1:N:352:GLN:HG2	2.15	0.46
1:N:502:SER:O	1:N:503:ALA:C	2.59	0.46
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.95	0.46
1:H:90:THR:OG1	4:H:1:AGS:S1G	2.69	0.46
1:L:319:GLN:HB3	1:L:336:VAL:CG2	2.45	0.46
1:B:77:VAL:HG23	1:B:510:VAL:HG21	1.97	0.46
1:G:224:ASP:HB3	1:G:302:SER:HB3	1.96	0.46
1:I:360:TYR:CE1	1:I:364:LYS:HE3	2.51	0.46
1:I:364:LYS:HA	1:I:364:LYS:HD3	1.70	0.46
1:D:57:ALA:O	1:D:75:LYS:CE	2.63	0.46
1:E:151:SER:HB2	1:E:399:ALA:HA	1.98	0.46
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.97	0.46
1:H:151:SER:HB2	1:H:399:ALA:HA	1.98	0.46
1:K:319:GLN:HB3	1:K:336:VAL:HG21	1.96	0.46
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.98	0.46
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.28	0.46
1:D:34:LYS:HE2	1:E:118:ARG:HH22	1.80	0.46
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.97	0.46
1:I:179:ASP:OD1	1:I:393:LYS:HE3	2.16	0.46
1:K:404:ARG:CG	1:K:404:ARG:NH1	2.79	0.46
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.98	0.46
1:M:179:ASP:HB3	1:M:389:MET:HE1	1.96	0.46
1:M:360:TYR:CE1	1:M:364:LYS:HE3	2.51	0.46
1:B:78:ALA:O	1:B:79:SER:C	2.55	0.46
1:B:179:ASP:HB3	1:B:389:MET:HE1	1.98	0.46
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.98	0.46
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.98	0.46
1:F:389:MET:CE	1:G:281:PHE:CE2	2.97	0.46
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.14	0.46
1:J:489:ILE:HD12	1:J:494:LEU:CD2	2.46	0.46
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.98	0.46
1:N:263:VAL:O	1:N:267:MET:HB2	2.16	0.46
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.97	0.46
1:B:191:GLU:O	1:B:334:ASP:HA	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:489:ILE:HD12	1:H:494:LEU:CD2	2.45	0.46
1:I:151:SER:HB2	1:I:399:ALA:HA	1.98	0.46
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.97	0.46
1:M:57:ALA:O	1:M:75:LYS:CE	2.63	0.46
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	0.46
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.81	0.46
1:I:57:ALA:O	1:I:75:LYS:CE	2.64	0.46
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.98	0.46
1:L:68:ASN:O	1:L:72:GLN:HG2	2.15	0.46
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.45
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.98	0.45
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.97	0.45
1:E:233:MET:HE1	1:E:249:ILE:HD12	1.98	0.45
1:E:305:ILE:HB	1:E:307:MET:HE2	1.97	0.45
1:C:514:MET:HE3	1:C:514:MET:HB3	1.80	0.45
1:F:449:ALA:N	1:F:450:PRO:CD	2.79	0.45
1:M:176:THR:HG22	1:M:177:VAL:H	1.80	0.45
1:M:236:VAL:O	1:M:240:VAL:HG23	2.17	0.45
1:N:360:TYR:CE1	1:N:364:LYS:HE3	2.52	0.45
1:C:266:THR:HG22	1:C:271:VAL:O	2.16	0.45
1:E:463:SER:HB2	5:E:649:HOH:O	2.16	0.45
1:G:284:ARG:HH11	1:G:364:LYS:HD2	1.80	0.45
1:N:351:GLN:HE21	1:N:351:GLN:HB3	1.65	0.45
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.98	0.45
1:F:386:GLU:O	1:F:390:LYS:HG2	2.16	0.45
1:H:35:GLY:O	1:H:51:LYS:HE2	2.16	0.45
1:B:263:VAL:O	1:B:267:MET:HB2	2.17	0.45
1:B:345:ARG:HA	1:B:348:GLN:NE2	2.27	0.45
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.82	0.45
1:H:63:GLU:OE2	1:I:526:LYS:HE2	2.16	0.45
1:J:305:ILE:HB	1:J:307:MET:HE2	1.98	0.45
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.97	0.45
1:F:360:TYR:CE1	1:F:364:LYS:HE3	2.52	0.45
1:H:177:VAL:CG2	1:H:397:GLU:HG3	2.40	0.45
1:H:263:VAL:O	1:H:267:MET:HB2	2.17	0.45
1:L:80:LYS:NZ	1:L:80:LYS:HG2	2.32	0.45
1:L:177:VAL:CG2	1:L:397:GLU:HG3	2.42	0.45
1:L:305:ILE:HB	1:L:307:MET:HE2	1.99	0.45
1:B:514:MET:HE3	1:B:514:MET:HB3	1.55	0.45
1:C:193:MET:HE2	1:C:193:MET:HB3	1.73	0.45
1:D:57:ALA:O	1:D:75:LYS:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.98	0.45
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.99	0.45
1:G:413:ALA:HB3	1:G:417:VAL:HG22	1.99	0.45
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.98	0.45
1:I:82:ASN:O	1:I:86:GLY:N	2.45	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:A:233:MET:HE1	1:A:249:ILE:HD12	1.97	0.45
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.99	0.45
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.98	0.45
1:E:224:ASP:HB3	1:E:302:SER:HB3	1.97	0.45
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.99	0.45
1:H:360:TYR:CE1	1:H:364:LYS:HE3	2.52	0.45
1:J:57:ALA:O	1:J:75:LYS:CE	2.65	0.45
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.98	0.45
1:K:321:LYS:HB2	1:K:334:ASP:HB3	1.98	0.45
1:L:78:ALA:HB1	1:L:89:THR:HB	1.99	0.45
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.99	0.45
1:M:305:ILE:HB	1:M:307:MET:HE2	1.98	0.45
1:C:449:ALA:N	1:C:450:PRO:CD	2.79	0.45
1:D:193:MET:HE2	1:D:193:MET:HB3	1.66	0.45
1:D:325:ILE:HG23	1:D:325:ILE:HD13	1.67	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.47	0.45
1:L:449:ALA:N	1:L:450:PRO:CD	2.79	0.45
1:C:57:ALA:O	1:C:75:LYS:HE3	2.17	0.45
1:D:233:MET:HE1	1:D:249:ILE:CD1	2.46	0.45
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.99	0.45
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.98	0.45
1:L:386:GLU:O	1:L:390:LYS:HG2	2.16	0.45
1:J:82:ASN:O	1:J:86:GLY:N	2.49	0.44
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.99	0.44
1:A:386:GLU:O	1:A:390:LYS:HG2	2.16	0.44
1:A:489:ILE:HD12	1:A:494:LEU:HD22	1.98	0.44
1:E:179:ASP:HB3	1:E:389:MET:HE1	1.99	0.44
1:E:458:CYS:SG	1:E:480:ALA:HB1	2.57	0.44
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.98	0.44
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.99	0.44
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.99	0.44
1:I:366:GLN:O	1:I:369:VAL:HG22	2.17	0.44
1:M:36:ARG:HG3	1:N:518:GLU:HG2	1.98	0.44
1:E:449:ALA:N	1:E:450:PRO:CD	2.80	0.44
1:F:236:VAL:O	1:F:240:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.44
1:I:64:ASP:C	1:I:64:ASP:OD1	2.60	0.44
1:K:186:GLU:HB2	1:K:380:LYS:HB2	2.00	0.44
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.99	0.44
1:K:224:ASP:HB3	1:K:302:SER:HB3	1.99	0.44
1:M:68:ASN:O	1:M:72:GLN:HG2	2.17	0.44
1:C:57:ALA:O	1:C:75:LYS:CE	2.66	0.44
1:G:288:MET:HG2	1:G:368:ARG:HD3	1.98	0.44
1:G:414:GLY:O	1:G:417:VAL:HG13	2.17	0.44
1:G:514:MET:HE3	1:G:514:MET:HB3	1.79	0.44
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.99	0.44
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.99	0.44
1:G:496:PRO:HB2	1:G:499:VAL:HG13	1.99	0.44
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.99	0.44
1:D:514:MET:HE3	1:D:514:MET:HB3	1.76	0.44
1:E:193:MET:HE2	1:E:193:MET:HB3	1.82	0.44
1:H:224:ASP:HB3	1:H:302:SER:HB3	2.00	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.17	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:J:90:THR:O	1:J:94:VAL:HG13	2.17	0.44
1:K:179:ASP:OD1	1:K:393:LYS:HE3	2.18	0.44
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.98	0.44
1:L:302:SER:H	1:L:307:MET:HE3	1.83	0.44
1:L:463:SER:HB2	5:L:612:HOH:O	2.17	0.44
1:D:217:SER:N	1:D:218:PRO:HD3	2.33	0.44
1:D:404:ARG:CG	1:D:404:ARG:NH1	2.79	0.44
1:F:36:ARG:HG3	1:G:518:GLU:HG2	1.98	0.44
1:H:386:GLU:O	1:H:390:LYS:HG2	2.17	0.44
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.99	0.44
1:K:82:ASN:HB2	1:K:89:THR:HG21	1.99	0.44
1:N:193:MET:HE1	1:N:292:ILE:CG1	2.42	0.44
1:N:236:VAL:O	1:N:240:VAL:HG23	2.17	0.44
1:A:77:VAL:O	1:A:78:ALA:C	2.60	0.44
1:D:77:VAL:O	1:D:78:ALA:C	2.60	0.44
1:F:524:LEU:O	1:F:526:LYS:N	2.51	0.44
1:I:514:MET:HE3	1:I:514:MET:HB3	1.94	0.44
1:J:63:GLU:HB2	1:K:524:LEU:HD21	2.00	0.44
1:J:151:SER:HB2	1:J:399:ALA:HA	1.99	0.44
1:J:325:ILE:HG22	1:J:330:THR:HG23	2.00	0.44
1:J:404:ARG:HH11	1:J:404:ARG:CG	2.29	0.44
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HB	1:A:307:MET:HE2	1.99	0.44
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.00	0.44
1:C:178:GLU:OE2	1:C:322:ARG:HD3	2.18	0.44
1:E:369:VAL:HG23	1:E:370:ALA:N	2.33	0.44
1:I:351:GLN:HE21	1:I:351:GLN:HB3	1.69	0.44
1:I:417:VAL:HG11	1:I:477:GLY:HA3	1.99	0.44
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.33	0.44
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.99	0.43
1:B:451:LEU:HD23	1:B:451:LEU:C	2.43	0.43
1:C:151:SER:HB2	1:C:399:ALA:HA	2.00	0.43
1:G:151:SER:HB2	1:G:399:ALA:HA	1.99	0.43
1:J:364:LYS:HA	1:J:364:LYS:HD3	1.84	0.43
1:L:179:ASP:HB3	1:L:389:MET:HE1	2.00	0.43
1:L:263:VAL:O	1:L:267:MET:HB2	2.18	0.43
1:F:263:VAL:O	1:F:267:MET:HB2	2.18	0.43
1:J:263:VAL:O	1:J:267:MET:HB2	2.18	0.43
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.99	0.43
1:N:319:GLN:HB3	1:N:336:VAL:CG2	2.48	0.43
1:A:525:PRO:O	1:A:526:LYS:CG	2.65	0.43
1:B:82:ASN:HB2	1:B:89:THR:HG21	2.00	0.43
1:E:166:MET:HE2	1:E:171:LYS:O	2.18	0.43
1:F:23:LEU:HD22	1:F:74:VAL:HG13	2.00	0.43
1:F:369:VAL:HG23	1:F:370:ALA:N	2.33	0.43
1:K:524:LEU:O	1:K:526:LYS:N	2.51	0.43
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.76	0.43
1:B:473:ASP:HB2	5:B:599:HOH:O	2.19	0.43
1:D:524:LEU:O	1:D:526:LYS:N	2.51	0.43
1:E:386:GLU:O	1:E:390:LYS:HG2	2.17	0.43
1:F:147:VAL:O	1:F:151:SER:OG	2.36	0.43
1:J:235:PRO:HG3	1:J:310:GLU:HA	2.00	0.43
1:G:305:ILE:HB	1:G:307:MET:HE2	1.99	0.43
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.00	0.43
1:L:151:SER:HB2	1:L:399:ALA:HA	2.00	0.43
1:L:489:ILE:HD12	1:L:494:LEU:CD2	2.49	0.43
1:A:118:ARG:HH22	1:G:34:LYS:HE2	1.84	0.43
1:A:151:SER:HB2	1:A:399:ALA:HA	2.01	0.43
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.16	0.43
1:H:218:PRO:HB3	1:H:246:PRO:HG2	2.00	0.43
1:B:221:LEU:HD23	1:B:249:ILE:HD12	2.01	0.43
1:E:37:ASN:ND2	1:E:51:LYS:HE3	2.33	0.43
1:E:186:GLU:HB2	1:E:380:LYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ASP:HB3	1:F:389:MET:HE1	2.00	0.43
1:F:351:GLN:HE21	1:F:351:GLN:HB3	1.64	0.43
1:H:366:GLN:O	1:H:369:VAL:HG22	2.18	0.43
1:J:351:GLN:HE21	1:J:351:GLN:HB3	1.66	0.43
1:N:305:ILE:HB	1:N:307:MET:HE2	2.00	0.43
1:B:224:ASP:HB3	1:B:302:SER:HB3	1.99	0.43
1:C:191:GLU:O	1:C:334:ASP:HA	2.18	0.43
1:D:325:ILE:HD12	1:D:325:ILE:HG21	1.64	0.43
1:H:351:GLN:HE21	1:H:351:GLN:HB3	1.68	0.43
1:K:364:LYS:HA	1:K:364:LYS:HD3	1.83	0.43
1:L:266:THR:HG22	1:L:271:VAL:O	2.18	0.43
1:M:178:GLU:HG2	1:M:322:ARG:NH1	2.33	0.43
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.43
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.49	0.43
1:C:284:ARG:HH11	1:C:364:LYS:HD2	1.84	0.43
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.43
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.58	0.43
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.01	0.43
1:J:186:GLU:HB2	1:J:380:LYS:HB2	2.01	0.43
1:K:366:GLN:O	1:K:369:VAL:HG22	2.19	0.43
1:M:404:ARG:CG	1:M:404:ARG:NH1	2.82	0.43
1:A:466:ALA:O	1:A:470:LYS:HG3	2.19	0.43
1:E:236:VAL:O	1:E:240:VAL:HG23	2.19	0.43
1:E:451:LEU:C	1:E:451:LEU:HD23	2.43	0.43
1:L:39:VAL:HG12	1:M:69:MET:CE	2.49	0.43
1:M:506:TYR:O	1:M:507:ALA:C	2.57	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.42
1:A:364:LYS:HA	1:A:364:LYS:HD3	1.85	0.42
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.82	0.42
1:D:186:GLU:HB2	1:D:380:LYS:HB2	2.01	0.42
1:F:366:GLN:O	1:F:369:VAL:HG22	2.18	0.42
1:G:325:ILE:HG23	1:G:325:ILE:HD13	1.78	0.42
1:K:63:GLU:OE2	1:L:526:LYS:HE2	2.18	0.42
1:K:284:ARG:HH11	1:K:364:LYS:HD2	1.84	0.42
1:B:218:PRO:HB3	1:B:246:PRO:HG2	2.01	0.42
1:C:272:LYS:NZ	1:D:228:SER:HB2	2.34	0.42
1:F:90:THR:OG1	4:F:1:AGS:S1G	2.72	0.42
1:F:177:VAL:CG2	1:F:397:GLU:HG3	2.43	0.42
1:F:193:MET:HE2	1:F:193:MET:HB3	1.88	0.42
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.00	0.42
1:L:345:ARG:HA	1:L:348:GLN:NE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:179:ASP:OD1	1:N:393:LYS:HE3	2.19	0.42
1:N:284:ARG:HH11	1:N:364:LYS:HD2	1.84	0.42
1:A:193:MET:HE1	1:A:292:ILE:CG1	2.42	0.42
1:G:179:ASP:HB3	1:G:389:MET:HE1	2.02	0.42
1:M:186:GLU:HB2	1:M:380:LYS:HB2	2.01	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.01	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.01	0.42
1:A:166:MET:HE2	1:A:171:LYS:O	2.18	0.42
1:C:263:VAL:O	1:C:267:MET:HB2	2.19	0.42
1:E:135:SER:HB3	5:E:618:HOH:O	2.18	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.50	0.42
1:F:413:ALA:HB3	1:F:417:VAL:HG22	2.00	0.42
1:H:404:ARG:NH1	1:H:404:ARG:HG2	2.32	0.42
1:J:360:TYR:CE1	1:J:364:LYS:HE3	2.54	0.42
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.34	0.42
1:A:193:MET:HB3	1:A:193:MET:HE2	1.78	0.42
1:A:263:VAL:O	1:A:267:MET:HB2	2.18	0.42
1:C:404:ARG:NH1	1:C:404:ARG:CG	2.81	0.42
1:D:404:ARG:HG2	1:D:404:ARG:NH1	2.30	0.42
1:F:288:MET:HG2	1:F:368:ARG:HD3	2.00	0.42
1:F:383:ALA:HB3	1:F:389:MET:HB2	2.01	0.42
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.86	0.42
1:H:514:MET:HE3	1:H:514:MET:HB3	1.74	0.42
1:N:506:TYR:O	1:N:507:ALA:C	2.56	0.42
1:B:386:GLU:O	1:B:390:LYS:HG2	2.19	0.42
1:C:489:ILE:HD12	1:C:494:LEU:CD2	2.49	0.42
1:F:109:ALA:HB2	1:H:109:ALA:HB2	2.02	0.42
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.01	0.42
1:F:389:MET:CE	1:G:281:PHE:HE2	2.33	0.42
1:F:466:ALA:O	1:F:470:LYS:HG3	2.20	0.42
1:G:18:ARG:CZ	5:G:595:HOH:O	2.66	0.42
1:I:218:PRO:HB3	1:I:246:PRO:HG2	2.01	0.42
1:J:217:SER:N	1:J:218:PRO:HD3	2.35	0.42
1:J:288:MET:HG2	1:J:368:ARG:HD3	2.02	0.42
1:M:193:MET:HE2	1:M:193:MET:HB3	1.85	0.42
1:N:57:ALA:O	1:N:75:LYS:CE	2.68	0.42
1:B:153:ASN:O	1:B:154:SER:HB2	2.20	0.42
1:C:63:GLU:HB2	1:D:524:LEU:HD21	2.01	0.42
1:E:171:LYS:HB2	1:E:407:VAL:HG11	2.02	0.42
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.49	0.42
1:G:144:ILE:HG23	1:G:403:THR:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:VAL:HG13	1:G:396:VAL:HG22	2.02	0.42
1:H:118:ARG:HG3	5:H:587:HOH:O	2.18	0.42
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.32	0.42
1:C:272:LYS:NZ	1:D:228:SER:HB3	2.35	0.42
1:E:351:GLN:HE21	1:E:351:GLN:HB3	1.66	0.42
1:F:348:GLN:O	1:F:352:GLN:HG2	2.20	0.42
1:G:118:ARG:HE	1:G:118:ARG:HB2	1.78	0.42
1:G:489:ILE:HD12	1:G:494:LEU:HD21	2.01	0.42
1:H:305:ILE:HG22	1:H:305:ILE:O	2.20	0.42
1:H:413:ALA:HB3	1:H:417:VAL:HG22	2.01	0.42
1:J:489:ILE:HD12	1:J:494:LEU:HD22	2.00	0.42
1:D:65:LYS:HG2	5:D:646:HOH:O	2.19	0.42
1:E:421:ARG:HH11	1:E:421:ARG:HD3	1.60	0.42
1:I:158:VAL:HG13	1:I:396:VAL:HG22	2.01	0.42
1:I:414:GLY:O	1:I:417:VAL:HG13	2.20	0.42
1:J:221:LEU:HD23	1:J:249:ILE:HD12	2.01	0.42
1:K:18:ARG:NE	5:K:590:HOH:O	2.47	0.42
1:L:171:LYS:HB2	1:L:407:VAL:HG11	2.02	0.42
1:L:218:PRO:HB3	1:L:246:PRO:HG2	2.00	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:E:118:ARG:HE	1:E:118:ARG:HB2	1.80	0.42
1:E:321:LYS:HB2	1:E:334:ASP:HB3	2.02	0.42
1:F:188:ASP:OD1	1:F:188:ASP:N	2.53	0.42
1:H:270:ILE:HG22	1:H:271:VAL:HG23	2.02	0.42
1:H:383:ALA:HB3	1:H:389:MET:HB2	2.01	0.42
1:N:193:MET:HE2	1:N:193:MET:HB3	1.84	0.42
1:A:37:ASN:ND2	1:A:51:LYS:HE3	2.35	0.41
1:A:236:VAL:O	1:A:240:VAL:HG23	2.20	0.41
1:F:321:LYS:HB2	1:F:334:ASP:HB3	2.02	0.41
1:H:18:ARG:NE	5:H:584:HOH:O	2.32	0.41
1:H:284:ARG:HH11	1:H:364:LYS:HD2	1.85	0.41
1:K:319:GLN:HB3	1:K:336:VAL:CG2	2.50	0.41
1:L:288:MET:HG2	1:L:368:ARG:HD3	2.02	0.41
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.60	0.41
1:M:366:GLN:O	1:M:369:VAL:HG22	2.20	0.41
1:M:409:GLU:OE1	5:M:578:HOH:O	2.22	0.41
1:N:489:ILE:HD12	1:N:494:LEU:HD22	2.00	0.41
1:D:179:ASP:HB3	1:D:389:MET:HE1	2.02	0.41
1:F:218:PRO:HB3	1:F:246:PRO:HG2	2.03	0.41
1:F:305:ILE:O	1:F:305:ILE:HG22	2.20	0.41
1:H:69:MET:O	1:H:73:MET:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.49	0.41
1:M:179:ASP:OD1	1:M:393:LYS:HE3	2.20	0.41
1:M:193:MET:HE1	1:M:292:ILE:CG1	2.42	0.41
1:M:263:VAL:O	1:M:267:MET:HB2	2.20	0.41
1:N:224:ASP:HB3	1:N:302:SER:HB3	2.02	0.41
1:A:319:GLN:HB3	1:A:336:VAL:HG21	2.02	0.41
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.02	0.41
1:C:118:ARG:HE	1:C:118:ARG:HB2	1.79	0.41
1:D:16:MET:O	1:D:20:VAL:HG13	2.21	0.41
1:A:351:GLN:HE21	1:A:351:GLN:HB3	1.65	0.41
1:H:179:ASP:HB3	1:H:389:MET:HE1	2.02	0.41
1:H:305:ILE:HB	1:H:307:MET:HE2	2.01	0.41
1:N:219:PHE:HB3	1:N:317:LEU:HD23	2.02	0.41
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.02	0.41
1:D:419:LEU:HA	1:D:419:LEU:HD23	1.82	0.41
1:E:417:VAL:HG11	1:E:477:GLY:HA3	2.01	0.41
4:I:1:AGS:S1G	4:I:1:AGS:O3B	2.59	0.41
1:J:269:GLY:HA3	1:K:257:GLU:HG3	2.03	0.41
1:M:221:LEU:HD23	1:M:249:ILE:HD12	2.02	0.41
1:M:360:TYR:CZ	1:M:364:LYS:HE3	2.55	0.41
1:M:451:LEU:C	1:M:451:LEU:HD23	2.45	0.41
1:A:266:THR:HG22	1:A:271:VAL:O	2.20	0.41
1:A:366:GLN:O	1:A:369:VAL:HG22	2.20	0.41
1:C:524:LEU:O	1:C:526:LYS:N	2.53	0.41
1:M:205:ILE:HA	1:M:213:VAL:HG22	2.03	0.41
1:N:366:GLN:O	1:N:369:VAL:HG22	2.21	0.41
1:B:37:ASN:ND2	5:B:628:HOH:O	2.47	0.41
1:G:266:THR:HG21	1:G:273:VAL:H	1.86	0.41
1:K:219:PHE:O	1:K:247:LEU:HD12	2.20	0.41
1:L:236:VAL:O	1:L:240:VAL:HG23	2.21	0.41
1:L:419:LEU:HD23	1:L:419:LEU:HA	1.96	0.41
1:M:70:GLY:HA2	1:M:73:MET:HE3	2.03	0.41
1:M:305:ILE:HG22	1:M:305:ILE:O	2.21	0.41
1:M:345:ARG:HA	1:M:348:GLN:NE2	2.32	0.41
1:N:419:LEU:HD23	1:N:419:LEU:HA	1.91	0.41
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.02	0.41
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.82	0.41
1:C:90:THR:O	1:C:94:VAL:HG13	2.21	0.41
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.03	0.41
1:C:260:ALA:O	1:C:264:VAL:HG23	2.20	0.41
1:D:39:VAL:HG23	1:E:517:THR:CG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ARG:O	1:D:446:ALA:C	2.62	0.41
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.50	0.41
1:I:235:PRO:CG	1:I:310:GLU:HA	2.51	0.41
1:J:73:MET:O	1:J:76:GLU:HB2	2.20	0.41
1:J:78:ALA:HB1	1:J:89:THR:HB	2.03	0.41
4:J:1:AGS:S1G	4:J:1:AGS:O3G	2.57	0.41
1:K:177:VAL:CG2	1:K:397:GLU:HG3	2.44	0.41
1:M:57:ALA:O	1:M:75:LYS:HE2	2.21	0.41
1:N:112:ASN:HA	1:N:113:PRO:HD3	1.96	0.41
1:N:221:LEU:HD23	1:N:249:ILE:HD12	2.02	0.41
1:A:69:MET:CE	1:G:39:VAL:HG12	2.50	0.41
1:A:514:MET:HE3	1:A:514:MET:HB3	1.76	0.41
1:C:224:ASP:HB3	1:C:302:SER:HB3	2.03	0.41
1:C:345:ARG:HA	1:C:348:GLN:NE2	2.31	0.41
1:D:18:ARG:NH2	5:D:587:HOH:O	2.51	0.41
1:E:16:MET:O	1:E:20:VAL:HG13	2.21	0.41
1:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:F:451:LEU:C	1:F:451:LEU:HD23	2.46	0.41
1:G:78:ALA:HB1	1:G:89:THR:HB	2.03	0.41
1:I:16:MET:O	1:I:20:VAL:HG13	2.21	0.41
1:I:191:GLU:O	1:I:334:ASP:HA	2.21	0.41
1:I:263:VAL:O	1:I:267:MET:HB2	2.21	0.41
1:K:348:GLN:O	1:K:352:GLN:HG2	2.20	0.41
1:L:364:LYS:HD3	1:L:364:LYS:HA	1.73	0.41
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.33	0.41
1:N:74:VAL:C	1:N:76:GLU:N	2.79	0.41
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.86	0.41
1:C:366:GLN:O	1:C:369:VAL:HG22	2.21	0.41
1:D:124:VAL:HG21	1:D:508:ALA:HB2	2.03	0.41
1:D:319:GLN:HB3	1:D:336:VAL:HG21	2.02	0.41
1:D:386:GLU:O	1:D:390:LYS:HG2	2.20	0.41
1:D:463:SER:HB2	5:D:644:HOH:O	2.20	0.41
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.61	0.41
1:F:233:MET:HE1	1:F:249:ILE:CD1	2.50	0.41
1:H:321:LYS:HB2	1:H:334:ASP:HB3	2.02	0.41
1:K:16:MET:O	1:K:20:VAL:HG13	2.21	0.41
1:K:325:ILE:HG22	1:K:330:THR:HG23	2.02	0.41
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.03	0.41
1:A:348:GLN:O	1:A:352:GLN:HG2	2.22	0.40
1:B:236:VAL:O	1:B:240:VAL:HG23	2.21	0.40
1:D:266:THR:HG22	1:D:271:VAL:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:496:PRO:HB2	1:F:499:VAL:HG13	2.03	0.40
1:J:39:VAL:HG12	1:K:69:MET:HE2	2.03	0.40
1:K:188:ASP:OD1	1:K:188:ASP:N	2.54	0.40
1:K:191:GLU:O	1:K:334:ASP:HA	2.22	0.40
1:M:364:LYS:HD3	1:M:364:LYS:HA	1.86	0.40
1:A:231:ARG:NH1	1:G:242:LYS:CG	2.83	0.40
1:E:360:TYR:CE1	1:E:364:LYS:HE3	2.56	0.40
1:F:178:GLU:HG2	1:F:322:ARG:NH1	2.36	0.40
1:G:66:PHE:CZ	1:G:522:THR:HG22	2.57	0.40
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.61	0.40
1:M:16:MET:O	1:M:20:VAL:HG13	2.21	0.40
1:N:466:ALA:O	1:N:470:LYS:HG3	2.21	0.40
1:A:69:MET:HE2	1:G:39:VAL:HG12	2.03	0.40
1:A:284:ARG:HH11	1:A:364:LYS:HD2	1.87	0.40
1:F:514:MET:HE3	1:F:514:MET:HB3	1.70	0.40
1:J:57:ALA:O	1:J:75:LYS:HE3	2.20	0.40
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.51	0.40
1:N:325:ILE:HG22	1:N:330:THR:HG23	2.02	0.40
1:A:34:LYS:HA	1:B:114:MET:HE2	2.02	0.40
1:C:360:TYR:CE1	1:C:364:LYS:HE3	2.56	0.40
1:H:404:ARG:NH1	1:H:404:ARG:CG	2.83	0.40
1:I:63:GLU:HB2	1:J:524:LEU:HD21	2.04	0.40
1:J:514:MET:HB3	1:J:514:MET:HE3	1.66	0.40
1:K:419:LEU:HD23	1:K:419:LEU:HA	1.94	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40
1:M:57:ALA:O	1:M:75:LYS:HE3	2.20	0.40
1:M:176:THR:HG22	1:M:177:VAL:N	2.36	0.40
1:M:514:MET:HE3	1:M:514:MET:HB3	1.69	0.40
1:A:404:ARG:CG	1:A:404:ARG:NH1	2.84	0.40
1:B:360:TYR:CE1	1:B:364:LYS:HE3	2.57	0.40
1:C:221:LEU:HD23	1:C:249:ILE:HD12	2.03	0.40
1:D:114:MET:CG	1:D:114:MET:CE	2.99	0.40
1:J:321:LYS:HB2	1:J:334:ASP:HB3	2.03	0.40
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.52	0.40
1:M:369:VAL:HG23	1:M:370:ALA:N	2.36	0.40
1:N:36:ARG:HD2	5:N:614:HOH:O	2.21	0.40

All (5) 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:I:142:LYS:NZ	1:N:354:GLU:O[2_646]	1.85	0.35
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.05	0.15
1:A:311:LYS:NZ	1:N:311:LYS:O[1_554]	2.09	0.11
1:H:350:ARG:NH1	1:L:354:GLU:OE1[1_455]	2.11	0.09
1:G:315:GLU:OE1	1:N:338:GLU:OE2[1_554]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	30	27
1	B	523/525 (100%)	506 (97%)	15 (3%)	2 (0%)	30	27
1	C	523/525 (100%)	505 (97%)	16 (3%)	2 (0%)	30	27
1	D	523/525 (100%)	509 (97%)	13 (2%)	1 (0%)	43	42
1	E	523/525 (100%)	507 (97%)	14 (3%)	2 (0%)	30	27
1	F	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	30	27
1	G	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	30	27
1	H	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	30	27
1	I	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	30	27
1	J	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	30	27
1	K	523/525 (100%)	505 (97%)	15 (3%)	3 (1%)	21	17
1	L	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	30	27
1	M	523/525 (100%)	512 (98%)	9 (2%)	2 (0%)	30	27
1	N	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	30	27
All	All	7322/7350 (100%)	7111 (97%)	183 (2%)	28 (0%)	30	27

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	GLY
1	A	256	GLY
1	B	256	GLY
1	C	256	GLY
1	E	256	GLY
1	F	256	GLY
1	G	256	GLY
1	H	256	GLY
1	I	256	GLY
1	J	256	GLY
1	K	256	GLY
1	L	256	GLY
1	M	256	GLY
1	N	256	GLY
1	N	270	ILE
1	I	270	ILE
1	H	270	ILE
1	K	270	ILE
1	L	270	ILE
1	M	270	ILE
1	B	270	ILE
1	C	270	ILE
1	E	270	ILE
1	F	270	ILE
1	G	270	ILE
1	K	77	VAL
1	A	270	ILE
1	J	270	ILE

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	404/405 (100%)	378 (94%)	26 (6%)	16	12
1	B	404/405 (100%)	374 (93%)	30 (7%)	13	9
1	C	404/405 (100%)	378 (94%)	26 (6%)	16	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/405 (100%)	372 (92%)	32 (8%)	11	8
1	E	404/405 (100%)	374 (93%)	30 (7%)	13	9
1	F	404/405 (100%)	378 (94%)	26 (6%)	16	12
1	G	404/405 (100%)	376 (93%)	28 (7%)	14	11
1	H	404/405 (100%)	378 (94%)	26 (6%)	16	12
1	I	404/405 (100%)	382 (95%)	22 (5%)	20	17
1	J	404/405 (100%)	377 (93%)	27 (7%)	15	11
1	K	404/405 (100%)	378 (94%)	26 (6%)	16	12
1	L	404/405 (100%)	374 (93%)	30 (7%)	13	9
1	M	404/405 (100%)	377 (93%)	27 (7%)	15	11
1	N	404/405 (100%)	380 (94%)	24 (6%)	18	14
All	All	5656/5670 (100%)	5276 (93%)	380 (7%)	15	11

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	14	VAL
1	A	20	VAL
1	A	23	LEU
1	A	75	LYS
1	A	94	VAL
1	A	151	SER
1	A	160	LYS
1	A	183	LEU
1	A	230	ILE
1	A	284	ARG
1	A	289	LEU
1	A	295	LEU
1	A	325	ILE
1	A	329	THR
1	A	331	THR
1	A	351	GLN
1	A	352	GLN
1	A	363	GLU
1	A	404	ARG
1	A	417	VAL
1	A	420	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	473	ASP
1	A	499	VAL
1	A	518	GLU
1	A	524	LEU
1	B	10	ASN
1	B	14	VAL
1	B	20	VAL
1	B	23	LEU
1	B	75	LYS
1	B	94	VAL
1	B	151	SER
1	B	160	LYS
1	B	176	THR
1	B	183	LEU
1	B	230	ILE
1	B	284	ARG
1	B	289	LEU
1	B	325	ILE
1	B	329	THR
1	B	331	THR
1	B	351	GLN
1	B	352	GLN
1	B	363	GLU
1	B	404	ARG
1	B	407	VAL
1	B	417	VAL
1	B	420	ILE
1	B	421	ARG
1	B	473	ASP
1	B	499	VAL
1	B	514	MET
1	B	518	GLU
1	B	524	LEU
1	B	526	LYS
1	C	10	ASN
1	C	14	VAL
1	C	20	VAL
1	C	23	LEU
1	C	75	LYS
1	C	94	VAL
1	C	151	SER
1	C	160	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	230	ILE
1	C	284	ARG
1	C	289	LEU
1	C	325	ILE
1	C	329	THR
1	C	331	THR
1	C	351	GLN
1	C	352	GLN
1	C	363	GLU
1	C	404	ARG
1	C	417	VAL
1	C	420	ILE
1	C	473	ASP
1	C	499	VAL
1	C	514	MET
1	C	518	GLU
1	C	524	LEU
1	C	526	LYS
1	D	10	ASN
1	D	14	VAL
1	D	20	VAL
1	D	75	LYS
1	D	94	VAL
1	D	135	SER
1	D	151	SER
1	D	160	LYS
1	D	177	VAL
1	D	183	LEU
1	D	188	ASP
1	D	230	ILE
1	D	267	MET
1	D	284	ARG
1	D	289	LEU
1	D	295	LEU
1	D	323	VAL
1	D	325	ILE
1	D	329	THR
1	D	331	THR
1	D	351	GLN
1	D	352	GLN
1	D	358	SER
1	D	404	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	417	VAL
1	D	420	ILE
1	D	473	ASP
1	D	489	ILE
1	D	499	VAL
1	D	514	MET
1	D	518	GLU
1	D	524	LEU
1	E	10	ASN
1	E	14	VAL
1	E	20	VAL
1	E	23	LEU
1	E	94	VAL
1	E	118	ARG
1	E	135	SER
1	E	146	GLN
1	E	151	SER
1	E	160	LYS
1	E	183	LEU
1	E	230	ILE
1	E	284	ARG
1	E	289	LEU
1	E	295	LEU
1	E	325	ILE
1	E	329	THR
1	E	331	THR
1	E	351	GLN
1	E	352	GLN
1	E	363	GLU
1	E	404	ARG
1	E	417	VAL
1	E	420	ILE
1	E	473	ASP
1	E	489	ILE
1	E	499	VAL
1	E	514	MET
1	E	518	GLU
1	E	524	LEU
1	F	10	ASN
1	F	14	VAL
1	F	20	VAL
1	F	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	94	VAL
1	F	151	SER
1	F	160	LYS
1	F	183	LEU
1	F	188	ASP
1	F	230	ILE
1	F	284	ARG
1	F	289	LEU
1	F	325	ILE
1	F	329	THR
1	F	331	THR
1	F	351	GLN
1	F	352	GLN
1	F	363	GLU
1	F	404	ARG
1	F	417	VAL
1	F	420	ILE
1	F	473	ASP
1	F	499	VAL
1	F	514	MET
1	F	518	GLU
1	F	524	LEU
1	G	10	ASN
1	G	14	VAL
1	G	20	VAL
1	G	75	LYS
1	G	94	VAL
1	G	151	SER
1	G	160	LYS
1	G	176	THR
1	G	183	LEU
1	G	188	ASP
1	G	230	ILE
1	G	284	ARG
1	G	325	ILE
1	G	329	THR
1	G	331	THR
1	G	351	GLN
1	G	352	GLN
1	G	358	SER
1	G	363	GLU
1	G	404	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	417	VAL
1	G	420	ILE
1	G	473	ASP
1	G	489	ILE
1	G	499	VAL
1	G	514	MET
1	G	518	GLU
1	G	524	LEU
1	H	10	ASN
1	H	14	VAL
1	H	20	VAL
1	H	23	LEU
1	H	75	LYS
1	H	94	VAL
1	H	118	ARG
1	H	151	SER
1	H	160	LYS
1	H	183	LEU
1	H	230	ILE
1	H	284	ARG
1	H	289	LEU
1	H	325	ILE
1	H	329	THR
1	H	331	THR
1	H	351	GLN
1	H	352	GLN
1	H	363	GLU
1	H	404	ARG
1	H	417	VAL
1	H	420	ILE
1	H	499	VAL
1	H	514	MET
1	H	518	GLU
1	H	524	LEU
1	I	10	ASN
1	I	14	VAL
1	I	20	VAL
1	I	75	LYS
1	I	94	VAL
1	I	151	SER
1	I	160	LYS
1	I	230	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	284	ARG
1	I	289	LEU
1	I	325	ILE
1	I	329	THR
1	I	331	THR
1	I	351	GLN
1	I	352	GLN
1	I	363	GLU
1	I	404	ARG
1	I	417	VAL
1	I	420	ILE
1	I	499	VAL
1	I	518	GLU
1	I	524	LEU
1	J	10	ASN
1	J	14	VAL
1	J	20	VAL
1	J	75	LYS
1	J	94	VAL
1	J	151	SER
1	J	160	LYS
1	J	183	LEU
1	J	230	ILE
1	J	231	ARG
1	J	284	ARG
1	J	289	LEU
1	J	325	ILE
1	J	329	THR
1	J	331	THR
1	J	351	GLN
1	J	352	GLN
1	J	358	SER
1	J	363	GLU
1	J	404	ARG
1	J	417	VAL
1	J	420	ILE
1	J	473	ASP
1	J	499	VAL
1	J	514	MET
1	J	518	GLU
1	J	524	LEU
1	K	10	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	14	VAL
1	K	20	VAL
1	K	75	LYS
1	K	80	LYS
1	K	94	VAL
1	K	118	ARG
1	K	151	SER
1	K	160	LYS
1	K	183	LEU
1	K	230	ILE
1	K	284	ARG
1	K	289	LEU
1	K	325	ILE
1	K	329	THR
1	K	331	THR
1	K	351	GLN
1	K	352	GLN
1	K	363	GLU
1	K	404	ARG
1	K	417	VAL
1	K	420	ILE
1	K	473	ASP
1	K	499	VAL
1	K	518	GLU
1	K	524	LEU
1	L	10	ASN
1	L	14	VAL
1	L	20	VAL
1	L	23	LEU
1	L	27	VAL
1	L	75	LYS
1	L	80	LYS
1	L	94	VAL
1	L	151	SER
1	L	160	LYS
1	L	183	LEU
1	L	230	ILE
1	L	284	ARG
1	L	289	LEU
1	L	325	ILE
1	L	328	ASP
1	L	329	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	331	THR
1	L	351	GLN
1	L	352	GLN
1	L	363	GLU
1	L	404	ARG
1	L	417	VAL
1	L	420	ILE
1	L	473	ASP
1	L	499	VAL
1	L	514	MET
1	L	518	GLU
1	L	524	LEU
1	L	526	LYS
1	M	10	ASN
1	M	14	VAL
1	M	20	VAL
1	M	23	LEU
1	M	75	LYS
1	M	94	VAL
1	M	151	SER
1	M	160	LYS
1	M	183	LEU
1	M	230	ILE
1	M	284	ARG
1	M	289	LEU
1	M	325	ILE
1	M	329	THR
1	M	331	THR
1	M	351	GLN
1	M	352	GLN
1	M	363	GLU
1	M	404	ARG
1	M	417	VAL
1	M	420	ILE
1	M	473	ASP
1	M	499	VAL
1	M	514	MET
1	M	518	GLU
1	M	524	LEU
1	M	526	LYS
1	N	10	ASN
1	N	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	20	VAL
1	N	23	LEU
1	N	75	LYS
1	N	94	VAL
1	N	151	SER
1	N	160	LYS
1	N	183	LEU
1	N	230	ILE
1	N	284	ARG
1	N	289	LEU
1	N	325	ILE
1	N	329	THR
1	N	331	THR
1	N	351	GLN
1	N	352	GLN
1	N	404	ARG
1	N	417	VAL
1	N	420	ILE
1	N	499	VAL
1	N	514	MET
1	N	518	GLU
1	N	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) 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	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	453	GLN
1	B	37	ASN
1	B	146	GLN
1	B	265	ASN
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	401	HIS
1	B	453	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	37	ASN
1	C	146	GLN
1	C	265	ASN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	401	HIS
1	D	37	ASN
1	D	146	GLN
1	D	229	ASN
1	D	265	ASN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	401	HIS
1	D	453	GLN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	475	ASN
1	F	146	GLN
1	F	265	ASN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	401	HIS
1	F	453	GLN
1	G	146	GLN
1	G	194	GLN
1	G	265	ASN
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	475	ASN
1	H	146	GLN
1	H	265	ASN
1	H	326	ASN
1	H	348	GLN
1	H	351	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	453	GLN
1	I	37	ASN
1	I	146	GLN
1	I	229	ASN
1	I	265	ASN
1	I	326	ASN
1	I	348	GLN
1	I	351	GLN
1	I	401	HIS
1	I	453	GLN
1	J	37	ASN
1	J	146	GLN
1	J	265	ASN
1	J	326	ASN
1	J	348	GLN
1	J	351	GLN
1	J	453	GLN
1	K	146	GLN
1	K	265	ASN
1	K	326	ASN
1	K	348	GLN
1	K	351	GLN
1	K	401	HIS
1	K	453	GLN
1	K	475	ASN
1	L	10	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN
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	265	ASN
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	N	37	ASN
1	N	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	265	ASN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	401	HIS
1	N	453	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 30 are monoatomic - leaving 14 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$
4	AGS	M	1	2,3	32,33,33	3.50	6 (18%)	45,52,52	2.39	13 (28%)
4	AGS	F	1	2,3	32,33,33	3.51	5 (15%)	45,52,52	1.91	12 (26%)
4	AGS	G	1	2,3	32,33,33	4.12	10 (31%)	45,52,52	2.23	17 (37%)
4	AGS	D	561	2,3	32,33,33	3.86	10 (31%)	45,52,52	2.07	14 (31%)
4	AGS	A	1	2,3	32,33,33	3.46	6 (18%)	45,52,52	2.27	16 (35%)
4	AGS	H	1	2,3	32,33,33	3.58	8 (25%)	45,52,52	2.43	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AGS	J	1	2,3	32,33,33	3.43	5 (15%)	45,52,52	2.10	14 (31%)
4	AGS	K	1	2,3	32,33,33	3.73	7 (21%)	45,52,52	2.02	12 (26%)
4	AGS	I	1	2,3	32,33,33	3.57	7 (21%)	45,52,52	1.96	15 (33%)
4	AGS	L	1	2,3	32,33,33	3.79	5 (15%)	45,52,52	2.56	14 (31%)
4	AGS	C	1	2,3	32,33,33	3.48	8 (25%)	45,52,52	2.14	10 (22%)
4	AGS	N	1	2,3	32,33,33	3.80	7 (21%)	45,52,52	2.57	16 (35%)
4	AGS	B	1	2,3	32,33,33	3.59	5 (15%)	45,52,52	2.14	14 (31%)
4	AGS	E	1	2,3	32,33,33	4.46	10 (31%)	45,52,52	2.58	19 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	M	1	2,3	-	3/21/38/38	0/3/3/3
4	AGS	F	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	G	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	D	561	2,3	-	4/21/38/38	0/3/3/3
4	AGS	A	1	2,3	-	3/21/38/38	0/3/3/3
4	AGS	H	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	J	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	K	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	I	1	2,3	-	3/21/38/38	0/3/3/3
4	AGS	L	1	2,3	-	1/21/38/38	0/3/3/3
4	AGS	C	1	2,3	-	3/21/38/38	0/3/3/3
4	AGS	N	1	2,3	-	2/21/38/38	0/3/3/3
4	AGS	B	1	2,3	-	3/21/38/38	0/3/3/3
4	AGS	E	1	2,3	-	3/21/38/38	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AGS	PG-S1G	-20.69	1.45	1.90
4	E	1	AGS	PG-S1G	-20.06	1.47	1.90
4	N	1	AGS	PG-S1G	-20.05	1.47	1.90
4	D	561	AGS	PG-S1G	-19.24	1.48	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1	AGS	PG-S1G	-18.84	1.49	1.90
4	I	1	AGS	PG-S1G	-18.48	1.50	1.90
4	F	1	AGS	PG-S1G	-18.24	1.51	1.90
4	C	1	AGS	PG-S1G	-18.23	1.51	1.90
4	H	1	AGS	PG-S1G	-18.22	1.51	1.90
4	K	1	AGS	PG-S1G	-18.15	1.51	1.90
4	M	1	AGS	PG-S1G	-18.10	1.51	1.90
4	B	1	AGS	PG-S1G	-17.73	1.52	1.90
4	J	1	AGS	PG-S1G	-17.63	1.52	1.90
4	A	1	AGS	PG-S1G	-17.09	1.53	1.90
4	E	1	AGS	PB-O3A	9.29	1.69	1.59
4	L	1	AGS	PB-O3A	7.19	1.67	1.59
4	B	1	AGS	PB-O3A	6.76	1.66	1.59
4	E	1	AGS	C8-N9	5.88	1.47	1.37
4	A	1	AGS	PA-O3A	5.85	1.65	1.59
4	K	1	AGS	PA-O3A	5.81	1.65	1.59
4	E	1	AGS	PA-O3A	5.57	1.65	1.59
4	G	1	AGS	PB-O3B	-5.43	1.53	1.59
4	J	1	AGS	PB-O3B	-5.25	1.53	1.59
4	K	1	AGS	PB-O3A	5.24	1.65	1.59
4	D	561	AGS	C4-N3	4.43	1.42	1.34
4	E	1	AGS	PA-O1A	-4.15	1.36	1.50
4	E	1	AGS	C5-N7	3.99	1.46	1.39
4	H	1	AGS	PB-O3A	3.79	1.63	1.59
4	A	1	AGS	C8-N7	3.75	1.38	1.31
4	D	561	AGS	C2-N1	3.64	1.40	1.33
4	M	1	AGS	C8-N7	3.59	1.38	1.31
4	F	1	AGS	PA-O1A	-3.55	1.38	1.50
4	I	1	AGS	C8-N7	3.41	1.38	1.31
4	E	1	AGS	C2-N3	3.40	1.40	1.33
4	E	1	AGS	C6-N1	3.35	1.45	1.35
4	D	561	AGS	C2-N3	3.34	1.39	1.33
4	F	1	AGS	C8-N7	3.30	1.38	1.31
4	G	1	AGS	C2-N3	3.25	1.39	1.33
4	F	1	AGS	O3'-C3'	-3.18	1.35	1.43
4	G	1	AGS	PA-O1A	-3.14	1.39	1.50
4	M	1	AGS	PB-O3A	3.13	1.62	1.59
4	D	561	AGS	PA-O3A	3.12	1.62	1.59
4	K	1	AGS	C8-N7	3.10	1.37	1.31
4	K	1	AGS	PB-O1B	-3.06	1.40	1.50
4	H	1	AGS	C5-N7	-3.04	1.33	1.39
4	G	1	AGS	C8-N9	3.01	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1	AGS	PA-O1A	-2.99	1.40	1.50
4	M	1	AGS	C8-N9	2.95	1.42	1.37
4	L	1	AGS	C2-N1	2.93	1.39	1.33
4	A	1	AGS	PB-O3A	2.93	1.62	1.59
4	E	1	AGS	C8-N7	2.91	1.37	1.31
4	N	1	AGS	O4'-C1'	-2.91	1.35	1.42
4	G	1	AGS	C2-N1	2.89	1.39	1.33
4	D	561	AGS	PG-O2G	2.88	1.64	1.54
4	C	1	AGS	C8-N7	2.86	1.37	1.31
4	I	1	AGS	O4'-C4'	-2.81	1.38	1.45
4	B	1	AGS	C8-N9	2.81	1.42	1.37
4	G	1	AGS	PB-O3A	-2.77	1.56	1.59
4	N	1	AGS	C2-N3	2.77	1.38	1.33
4	C	1	AGS	PA-O3A	2.74	1.62	1.59
4	A	1	AGS	C2-N3	2.73	1.38	1.33
4	N	1	AGS	PA-O1A	-2.73	1.41	1.50
4	N	1	AGS	PA-O3A	2.70	1.62	1.59
4	L	1	AGS	PB-O3B	2.63	1.62	1.59
4	B	1	AGS	PA-O1A	-2.60	1.41	1.50
4	D	561	AGS	PB-O3B	-2.59	1.56	1.59
4	G	1	AGS	C4-N9	-2.50	1.32	1.37
4	D	561	AGS	C8-N9	2.48	1.41	1.37
4	K	1	AGS	C2-N3	2.48	1.38	1.33
4	C	1	AGS	C2-N1	2.47	1.38	1.33
4	E	1	AGS	PB-O1B	-2.46	1.42	1.50
4	I	1	AGS	C2-N3	2.42	1.38	1.33
4	B	1	AGS	C8-N7	2.42	1.36	1.31
4	D	561	AGS	PA-O1A	-2.38	1.42	1.50
4	N	1	AGS	C2-N1	2.38	1.38	1.33
4	G	1	AGS	O3'-C3'	-2.37	1.37	1.43
4	D	561	AGS	C8-N7	2.36	1.36	1.31
4	H	1	AGS	O2'-C2'	-2.33	1.37	1.43
4	F	1	AGS	PB-O3A	2.31	1.62	1.59
4	C	1	AGS	PB-O3B	2.26	1.61	1.59
4	H	1	AGS	C8-N7	2.25	1.36	1.31
4	G	1	AGS	C8-N7	2.24	1.36	1.31
4	C	1	AGS	PA-O1A	-2.23	1.43	1.50
4	I	1	AGS	PA-O2A	2.23	1.65	1.55
4	J	1	AGS	O4'-C4'	-2.21	1.40	1.45
4	C	1	AGS	PB-O3A	2.19	1.61	1.59
4	I	1	AGS	PB-O3B	-2.18	1.57	1.59
4	M	1	AGS	O2'-C2'	-2.17	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	AGS	C8-N7	2.15	1.35	1.31
4	K	1	AGS	C2-N1	2.13	1.37	1.33
4	M	1	AGS	C2-N3	2.12	1.37	1.33
4	N	1	AGS	PB-O3A	2.11	1.61	1.59
4	H	1	AGS	PB-O1B	-2.10	1.43	1.50
4	J	1	AGS	C2-N1	2.08	1.37	1.33
4	A	1	AGS	PA-O1A	-2.08	1.43	1.50
4	H	1	AGS	C2-N3	2.07	1.37	1.33
4	H	1	AGS	C4-N9	-2.06	1.33	1.37
4	C	1	AGS	C2-N3	2.05	1.37	1.33
4	I	1	AGS	C2-N1	2.03	1.37	1.33

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	AGS	N3-C2-N1	-9.10	114.81	128.58
4	L	1	AGS	N3-C2-N1	-8.55	115.64	128.58
4	C	1	AGS	N3-C2-N1	-8.46	115.77	128.58
4	A	1	AGS	N3-C2-N1	-7.30	117.53	128.58
4	E	1	AGS	N9-C8-N7	-6.83	104.24	113.94
4	N	1	AGS	N9-C8-N7	-6.64	104.51	113.94
4	H	1	AGS	N9-C8-N7	-6.58	104.61	113.94
4	B	1	AGS	N9-C8-N7	-6.51	104.70	113.94
4	L	1	AGS	N9-C8-N7	-6.40	104.86	113.94
4	G	1	AGS	N9-C8-N7	-6.16	105.19	113.94
4	N	1	AGS	N3-C2-N1	-5.83	119.75	128.58
4	N	1	AGS	C5-N7-C8	5.80	112.56	103.45
4	K	1	AGS	O4'-C1'-N9	5.76	119.15	108.09
4	M	1	AGS	C2-N3-C4	5.61	125.54	111.83
4	E	1	AGS	O2B-PB-O3A	-5.43	92.59	107.27
4	D	561	AGS	N9-C8-N7	-5.43	106.24	113.94
4	H	1	AGS	O2B-PB-O3A	5.42	121.94	107.27
4	E	1	AGS	N3-C2-N1	-5.39	120.43	128.58
4	B	1	AGS	N3-C2-N1	-5.37	120.46	128.58
4	E	1	AGS	O3B-PB-O1B	5.19	126.31	110.70
4	F	1	AGS	N9-C8-N7	-5.03	106.79	113.94
4	E	1	AGS	C4-N9-C8	5.01	111.00	105.74
4	J	1	AGS	C5-C4-N3	-5.01	119.81	126.72
4	A	1	AGS	O2B-PB-O3A	-4.96	93.88	107.27
4	G	1	AGS	N3-C2-N1	-4.94	121.11	128.58
4	L	1	AGS	C4-N9-C8	4.84	110.82	105.74
4	J	1	AGS	C5-N7-C8	4.83	111.05	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	AGS	O3'-C3'-C4'	-4.83	97.21	111.08
4	L	1	AGS	O4'-C1'-N9	4.80	117.31	108.09
4	N	1	AGS	C4-C5-N7	-4.80	105.10	110.58
4	I	1	AGS	N9-C8-N7	-4.78	107.15	113.94
4	J	1	AGS	N3-C2-N1	-4.74	121.40	128.58
4	H	1	AGS	O5'-PA-O1A	-4.74	90.15	108.94
4	N	1	AGS	O5'-PA-O1A	-4.73	90.20	108.94
4	L	1	AGS	C2-N3-C4	4.68	123.27	111.83
4	H	1	AGS	N3-C2-N1	-4.67	121.51	128.58
4	D	561	AGS	C4-N9-C8	4.59	110.56	105.74
4	M	1	AGS	O4'-C1'-C2'	-4.55	96.88	106.62
4	I	1	AGS	N3-C2-N1	-4.50	121.77	128.58
4	C	1	AGS	C2-N3-C4	4.48	122.78	111.83
4	B	1	AGS	C4-N9-C8	4.47	110.43	105.74
4	J	1	AGS	N9-C8-N7	-4.43	107.65	113.94
4	H	1	AGS	C5-N7-C8	4.41	110.38	103.45
4	K	1	AGS	N3-C2-N1	-4.37	121.96	128.58
4	C	1	AGS	O4'-C1'-N9	4.34	116.42	108.09
4	M	1	AGS	N9-C8-N7	-4.32	107.81	113.94
4	L	1	AGS	C5-N7-C8	4.25	110.13	103.45
4	C	1	AGS	C5-C4-N3	-4.19	120.95	126.72
4	J	1	AGS	C4-C5-N7	-4.17	105.82	110.58
4	G	1	AGS	C4-N9-C8	4.12	110.06	105.74
4	N	1	AGS	C4-N9-C8	4.06	110.00	105.74
4	B	1	AGS	C5-N7-C8	3.98	109.71	103.45
4	N	1	AGS	C5-C4-N3	-3.97	121.25	126.72
4	N	1	AGS	C2-N3-C4	3.97	121.53	111.83
4	K	1	AGS	N9-C8-N7	-3.95	108.34	113.94
4	F	1	AGS	N3-C2-N1	-3.88	122.70	128.58
4	G	1	AGS	C5-N7-C8	3.87	109.53	103.45
4	F	1	AGS	C5'-C4'-C3'	-3.84	101.38	115.21
4	M	1	AGS	C5-C4-N3	-3.81	121.47	126.72
4	I	1	AGS	O4'-C1'-N9	3.79	115.37	108.09
4	H	1	AGS	O3B-PB-O1B	3.76	122.01	110.70
4	D	561	AGS	N3-C4-N9	3.74	133.53	127.17
4	K	1	AGS	C5-C4-N3	-3.74	121.57	126.72
4	A	1	AGS	C2-N3-C4	3.74	120.96	111.83
4	I	1	AGS	C5-N7-C8	3.64	109.16	103.45
4	F	1	AGS	C5-C4-N3	-3.62	121.73	126.72
4	H	1	AGS	C4-N9-C8	3.61	109.53	105.74
4	C	1	AGS	O3B-PB-O1B	-3.58	99.94	110.70
4	E	1	AGS	C5-N7-C8	3.52	108.99	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	561	AGS	C5-C4-N3	-3.50	121.89	126.72
4	K	1	AGS	PB-O3B-PG	-3.49	120.39	133.17
4	N	1	AGS	C5'-C4'-C3'	-3.48	102.68	115.21
4	F	1	AGS	C5-N7-C8	3.47	108.90	103.45
4	G	1	AGS	O2A-PA-O3A	-3.46	97.92	107.27
4	E	1	AGS	C2-N3-C4	3.45	120.26	111.83
4	D	561	AGS	N3-C2-N1	-3.44	123.37	128.58
4	I	1	AGS	C5-C4-N3	-3.43	122.00	126.72
4	K	1	AGS	O3B-PB-O1B	3.40	120.93	110.70
4	D	561	AGS	C5-N7-C8	3.36	108.73	103.45
4	F	1	AGS	C4-N9-C8	3.34	109.24	105.74
4	J	1	AGS	C2-N3-C4	3.32	119.94	111.83
4	N	1	AGS	O2B-PB-O3A	3.30	116.18	107.27
4	G	1	AGS	C4-N9-C1'	-3.30	118.93	126.63
4	K	1	AGS	O2G-PG-O3B	3.28	115.60	104.64
4	H	1	AGS	C5-C4-N3	-3.28	122.20	126.72
4	N	1	AGS	C4-N9-C1'	-3.27	118.98	126.63
4	L	1	AGS	C4-N9-C1'	-3.25	119.02	126.63
4	E	1	AGS	O2A-PA-O5'	3.25	122.31	107.57
4	L	1	AGS	O3'-C3'-C4'	-3.25	101.75	111.08
4	H	1	AGS	PB-O3B-PG	-3.20	121.47	133.17
4	E	1	AGS	C5'-C4'-C3'	-3.17	103.79	115.21
4	E	1	AGS	O3G-PG-O3B	3.17	115.23	104.64
4	D	561	AGS	O5'-PA-O1A	-3.15	96.44	108.94
4	A	1	AGS	N9-C8-N7	-3.15	109.47	113.94
4	I	1	AGS	O2B-PB-O3A	3.11	115.67	107.27
4	N	1	AGS	PB-O3B-PG	-3.08	121.90	133.17
4	A	1	AGS	C5-C4-N3	-3.06	122.51	126.72
4	E	1	AGS	C2'-C1'-N9	-3.01	105.83	113.30
4	B	1	AGS	O3B-PB-O1B	3.01	119.75	110.70
4	F	1	AGS	C4-C5-N7	-3.00	107.15	110.58
4	M	1	AGS	C6-C5-N7	2.96	137.80	132.09
4	K	1	AGS	C2-N3-C4	2.96	119.05	111.83
4	A	1	AGS	O4'-C1'-N9	2.94	113.74	108.09
4	M	1	AGS	C6-C5-C4	-2.94	113.17	117.18
4	H	1	AGS	O3G-PG-O3B	2.91	114.35	104.64
4	D	561	AGS	C5'-C4'-C3'	-2.91	104.75	115.21
4	J	1	AGS	O4'-C1'-N9	2.91	113.67	108.09
4	I	1	AGS	C4-N9-C1'	-2.89	119.88	126.63
4	G	1	AGS	C4-C5-N7	-2.88	107.29	110.58
4	F	1	AGS	C2-N3-C4	2.86	118.82	111.83
4	G	1	AGS	O2B-PB-O3A	2.84	114.96	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	561	AGS	O2B-PB-O1B	2.83	125.59	112.44
4	C	1	AGS	C2-N1-C6	2.82	123.36	118.73
4	L	1	AGS	C5-C4-N3	-2.80	122.86	126.72
4	B	1	AGS	C2'-C1'-N9	-2.80	106.35	113.30
4	E	1	AGS	O4'-C1'-C2'	-2.80	100.62	106.62
4	D	561	AGS	O3B-PB-O1B	-2.80	102.28	110.70
4	I	1	AGS	C2-N3-C4	2.79	118.64	111.83
4	M	1	AGS	C4-N9-C1'	-2.78	120.14	126.63
4	I	1	AGS	C5'-C4'-C3'	-2.77	105.22	115.21
4	G	1	AGS	C2-N3-C4	2.77	118.60	111.83
4	J	1	AGS	N3-C4-N9	2.75	131.85	127.17
4	L	1	AGS	C5'-C4'-C3'	-2.74	105.34	115.21
4	C	1	AGS	C5'-C4'-C3'	-2.73	105.39	115.21
4	C	1	AGS	N9-C8-N7	-2.72	110.08	113.94
4	M	1	AGS	C4-N9-C8	2.71	108.59	105.74
4	B	1	AGS	C5'-C4'-C3'	-2.70	105.49	115.21
4	A	1	AGS	O2B-PB-O3B	2.70	114.56	107.27
4	E	1	AGS	O2A-PA-O3A	-2.69	99.99	107.27
4	E	1	AGS	C5-C4-N3	-2.69	123.01	126.72
4	I	1	AGS	C4-C5-N7	-2.68	107.52	110.58
4	C	1	AGS	N3-C4-N9	2.67	131.70	127.17
4	H	1	AGS	C2-N3-C4	2.63	118.25	111.83
4	N	1	AGS	O2A-PA-O1A	2.63	124.67	112.44
4	N	1	AGS	C6-C5-N7	2.62	137.15	132.09
4	E	1	AGS	C3'-C2'-C1'	-2.62	96.51	101.46
4	J	1	AGS	O3B-PB-O1B	-2.61	102.84	110.70
4	I	1	AGS	PB-O3B-PG	-2.61	123.63	133.17
4	G	1	AGS	O3G-PG-O3B	2.60	113.32	104.64
4	J	1	AGS	O2B-PB-O3A	2.57	114.23	107.27
4	G	1	AGS	PB-O3B-PG	-2.57	123.77	133.17
4	K	1	AGS	C5-C4-N9	2.57	108.61	105.81
4	M	1	AGS	C5-C6-N1	2.56	124.02	117.51
4	B	1	AGS	C4-N9-C1'	-2.56	120.65	126.63
4	K	1	AGS	O2A-PA-O5'	2.55	119.12	107.57
4	E	1	AGS	C4-N9-C1'	-2.54	120.69	126.63
4	D	561	AGS	O4'-C1'-N9	2.54	112.96	108.09
4	E	1	AGS	PB-O3B-PG	-2.53	123.90	133.17
4	G	1	AGS	C3'-C2'-C1'	-2.52	96.70	101.46
4	B	1	AGS	C2-N3-C4	2.50	117.94	111.83
4	H	1	AGS	O4'-C1'-N9	2.50	112.89	108.09
4	J	1	AGS	O4'-C1'-C2'	-2.48	101.31	106.62
4	B	1	AGS	O4'-C1'-N9	2.46	112.82	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	AGS	C4-N9-C1'	-2.46	120.88	126.63
4	J	1	AGS	O2A-PA-O3A	-2.44	100.67	107.27
4	L	1	AGS	C6-C5-N7	2.43	136.78	132.09
4	K	1	AGS	O2B-PB-O3A	-2.42	100.73	107.27
4	A	1	AGS	O2G-PG-O3B	2.39	112.63	104.64
4	M	1	AGS	N6-C6-N1	-2.38	113.08	118.38
4	D	561	AGS	O2B-PB-O3A	-2.36	100.89	107.27
4	H	1	AGS	C4-C5-N7	-2.36	107.88	110.58
4	F	1	AGS	C2'-C1'-N9	-2.36	107.44	113.30
4	C	1	AGS	O2B-PB-O3A	2.35	113.61	107.27
4	G	1	AGS	O2A-PA-O5'	2.32	118.10	107.57
4	E	1	AGS	O4'-C4'-C3'	-2.32	100.55	105.15
4	J	1	AGS	C5-C4-N9	2.31	108.33	105.81
4	A	1	AGS	O5'-PA-O1A	-2.30	99.82	108.94
4	L	1	AGS	C4-C5-N7	-2.29	107.97	110.58
4	A	1	AGS	O2A-PA-O5'	2.29	117.93	107.57
4	F	1	AGS	O2B-PB-O3B	2.28	113.43	107.27
4	A	1	AGS	C5-C4-N9	2.27	108.28	105.81
4	I	1	AGS	C1'-N9-C8	2.26	132.12	127.09
4	B	1	AGS	O2B-PB-O3B	-2.26	101.17	107.27
4	H	1	AGS	O3A-PB-O1B	-2.25	103.92	110.70
4	F	1	AGS	O3'-C3'-C4'	-2.24	104.64	111.08
4	H	1	AGS	O2B-PB-O3B	-2.23	101.23	107.27
4	D	561	AGS	O3'-C3'-C4'	-2.23	104.67	111.08
4	I	1	AGS	O2B-PB-O3B	-2.23	101.25	107.27
4	H	1	AGS	C4-N9-C1'	-2.21	121.46	126.63
4	N	1	AGS	N3-C4-N9	2.21	130.93	127.17
4	L	1	AGS	O3A-PA-O1A	2.17	117.24	110.70
4	E	1	AGS	C2'-C3'-C4'	2.17	106.79	102.61
4	L	1	AGS	N3-C4-N9	2.16	130.85	127.17
4	G	1	AGS	O3'-C3'-C4'	-2.16	104.89	111.08
4	I	1	AGS	C4-N9-C8	2.15	108.00	105.74
4	I	1	AGS	C5-C4-N9	2.14	108.14	105.81
4	B	1	AGS	O3A-PB-O1B	2.13	117.12	110.70
4	M	1	AGS	C5-N7-C8	2.13	106.80	103.45
4	A	1	AGS	C1'-N9-C8	2.13	131.82	127.09
4	G	1	AGS	C5'-C4'-C3'	-2.12	107.58	115.21
4	G	1	AGS	O3B-PB-O1B	-2.12	104.33	110.70
4	N	1	AGS	O5'-C5'-C4'	2.11	116.17	108.99
4	K	1	AGS	C4-N9-C8	2.10	107.94	105.74
4	B	1	AGS	O4'-C4'-C3'	2.10	109.32	105.15
4	H	1	AGS	O3'-C3'-C4'	-2.09	105.09	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	AGS	O3G-PG-O3B	2.08	111.58	104.64
4	M	1	AGS	N3-C4-N9	2.07	130.69	127.17
4	B	1	AGS	C4-C5-N7	-2.07	108.21	110.58
4	A	1	AGS	PB-O3B-PG	-2.05	125.67	133.17
4	D	561	AGS	PB-O3B-PG	-2.04	125.70	133.17
4	F	1	AGS	O4'-C1'-C2'	-2.04	102.25	106.62
4	G	1	AGS	C5-C4-N3	-2.03	123.92	126.72
4	A	1	AGS	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	AGS	PB-O3B-PG-O3G
4	B	1	AGS	PB-O3B-PG-O3G
4	C	1	AGS	PB-O3B-PG-O2G
4	C	1	AGS	PB-O3B-PG-O3G
4	D	561	AGS	PB-O3B-PG-O2G
4	D	561	AGS	PB-O3B-PG-O3G
4	E	1	AGS	PB-O3B-PG-O3G
4	F	1	AGS	PB-O3B-PG-O3G
4	G	1	AGS	PB-O3B-PG-O2G
4	G	1	AGS	PB-O3B-PG-O3G
4	H	1	AGS	PB-O3B-PG-O3G
4	I	1	AGS	PB-O3B-PG-O2G
4	I	1	AGS	PB-O3B-PG-O3G
4	J	1	AGS	PB-O3B-PG-O2G
4	J	1	AGS	PB-O3B-PG-O3G
4	K	1	AGS	PB-O3B-PG-O3G
4	M	1	AGS	PB-O3B-PG-O2G
4	M	1	AGS	PB-O3B-PG-O3G
4	N	1	AGS	PB-O3B-PG-O3G
4	E	1	AGS	PB-O3A-PA-O1A
4	F	1	AGS	PA-O3A-PB-O1B
4	B	1	AGS	PA-O3A-PB-O1B
4	L	1	AGS	PA-O3A-PB-O1B
4	H	1	AGS	PB-O3B-PG-O2G
4	A	1	AGS	PA-O3A-PB-O1B
4	D	561	AGS	PA-O3A-PB-O2B
4	E	1	AGS	PA-O3A-PB-O2B
4	K	1	AGS	PA-O3A-PB-O1B
4	M	1	AGS	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1	AGS	PA-O3A-PB-O2B
4	B	1	AGS	PA-O3A-PB-O2B
4	C	1	AGS	PA-O3A-PB-O2B
4	D	561	AGS	PA-O3A-PB-O1B
4	I	1	AGS	PA-O3A-PB-O2B
4	N	1	AGS	PA-O3A-PB-O2B

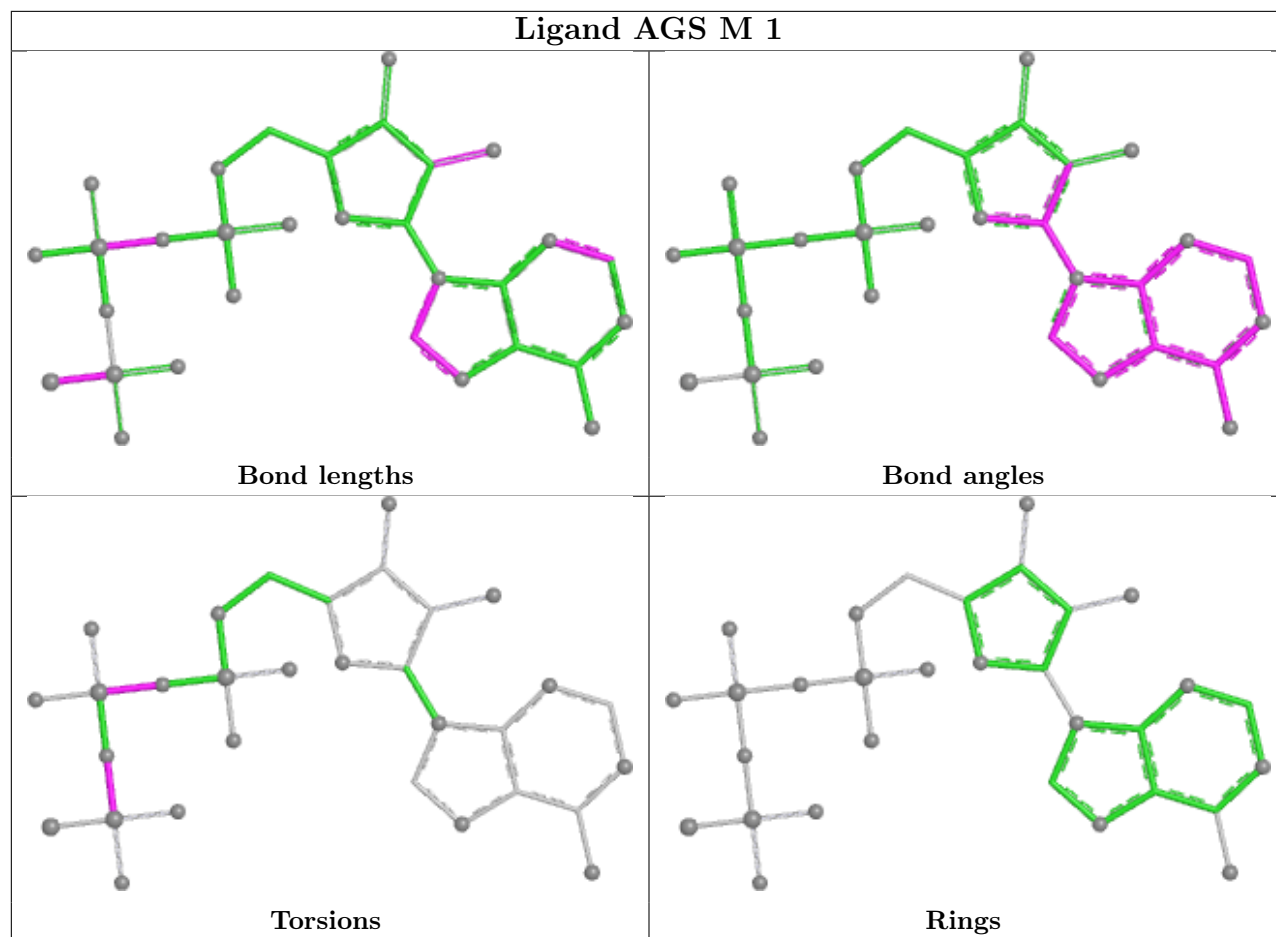
There are no ring outliers.

14 monomers are involved in 50 short contacts:

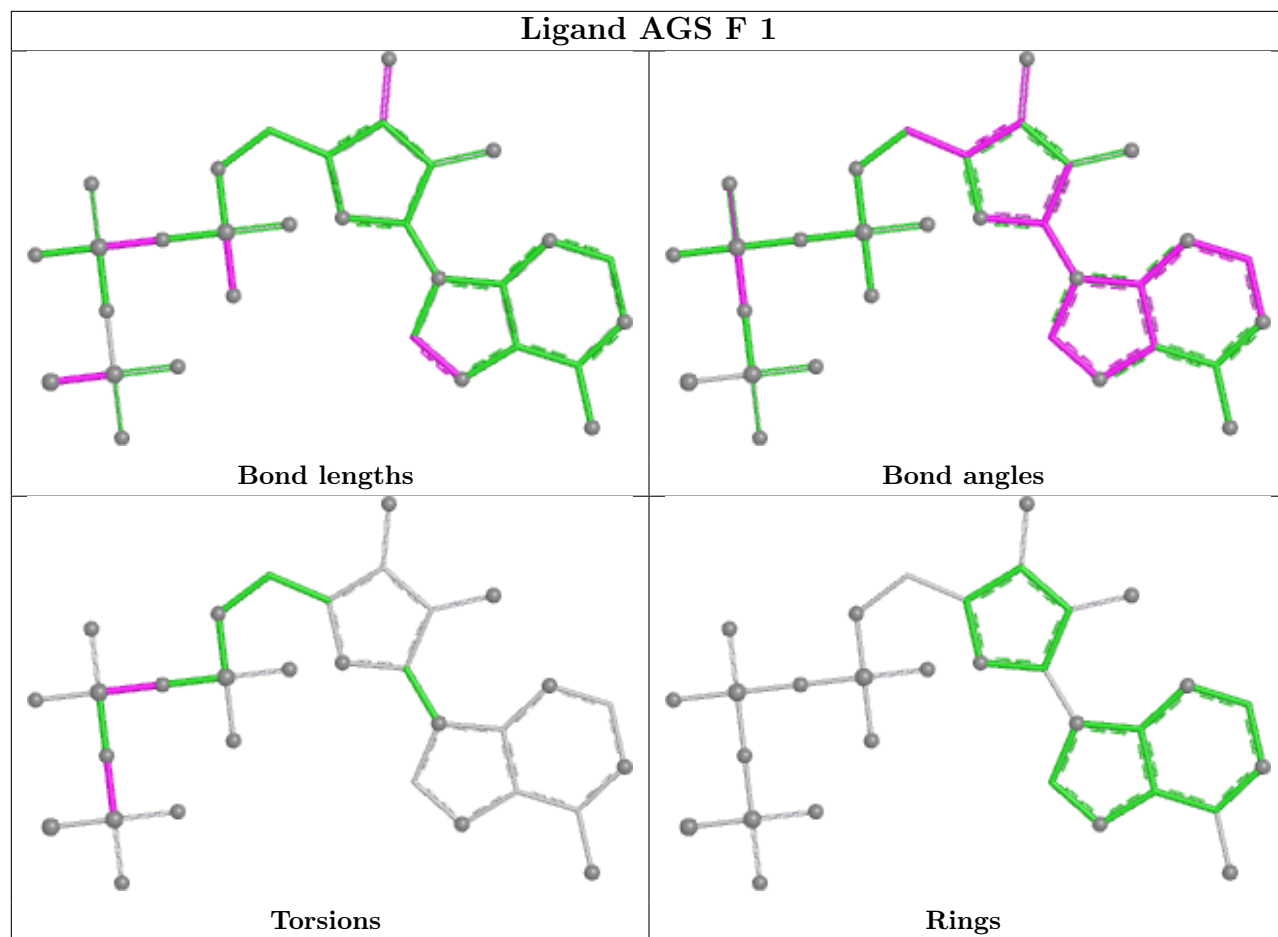
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	AGS	3	0
4	F	1	AGS	4	0
4	G	1	AGS	4	0
4	D	561	AGS	4	0
4	A	1	AGS	3	0
4	H	1	AGS	4	0
4	J	1	AGS	5	0
4	K	1	AGS	2	0
4	I	1	AGS	4	0
4	L	1	AGS	3	0
4	C	1	AGS	2	0
4	N	1	AGS	5	0
4	B	1	AGS	4	0
4	E	1	AGS	3	0

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.

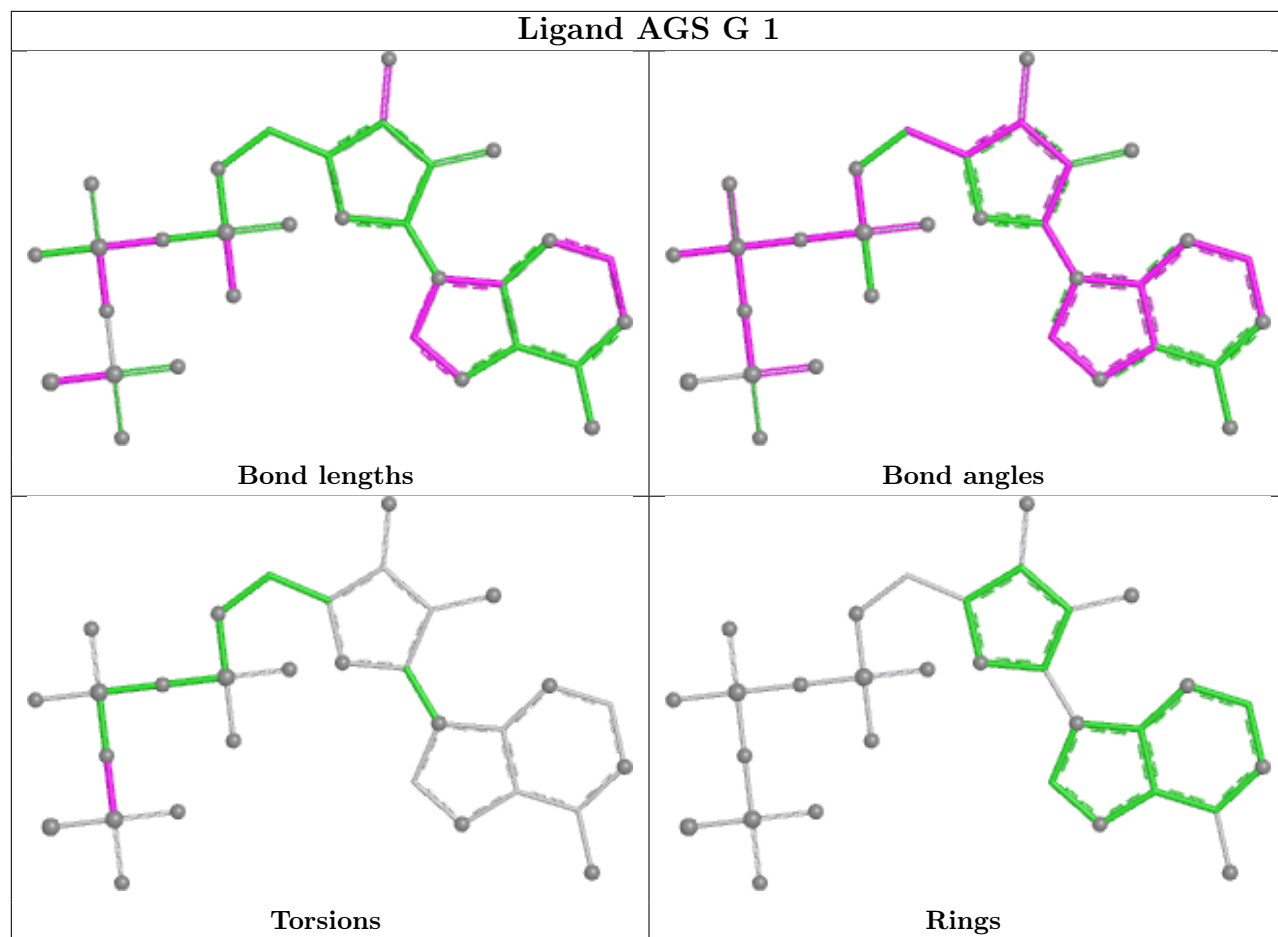
Ligand AGS M 1



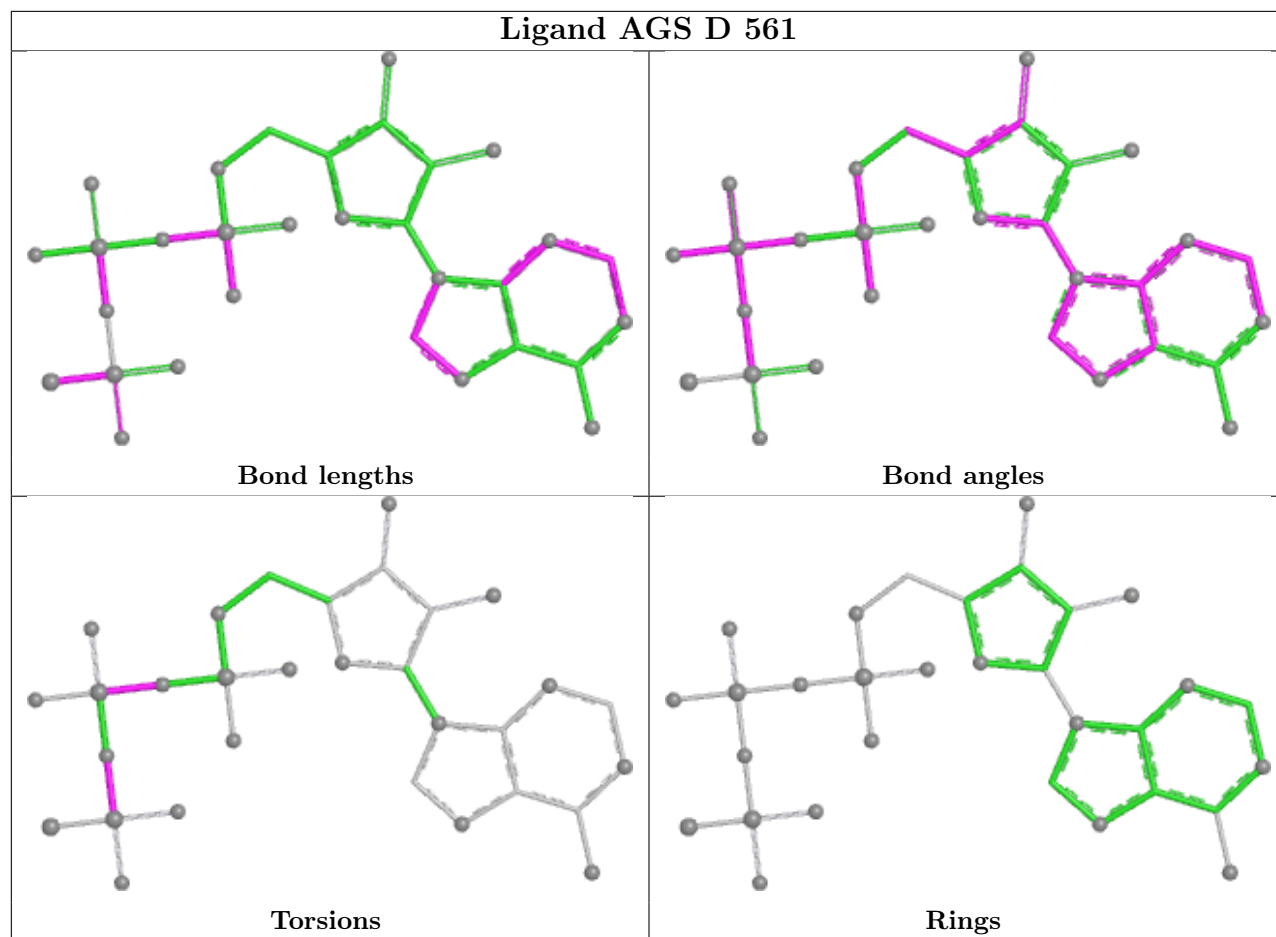
Ligand AGS F 1



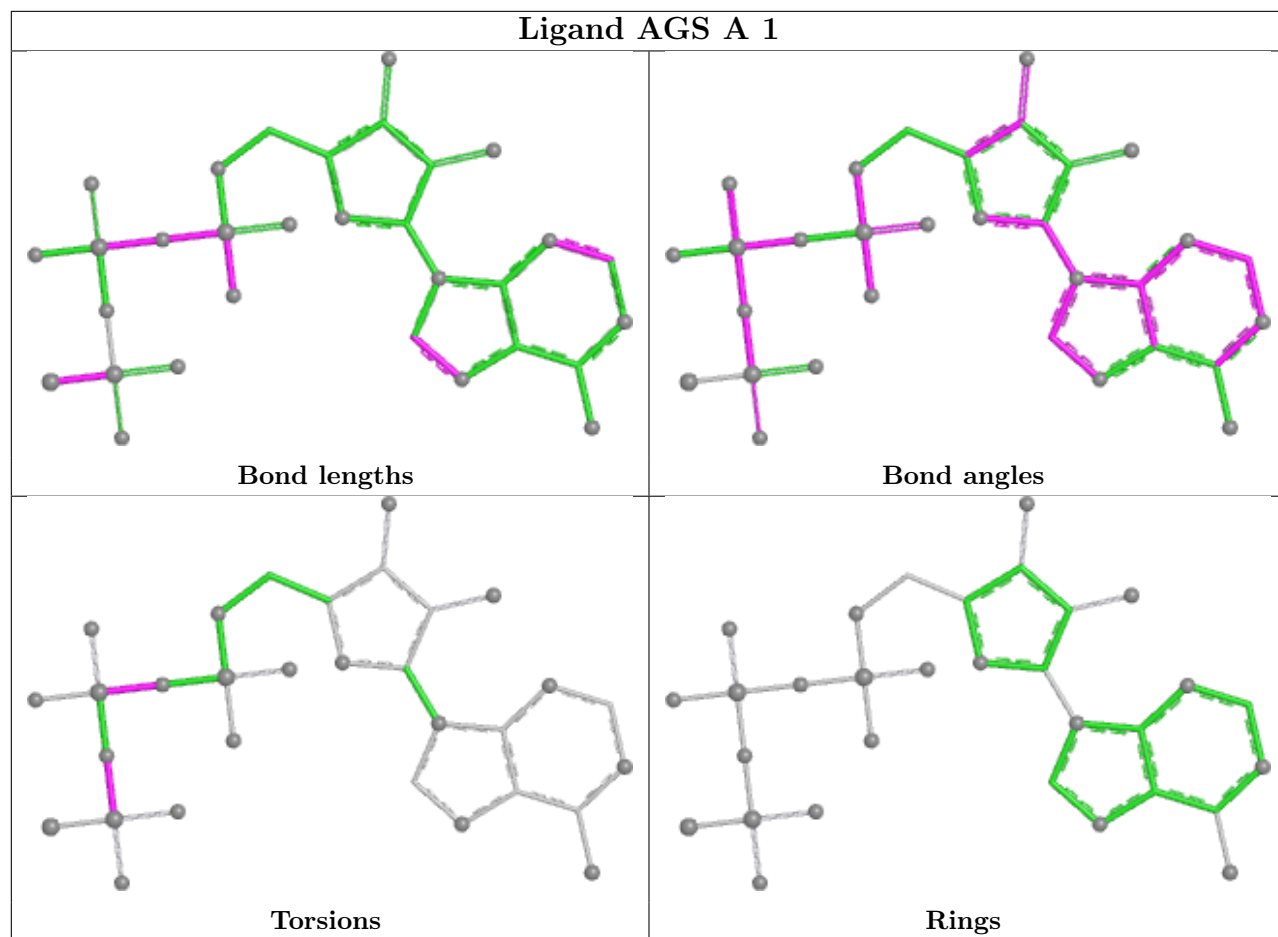
Ligand AGS G 1



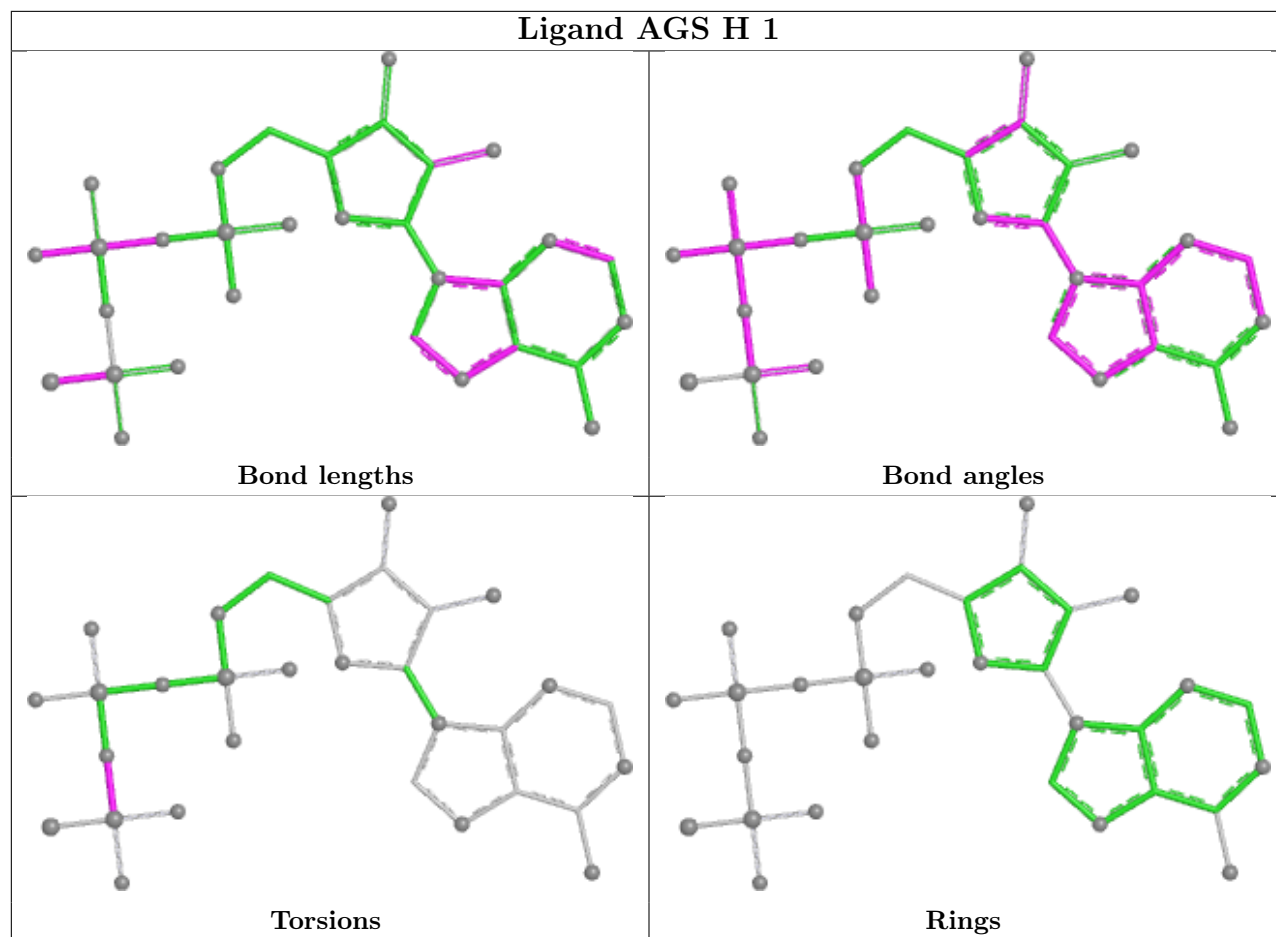
Ligand AGS D 561



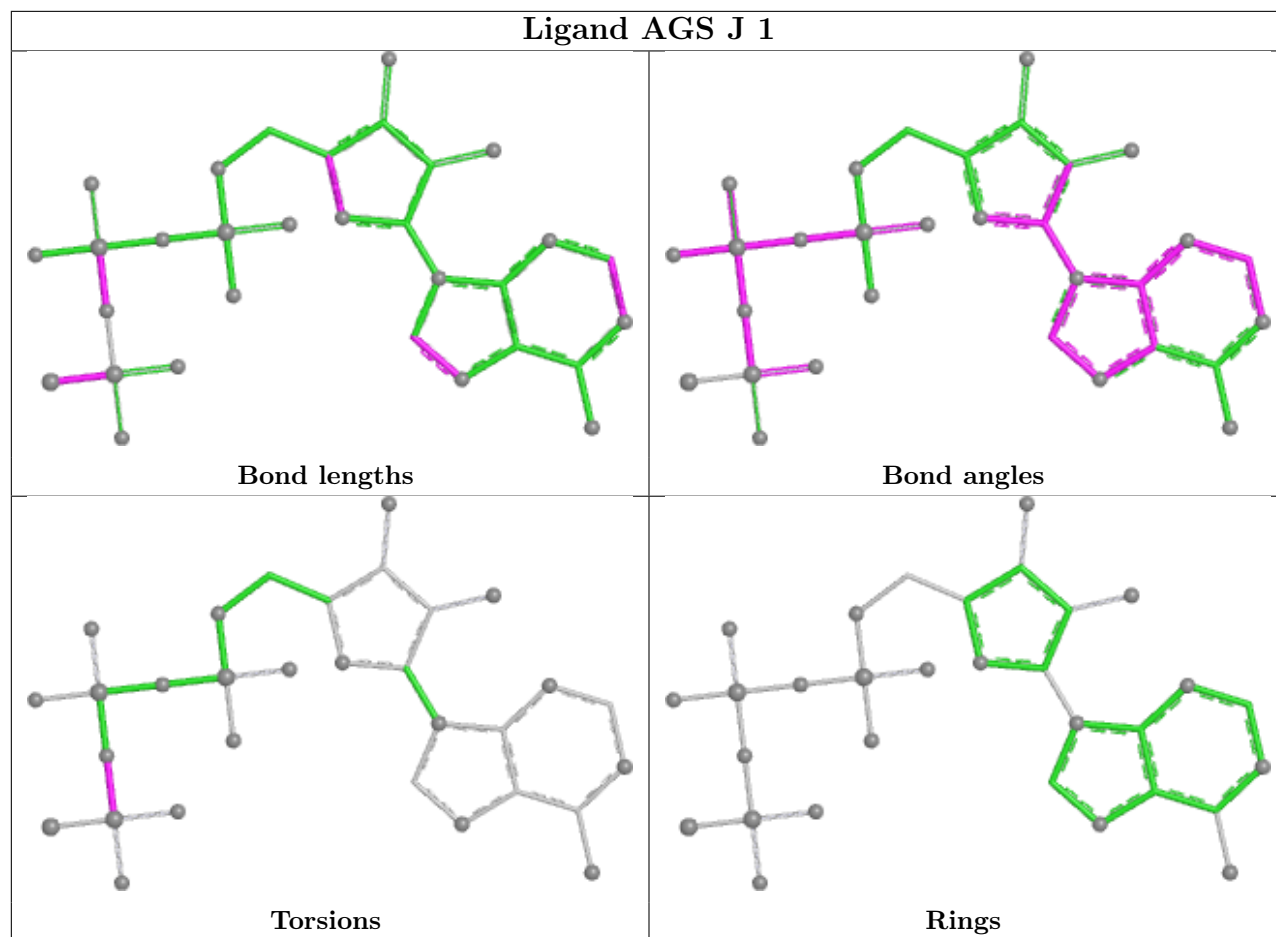
Ligand AGS A 1



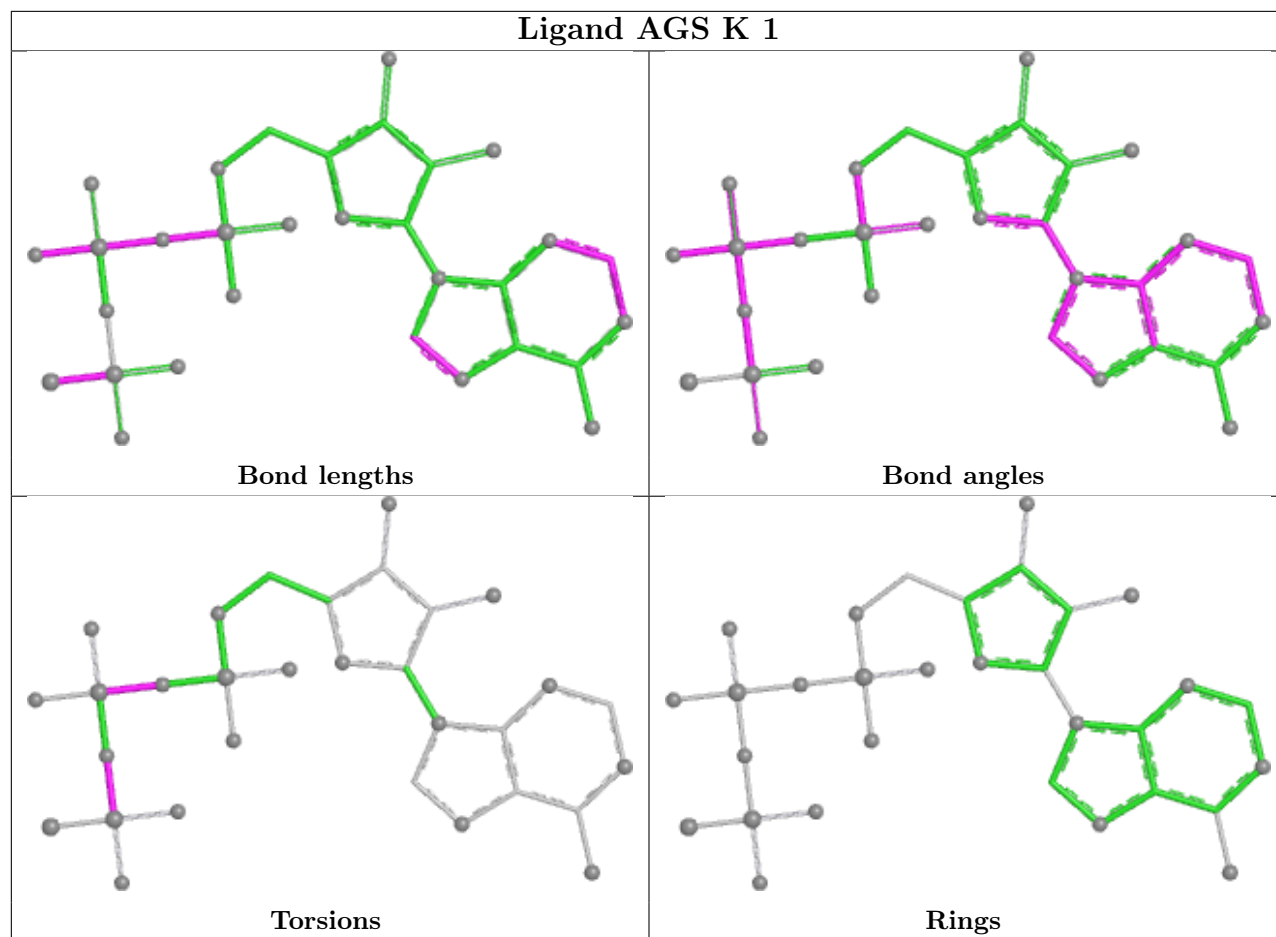
Ligand AGS H 1



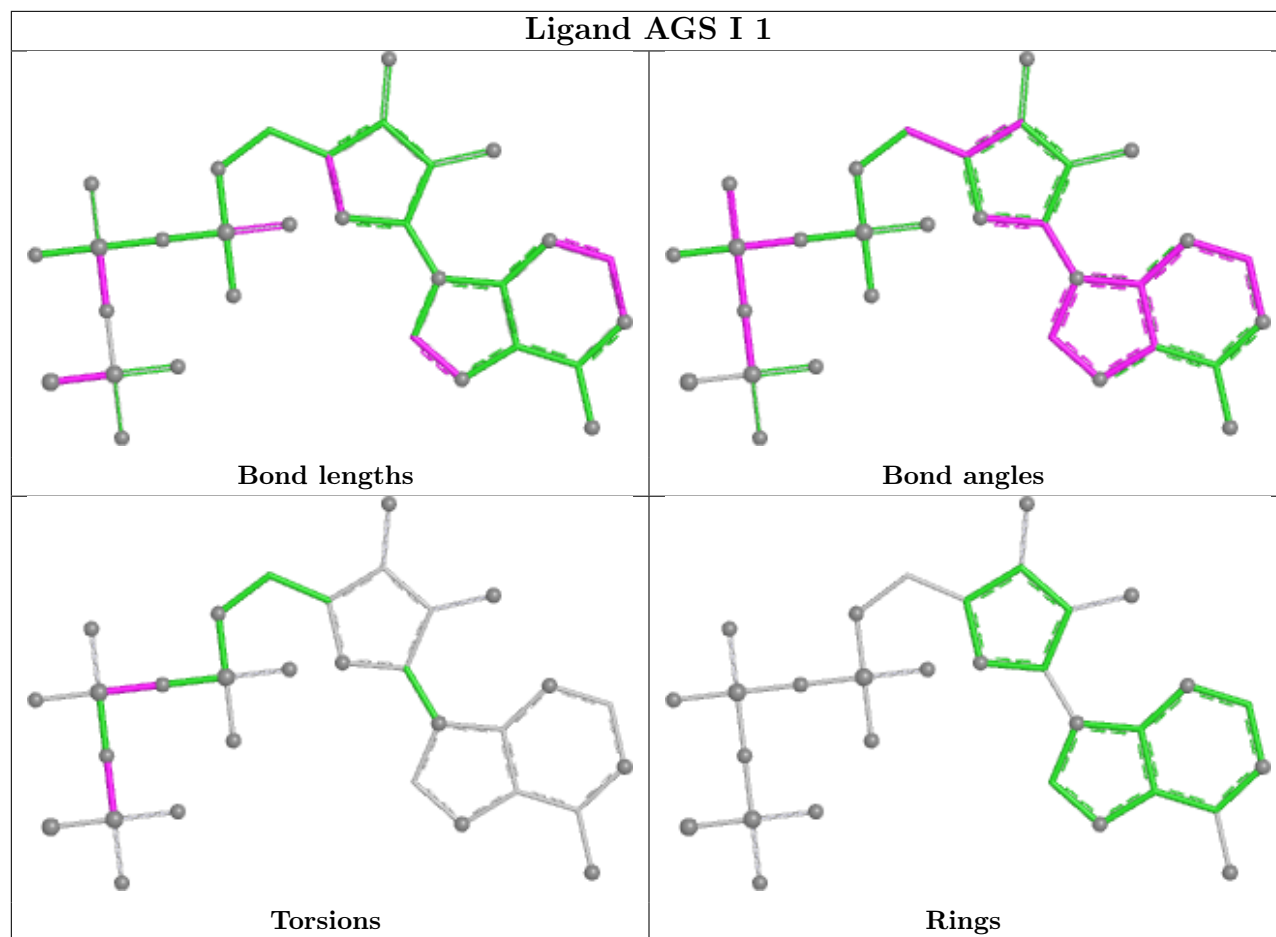
Ligand AGS J 1



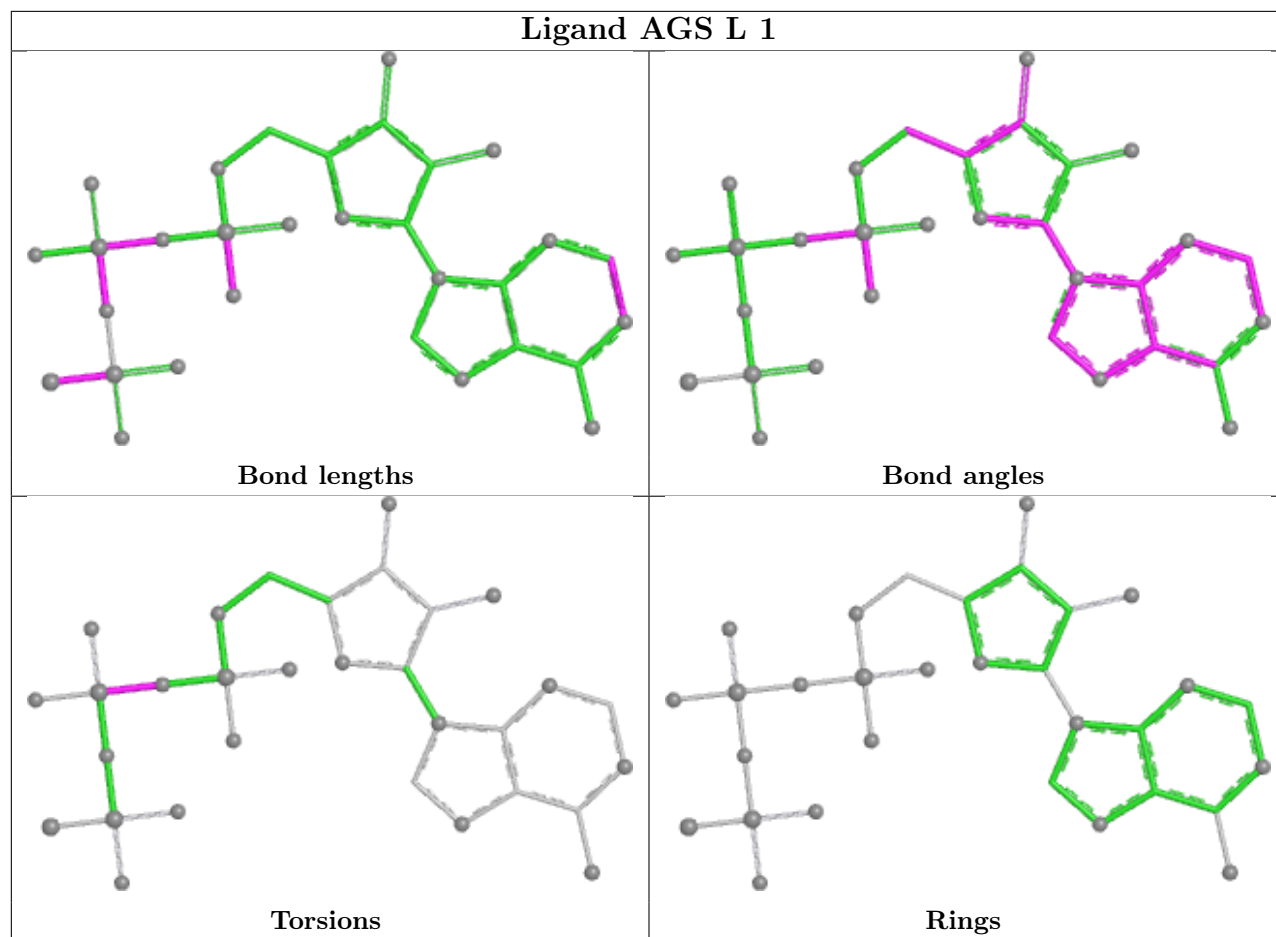
Ligand AGS K 1



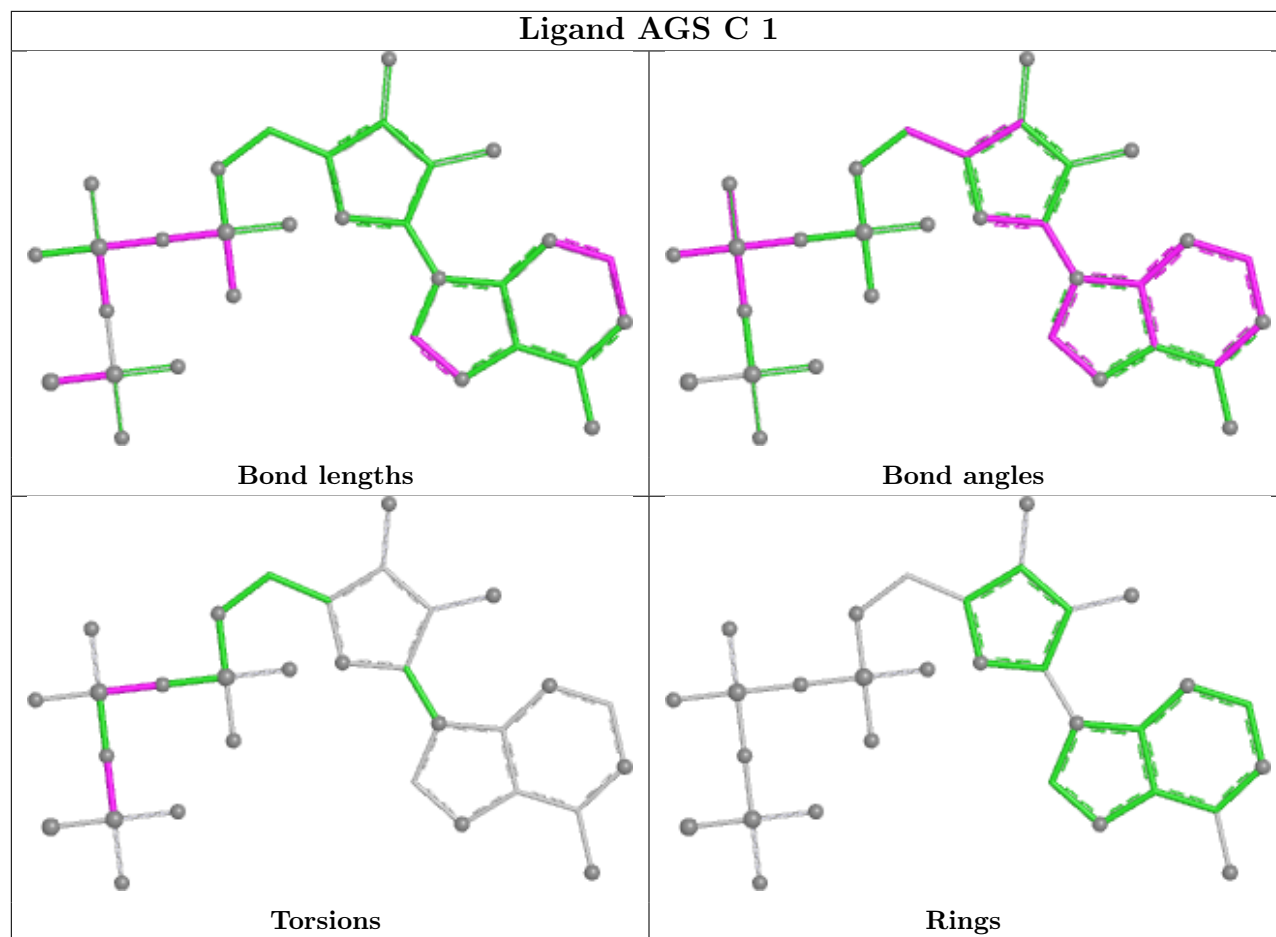
Ligand AGS I 1



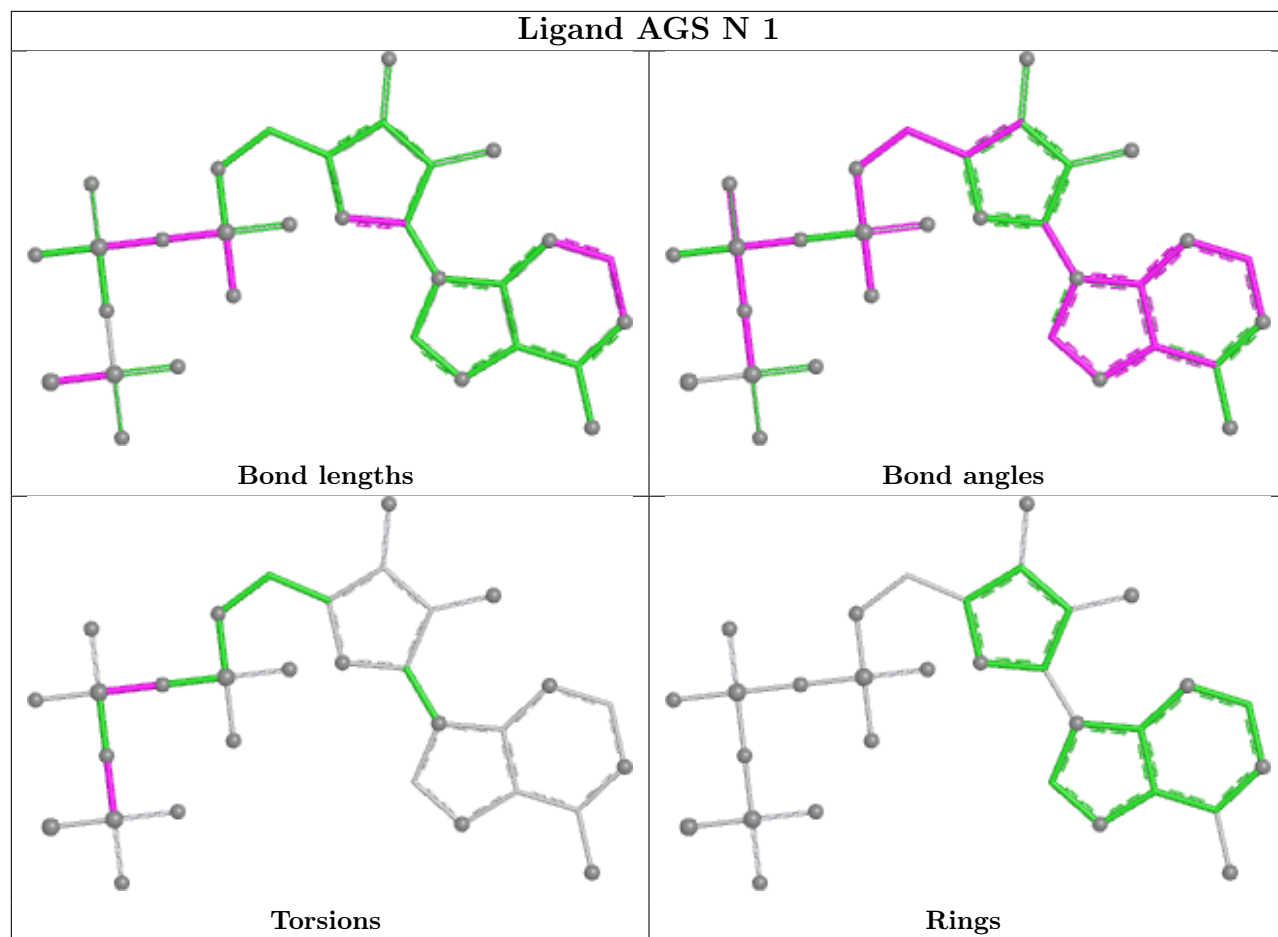
Ligand AGS L 1



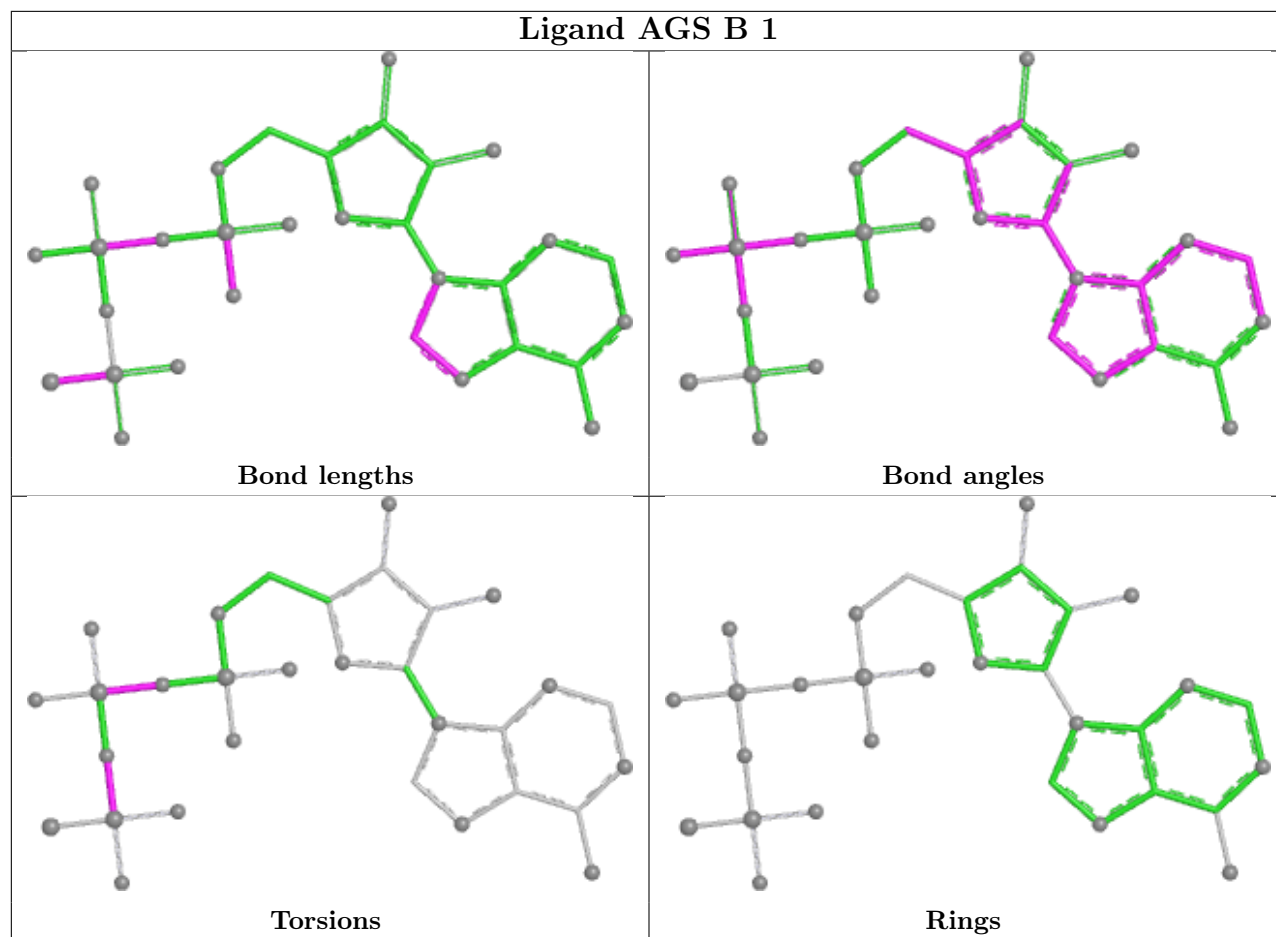
Ligand AGS C 1

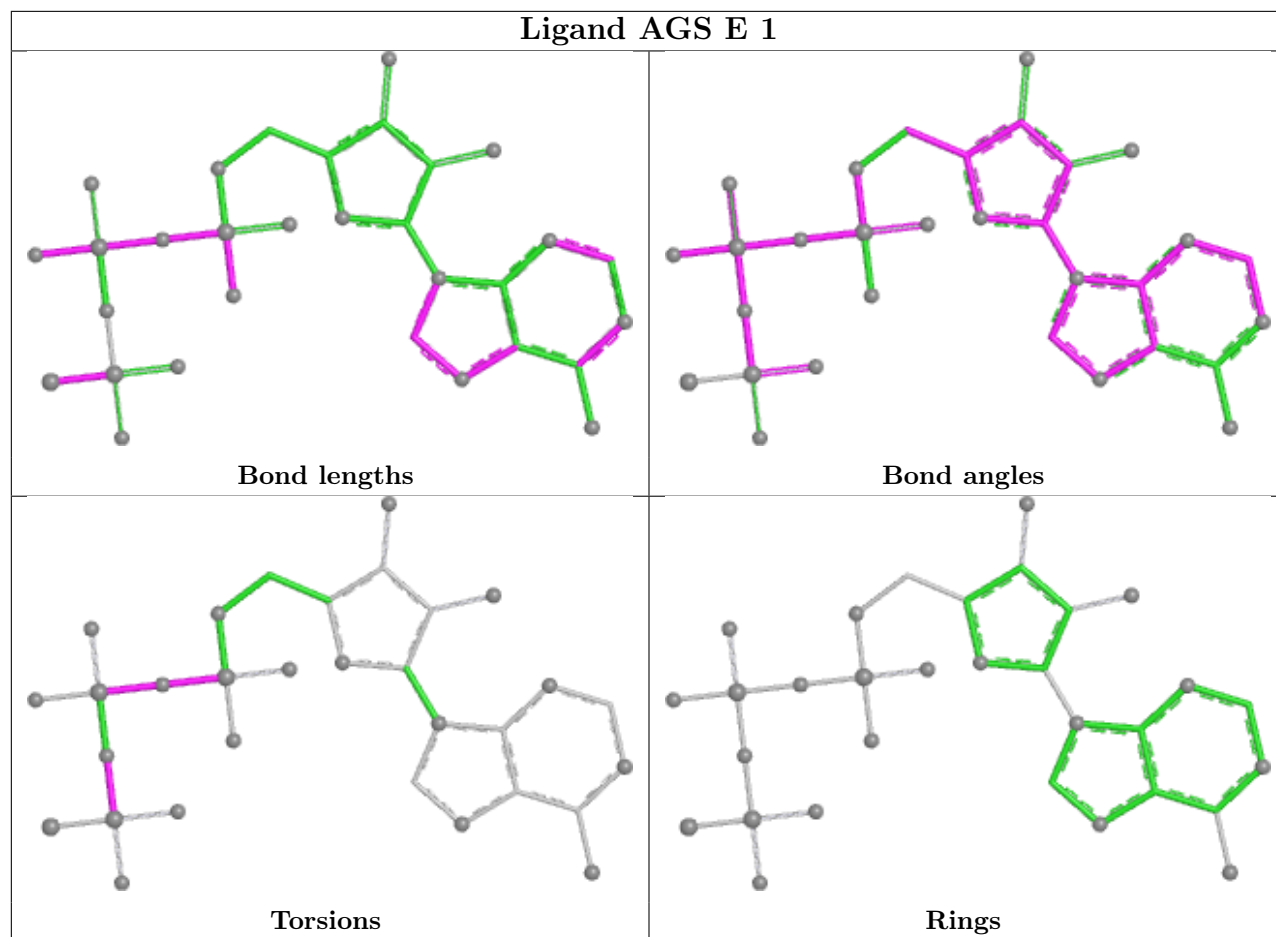


Ligand AGS N 1



Ligand AGS B 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	525/525 (100%)	0.24	33 (6%)	26 24	10, 14, 16, 20	0
1	B	525/525 (100%)	0.41	48 (9%)	15 13	10, 14, 16, 20	0
1	C	525/525 (100%)	0.47	62 (11%)	9 8	10, 14, 16, 20	0
1	D	525/525 (100%)	0.10	23 (4%)	39 38	10, 14, 16, 20	0
1	E	525/525 (100%)	0.24	35 (6%)	24 22	9, 14, 16, 20	0
1	F	525/525 (100%)	0.30	46 (8%)	15 14	10, 14, 16, 20	0
1	G	525/525 (100%)	0.28	28 (5%)	32 31	10, 14, 16, 20	0
1	H	525/525 (100%)	0.21	30 (5%)	29 28	9, 14, 16, 20	0
1	I	525/525 (100%)	0.17	28 (5%)	32 31	9, 14, 16, 20	0
1	J	525/525 (100%)	0.22	19 (3%)	46 45	10, 14, 16, 20	0
1	K	525/525 (100%)	0.47	59 (11%)	10 9	10, 14, 16, 20	0
1	L	525/525 (100%)	0.22	25 (4%)	35 34	10, 14, 16, 20	0
1	M	525/525 (100%)	0.66	77 (14%)	6 5	10, 14, 16, 20	0
1	N	525/525 (100%)	0.09	13 (2%)	58 58	10, 14, 16, 20	0
All	All	7350/7350 (100%)	0.29	526 (7%)	21 20	9, 14, 16, 20	0

All (526) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	231	ARG	6.2
1	B	77	VAL	6.1
1	K	242	LYS	5.8
1	H	44	PHE	5.8
1	M	320	ALA	5.5
1	F	231	ARG	5.5
1	A	387	VAL	5.5
1	F	240	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	223	ALA	5.2
1	M	387	VAL	4.9
1	K	203	TYR	4.9
1	B	349	ILE	4.9
1	G	44	PHE	4.9
1	B	182	GLY	4.8
1	K	335	GLY	4.8
1	M	256	GLY	4.8
1	M	335	GLY	4.7
1	C	231	ARG	4.7
1	D	526	LYS	4.7
1	M	223	ALA	4.6
1	I	270	ILE	4.6
1	K	231	ARG	4.5
1	E	264	VAL	4.5
1	E	387	VAL	4.5
1	L	231	ARG	4.5
1	C	292	ILE	4.4
1	C	242	LYS	4.4
1	H	297	GLY	4.3
1	F	233	MET	4.3
1	I	305	ILE	4.3
1	B	44	PHE	4.2
1	C	340	ALA	4.2
1	A	383	ALA	4.2
1	C	349	ILE	4.2
1	B	203	TYR	4.2
1	C	305	ILE	4.2
1	K	188	ASP	4.2
1	H	264	VAL	4.1
1	K	340	ALA	4.1
1	M	268	ARG	4.1
1	M	181	THR	4.1
1	M	218	PRO	4.1
1	H	231	ARG	4.0
1	F	311	LYS	4.0
1	H	526	LYS	4.0
1	L	242	LYS	4.0
1	K	341	ALA	3.9
1	G	525	PRO	3.9
1	F	219	PHE	3.9
1	K	160	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	177	VAL	3.9
1	K	349	ILE	3.9
1	C	203	TYR	3.8
1	M	386	GLU	3.8
1	N	263	VAL	3.8
1	B	293	ALA	3.8
1	M	333	ILE	3.7
1	M	383	ALA	3.7
1	M	385	THR	3.7
1	J	248	LEU	3.7
1	K	234	LEU	3.7
1	J	305	ILE	3.7
1	A	187	LEU	3.7
1	C	234	LEU	3.7
1	F	309	LEU	3.7
1	M	234	LEU	3.7
1	A	378	VAL	3.7
1	C	254	VAL	3.7
1	C	180	GLY	3.7
1	N	526	LYS	3.6
1	M	394	ALA	3.6
1	B	231	ARG	3.6
1	M	189	VAL	3.6
1	C	44	PHE	3.6
1	B	526	LYS	3.6
1	M	221	LEU	3.5
1	D	271	VAL	3.5
1	F	214	GLU	3.5
1	K	181	THR	3.5
1	H	335	GLY	3.5
1	K	334	ASP	3.5
1	G	189	VAL	3.5
1	M	272	LYS	3.5
1	I	266	THR	3.5
1	K	331	THR	3.5
1	M	340	ALA	3.5
1	G	267	MET	3.4
1	I	44	PHE	3.4
1	E	136	VAL	3.4
1	C	334	ASP	3.4
1	M	334	ASP	3.4
1	J	233	MET	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	270	ILE	3.4
1	M	305	ILE	3.4
1	H	203	TYR	3.3
1	C	174	VAL	3.3
1	C	249	ILE	3.3
1	B	134	LEU	3.3
1	K	268	ARG	3.3
1	A	263	VAL	3.3
1	K	271	VAL	3.3
1	K	219	PHE	3.3
1	M	264	VAL	3.2
1	F	242	LYS	3.2
1	G	182	GLY	3.2
1	E	172	GLU	3.2
1	K	311	LYS	3.2
1	M	384	ALA	3.2
1	B	240	VAL	3.2
1	G	378	VAL	3.2
1	A	394	ALA	3.2
1	F	383	ALA	3.2
1	F	230	ILE	3.2
1	A	284	ARG	3.2
1	A	209	GLU	3.2
1	J	526	LYS	3.2
1	E	526	LYS	3.1
1	G	526	LYS	3.1
1	H	525	PRO	3.1
1	B	258	ALA	3.1
1	E	273	VAL	3.1
1	M	323	VAL	3.1
1	N	349	ILE	3.1
1	F	182	GLY	3.1
1	B	189	VAL	3.1
1	K	264	VAL	3.1
1	A	375	GLY	3.1
1	G	357	THR	3.1
1	F	44	PHE	3.1
1	J	44	PHE	3.1
1	I	268	ARG	3.1
1	E	78	ALA	3.1
1	I	239	ALA	3.1
1	G	271	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	270	ILE	3.1
1	D	44	PHE	3.0
1	C	255	GLU	3.0
1	H	242	LYS	3.0
1	J	384	ALA	3.0
1	C	307	MET	3.0
1	K	381	VAL	3.0
1	H	198	GLY	3.0
1	F	222	LEU	3.0
1	K	227	ILE	3.0
1	M	249	ILE	3.0
1	F	256	GLY	3.0
1	I	265	ASN	3.0
1	M	238	GLU	3.0
1	A	176	THR	3.0
1	A	44	PHE	3.0
1	N	44	PHE	3.0
1	E	233	MET	3.0
1	C	268	ARG	3.0
1	I	240	VAL	3.0
1	A	214	GLU	3.0
1	C	270	ILE	3.0
1	E	242	LYS	3.0
1	G	174	VAL	2.9
1	J	333	ILE	2.9
1	K	270	ILE	2.9
1	M	175	ILE	2.9
1	F	385	THR	2.9
1	C	311	LYS	2.9
1	I	269	GLY	2.9
1	C	300	VAL	2.9
1	D	301	ILE	2.9
1	L	301	ILE	2.9
1	M	379	ILE	2.9
1	F	180	GLY	2.9
1	F	237	LEU	2.9
1	K	387	VAL	2.9
1	E	394	ALA	2.9
1	B	365	LEU	2.8
1	I	233	MET	2.8
1	I	267	MET	2.8
1	K	237	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	305	ILE	2.8
1	K	162	ILE	2.8
1	C	526	LYS	2.8
1	K	244	GLY	2.8
1	K	305	ILE	2.8
1	E	44	PHE	2.8
1	J	334	ASP	2.8
1	G	269	GLY	2.8
1	C	356	ALA	2.8
1	L	174	VAL	2.8
1	G	227	ILE	2.8
1	M	270	ILE	2.8
1	M	217	SER	2.8
1	B	260	ALA	2.8
1	D	254	VAL	2.8
1	H	254	VAL	2.8
1	C	301	ILE	2.8
1	M	349	ILE	2.8
1	A	335	GLY	2.7
1	M	327	LYS	2.7
1	J	208	PRO	2.7
1	M	263	VAL	2.7
1	H	227	ILE	2.7
1	A	223	ALA	2.7
1	C	181	THR	2.7
1	C	262	LEU	2.7
1	F	317	LEU	2.7
1	M	262	LEU	2.7
1	M	203	TYR	2.7
1	C	191	GLU	2.7
1	C	264	VAL	2.7
1	E	396	VAL	2.7
1	K	236	VAL	2.7
1	D	227	ILE	2.7
1	F	241	ALA	2.7
1	H	241	ALA	2.7
1	K	377	ALA	2.7
1	E	309	LEU	2.7
1	B	129	GLU	2.7
1	I	203	TYR	2.7
1	B	387	VAL	2.7
1	E	271	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	349	ILE	2.7
1	H	270	ILE	2.7
1	I	230	ILE	2.7
1	L	313	THR	2.6
1	M	283	ASP	2.6
1	C	327	LYS	2.6
1	C	387	VAL	2.6
1	F	387	VAL	2.6
1	H	190	VAL	2.6
1	J	231	ARG	2.6
1	M	267	MET	2.6
1	K	320	ALA	2.6
1	J	349	ILE	2.6
1	D	375	GLY	2.6
1	I	211	GLY	2.6
1	C	313	THR	2.6
1	M	377	ALA	2.6
1	B	202	PRO	2.6
1	J	309	LEU	2.6
1	M	242	LYS	2.6
1	A	379	ILE	2.6
1	B	342	ILE	2.6
1	F	249	ILE	2.6
1	I	272	LYS	2.6
1	L	312	ALA	2.6
1	E	490	ASP	2.6
1	B	262	LEU	2.6
1	M	228	SER	2.6
1	E	250	ILE	2.5
1	F	349	ILE	2.5
1	G	190	VAL	2.5
1	J	271	VAL	2.5
1	N	77	VAL	2.5
1	A	244	GLY	2.5
1	B	384	ALA	2.5
1	D	266	THR	2.5
1	L	357	THR	2.5
1	C	184	GLN	2.5
1	K	248	LEU	2.5
1	D	189	VAL	2.5
1	L	230	ILE	2.5
1	F	266	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	228	SER	2.5
1	B	256	GLY	2.5
1	F	189	VAL	2.5
1	J	264	VAL	2.5
1	K	254	VAL	2.5
1	M	336	VAL	2.5
1	F	360	TYR	2.5
1	M	303	GLU	2.5
1	B	223	ALA	2.5
1	K	275	ALA	2.5
1	C	289	LEU	2.5
1	N	314	LEU	2.5
1	G	231	ARG	2.5
1	E	269	GLY	2.5
1	A	264	VAL	2.4
1	C	236	VAL	2.4
1	K	191	GLU	2.4
1	H	43	SER	2.4
1	M	176	THR	2.4
1	H	384	ALA	2.4
1	M	251	ALA	2.4
1	I	526	LYS	2.4
1	K	200	LEU	2.4
1	M	309	LEU	2.4
1	M	314	LEU	2.4
1	B	374	GLY	2.4
1	K	269	GLY	2.4
1	L	256	GLY	2.4
1	B	206	ASN	2.4
1	D	363	GLU	2.4
1	F	292	ILE	2.4
1	F	308	GLU	2.4
1	M	254	VAL	2.4
1	K	141	SER	2.4
1	M	266	THR	2.4
1	D	284	ARG	2.4
1	H	311	LYS	2.4
1	I	260	ALA	2.4
1	M	187	LEU	2.4
1	C	375	GLY	2.4
1	K	283	ASP	2.4
1	A	353	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	174	VAL	2.4
1	H	300	VAL	2.4
1	M	346	VAL	2.4
1	B	312	ALA	2.4
1	H	314	LEU	2.4
1	K	262	LEU	2.4
1	M	248	LEU	2.4
1	K	238	GLU	2.4
1	G	282	GLY	2.4
1	A	175	ILE	2.4
1	B	233	MET	2.4
1	G	236	VAL	2.4
1	N	300	VAL	2.4
1	I	255	GLU	2.3
1	C	306	GLY	2.3
1	C	155	ASP	2.3
1	F	283	ASP	2.3
1	C	277	LYS	2.3
1	M	225	LYS	2.3
1	M	307	MET	2.3
1	I	325	ILE	2.3
1	A	271	VAL	2.3
1	K	276	VAL	2.3
1	K	369	VAL	2.3
1	D	357	THR	2.3
1	M	255	GLU	2.3
1	F	340	ALA	2.3
1	K	152	ALA	2.3
1	M	360	TYR	2.3
1	A	234	LEU	2.3
1	C	221	LEU	2.3
1	F	382	GLY	2.3
1	G	234	LEU	2.3
1	H	309	LEU	2.3
1	M	372	LEU	2.3
1	D	58	ARG	2.3
1	F	389	MET	2.3
1	C	281	PHE	2.3
1	B	43	SER	2.3
1	F	342	ILE	2.3
1	A	189	VAL	2.3
1	A	254	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	376	VAL	2.3
1	G	172	GLU	2.3
1	M	216	GLU	2.3
1	K	235	PRO	2.3
1	A	243	ALA	2.3
1	B	244	GLY	2.3
1	B	284	ARG	2.3
1	C	295	LEU	2.3
1	D	269	GLY	2.3
1	D	398	ASP	2.3
1	E	234	LEU	2.3
1	F	335	GLY	2.3
1	K	88	GLY	2.3
1	M	337	GLY	2.3
1	E	342	ILE	2.3
1	F	175	ILE	2.3
1	F	333	ILE	2.3
1	K	292	ILE	2.3
1	M	332	ILE	2.3
1	C	189	VAL	2.3
1	C	273	VAL	2.3
1	G	254	VAL	2.3
1	K	174	VAL	2.3
1	A	402	ALA	2.3
1	B	133	ALA	2.3
1	C	283	ASP	2.3
1	H	277	LYS	2.3
1	I	258	ALA	2.3
1	M	317	LEU	2.3
1	L	172	GLU	2.2
1	A	305	ILE	2.2
1	B	270	ILE	2.2
1	C	333	ILE	2.2
1	J	270	ILE	2.2
1	I	202	PRO	2.2
1	M	208	PRO	2.2
1	M	236	VAL	2.2
1	A	58	ARG	2.2
1	M	526	LYS	2.2
1	C	280	GLY	2.2
1	E	337	GLY	2.2
1	K	258	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	203	TYR	2.2
1	A	391	GLU	2.2
1	B	175	ILE	2.2
1	C	229	ASN	2.2
1	K	175	ILE	2.2
1	K	342	ILE	2.2
1	L	240	VAL	2.2
1	F	280	GLY	2.2
1	M	182	GLY	2.2
1	B	130	GLU	2.2
1	E	356	ALA	2.2
1	E	373	ALA	2.2
1	F	275	ALA	2.2
1	M	356	ALA	2.2
1	F	215	LEU	2.2
1	M	289	LEU	2.2
1	L	184	GLN	2.2
1	E	203	TYR	2.2
1	L	203	TYR	2.2
1	C	210	THR	2.2
1	G	305	ILE	2.2
1	J	385	THR	2.2
1	K	185	ASP	2.2
1	K	379	ILE	2.2
1	B	264	VAL	2.2
1	C	369	VAL	2.2
1	D	264	VAL	2.2
1	H	387	VAL	2.2
1	I	271	VAL	2.2
1	J	158	VAL	2.2
1	L	264	VAL	2.2
1	B	282	GLY	2.2
1	E	339	GLU	2.2
1	M	191	GLU	2.2
1	F	251	ALA	2.2
1	G	377	ALA	2.2
1	L	384	ALA	2.2
1	K	401	HIS	2.2
1	C	200	LEU	2.2
1	C	222	LEU	2.2
1	C	299	THR	2.2
1	D	359	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	191	GLU	2.1
1	B	204	PHE	2.1
1	B	257	GLU	2.1
1	L	333	ILE	2.1
1	N	281	PHE	2.1
1	F	346	VAL	2.1
1	B	180	GLY	2.1
1	K	306	GLY	2.1
1	B	259	LEU	2.1
1	D	473	ASP	2.1
1	C	266	THR	2.1
1	N	525	PRO	2.1
1	B	230	ILE	2.1
1	G	230	ILE	2.1
1	G	270	ILE	2.1
1	G	325	ILE	2.1
1	L	44	PHE	2.1
1	B	211	GLY	2.1
1	F	271	VAL	2.1
1	H	177	VAL	2.1
1	A	341	ALA	2.1
1	M	243	ALA	2.1
1	N	383	ALA	2.1
1	I	242	LYS	2.1
1	G	358	SER	2.1
1	J	234	LEU	2.1
1	K	139	SER	2.1
1	K	247	LEU	2.1
1	I	310	GLU	2.1
1	F	261	THR	2.1
1	H	266	THR	2.1
1	M	210	THR	2.1
1	E	318	GLY	2.1
1	H	301	ILE	2.1
1	L	175	ILE	2.1
1	M	159	GLY	2.1
1	D	281	PHE	2.1
1	B	136	VAL	2.1
1	C	77	VAL	2.1
1	F	174	VAL	2.1
1	C	286	LYS	2.1
1	M	311	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	165	ALA	2.1
1	C	217	SER	2.1
1	I	234	LEU	2.1
1	L	234	LEU	2.1
1	M	222	LEU	2.1
1	C	308	GLU	2.1
1	D	214	GLU	2.1
1	E	216	GLU	2.1
1	H	156	GLU	2.1
1	I	238	GLU	2.1
1	L	224	ASP	2.1
1	F	203	TYR	2.1
1	M	322	ARG	2.1
1	B	311	LYS	2.1
1	D	325	ILE	2.1
1	E	230	ILE	2.1
1	E	292	ILE	2.1
1	C	271	VAL	2.1
1	E	158	VAL	2.1
1	E	254	VAL	2.1
1	H	189	VAL	2.1
1	L	254	VAL	2.1
1	L	271	VAL	2.1
1	M	378	VAL	2.1
1	D	339	GLU	2.0
1	H	172	GLU	2.0
1	I	341	ALA	2.1
1	K	166	MET	2.0
1	N	308	GLU	2.0
1	G	283	ASP	2.0
1	N	350	ARG	2.0
1	G	353	ILE	2.0
1	N	301	ILE	2.0
1	E	240	VAL	2.0
1	F	178	GLU	2.0
1	G	209	GLU	2.0
1	J	77	VAL	2.0
1	K	386	GLU	2.0
1	L	381	VAL	2.0
1	M	190	VAL	2.0
1	D	228	SER	2.0
1	F	228	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	243	ALA	2.0
1	K	243	ALA	2.0
1	M	152	ALA	2.0
1	A	259	LEU	2.0
1	C	161	LEU	2.0
1	E	222	LEU	2.0
1	L	185	ASP	2.0
1	B	362	ARG	2.0
1	C	284	ARG	2.0
1	K	357	THR	2.0
1	A	173	GLY	2.0
1	B	306	GLY	2.0
1	C	337	GLY	2.0
1	M	269	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
2	MG	L	550	1/1	0.93	0.03	9,9,9,9	0
4	AGS	E	1	31/31	0.95	0.06	2,11,19,20	0
4	AGS	G	1	31/31	0.95	0.05	4,9,16,16	0
4	AGS	J	1	31/31	0.95	0.06	2,7,14,15	0
4	AGS	K	1	31/31	0.95	0.06	6,14,21,24	0
4	AGS	L	1	31/31	0.95	0.06	2,8,11,18	0
4	AGS	M	1	31/31	0.95	0.05	5,12,18,21	0
4	AGS	I	1	31/31	0.96	0.05	5,12,16,20	0
4	AGS	D	561	31/31	0.96	0.05	2,11,18,21	0

Continued on next page...

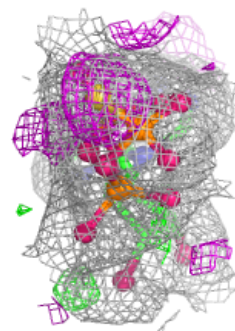
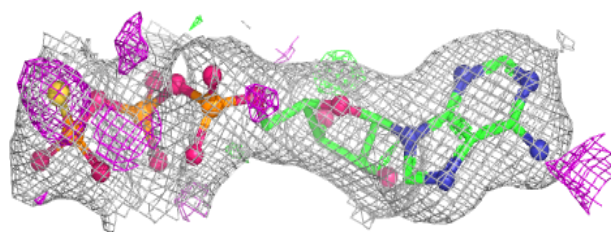
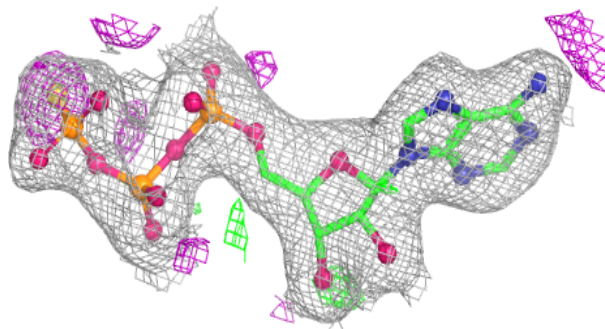
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	N	550	1/1	0.96	0.04	7,7,7,7	0
4	AGS	F	1	31/31	0.96	0.05	2,11,22,23	0
4	AGS	C	1	31/31	0.96	0.05	8,13,19,20	0
4	AGS	N	1	31/31	0.96	0.06	4,10,17,19	0
3	K	B	560	1/1	0.97	0.05	13,13,13,13	0
3	K	D	1	1/1	0.97	0.22	29,29,29,29	0
3	K	E	560	1/1	0.97	0.02	11,11,11,11	0
3	K	F	560	1/1	0.97	0.03	13,13,13,13	0
4	AGS	H	1	31/31	0.97	0.04	3,9,15,17	0
3	K	L	560	1/1	0.97	0.04	6,6,6,6	0
3	K	M	560	1/1	0.97	0.02	14,14,14,14	0
3	K	N	560	1/1	0.97	0.02	11,11,11,11	0
4	AGS	A	1	31/31	0.97	0.04	4,11,16,20	0
4	AGS	B	1	31/31	0.97	0.05	8,13,21,24	0
2	MG	A	550	1/1	0.97	0.02	7,7,7,7	0
2	MG	B	550	1/1	0.98	0.02	8,8,8,8	0
2	MG	M	550	1/1	0.98	0.01	7,7,7,7	0
3	K	G	560	1/1	0.98	0.02	16,16,16,16	0
3	K	J	560	1/1	0.98	0.02	11,11,11,11	0
3	K	K	560	1/1	0.98	0.05	11,11,11,11	0
2	MG	E	550	1/1	0.98	0.02	6,6,6,6	0
3	K	A	560	1/1	0.98	0.02	13,13,13,13	0
2	MG	H	550	1/1	0.98	0.04	4,4,4,4	0
2	MG	J	550	1/1	0.98	0.02	8,8,8,8	0
3	K	D	560	1/1	0.98	0.03	16,16,16,16	0
3	K	E	527	1/1	0.98	0.03	31,31,31,31	0
2	MG	K	550	1/1	0.99	0.04	7,7,7,7	0
2	MG	F	550	1/1	0.99	0.03	7,7,7,7	0
2	MG	G	550	1/1	0.99	0.03	9,9,9,9	0
2	MG	D	550	1/1	0.99	0.01	10,10,10,10	0
2	MG	I	550	1/1	0.99	0.03	9,9,9,9	0
2	MG	C	550	1/1	0.99	0.02	9,9,9,9	0
3	K	H	560	1/1	0.99	0.01	15,15,15,15	0
3	K	I	560	1/1	0.99	0.01	11,11,11,11	0
3	K	C	560	1/1	0.99	0.07	19,19,19,19	0

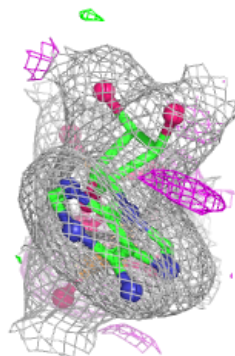
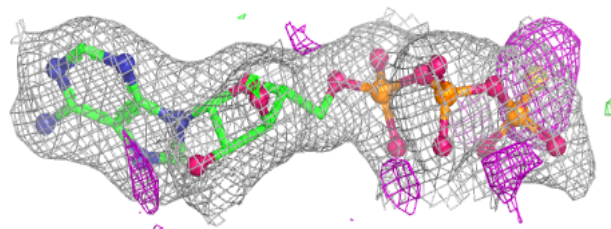
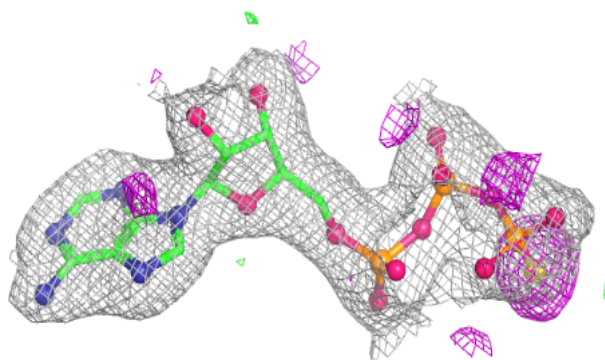
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS E 1:

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

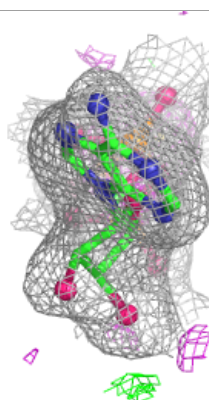
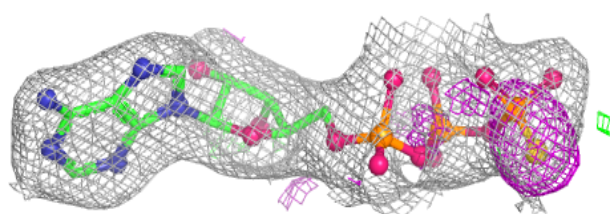
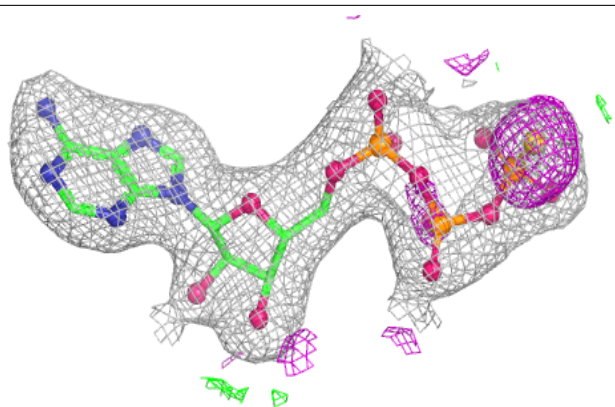
**Electron density around AGS G 1:**

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

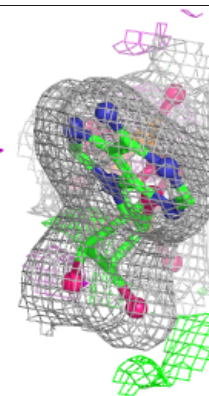
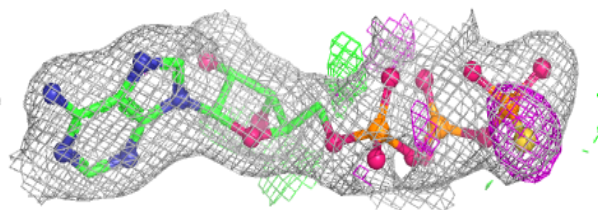
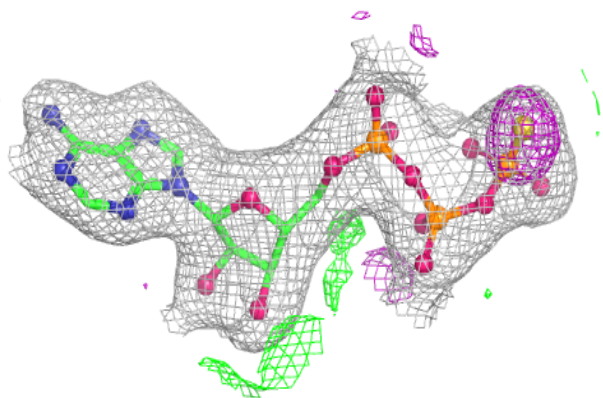


Electron density around AGS J 1:

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

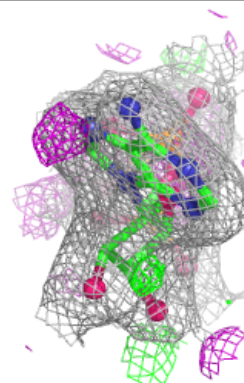
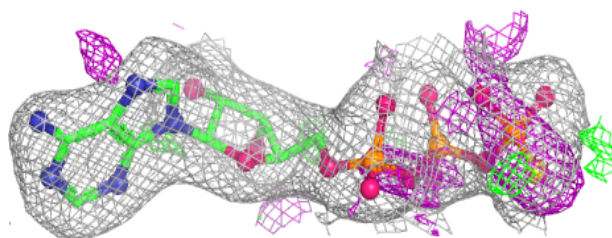
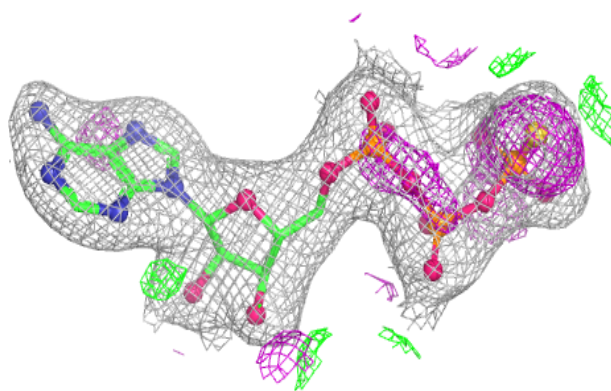
**Electron density around AGS K 1:**

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

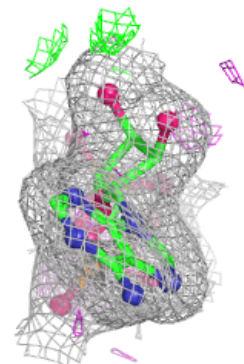
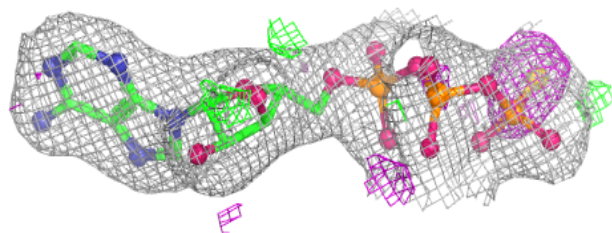
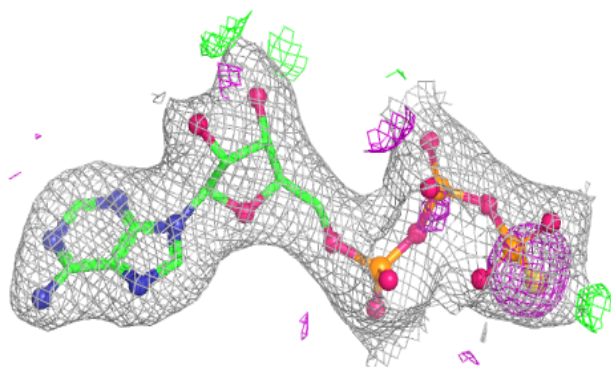


Electron density around AGS L 1:

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

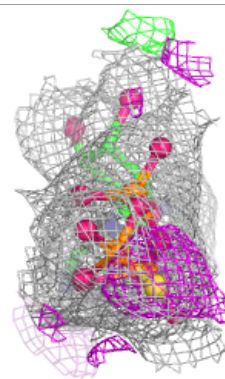
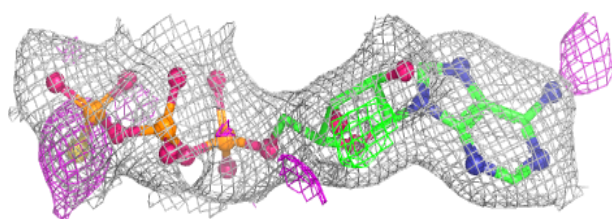
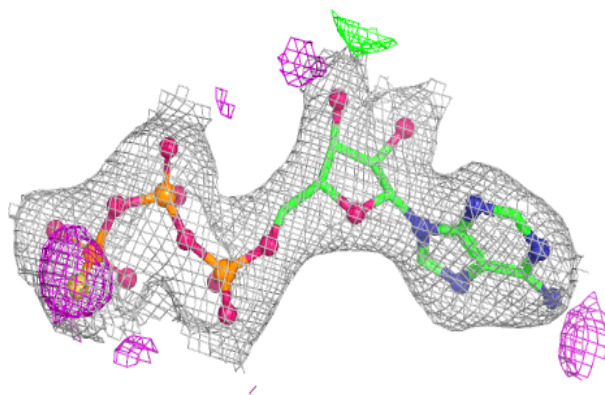
**Electron density around AGS M 1:**

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

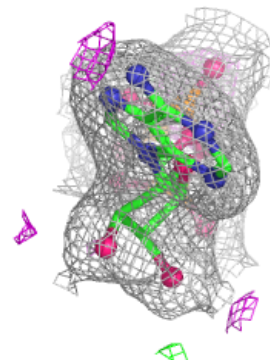
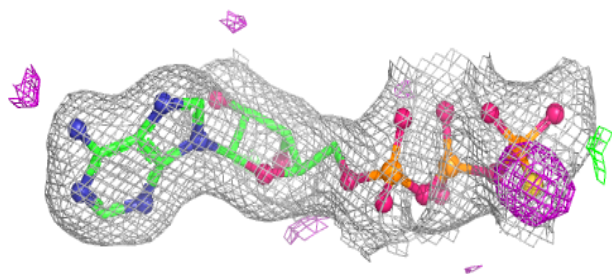
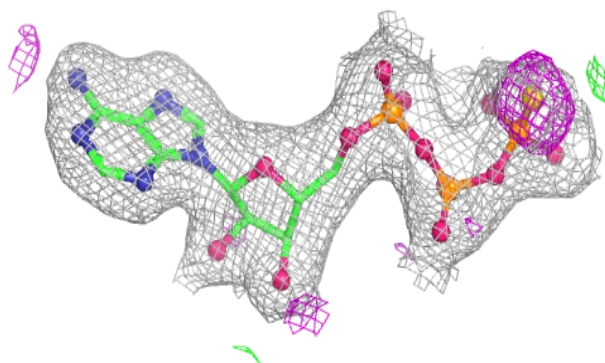


Electron density around AGS I 1:

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

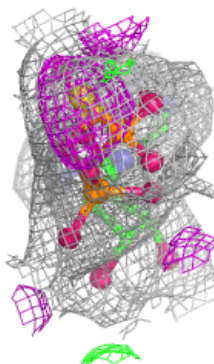
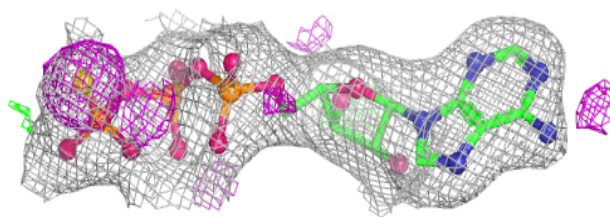
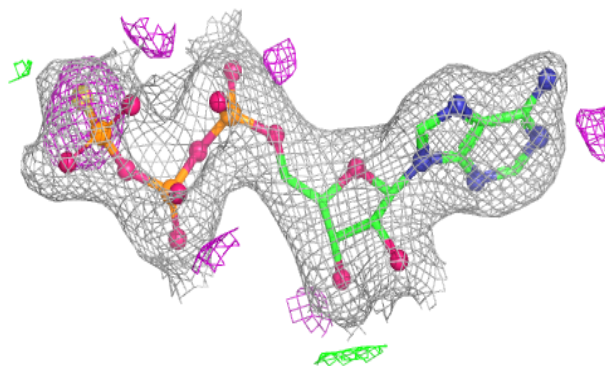
**Electron density around AGS D 561:**

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

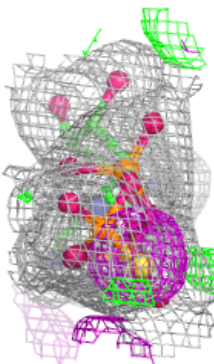
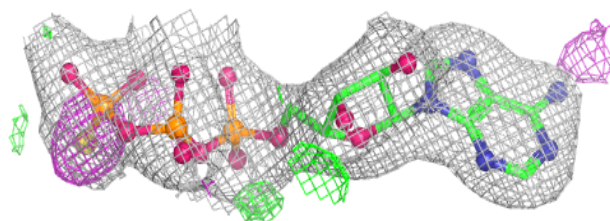
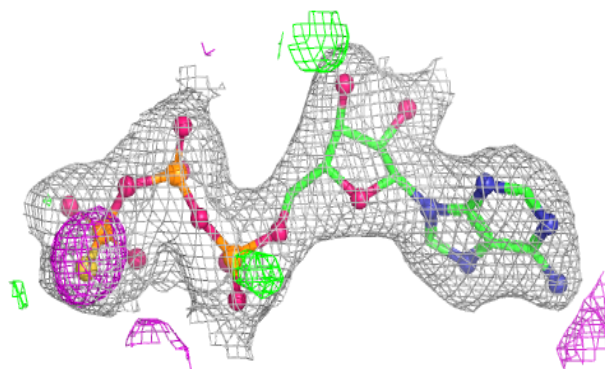


Electron density around AGS F 1:

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

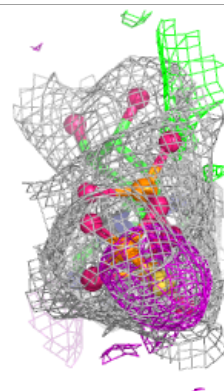
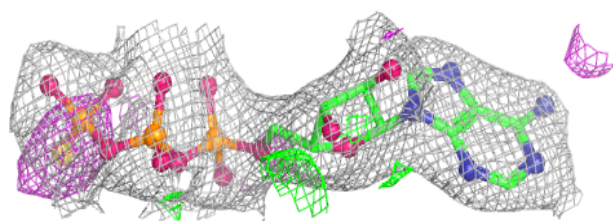
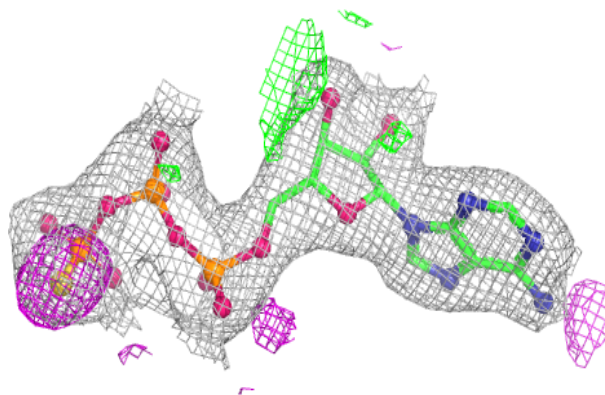
**Electron density around AGS C 1:**

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

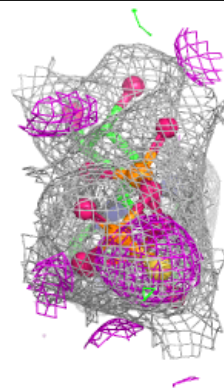
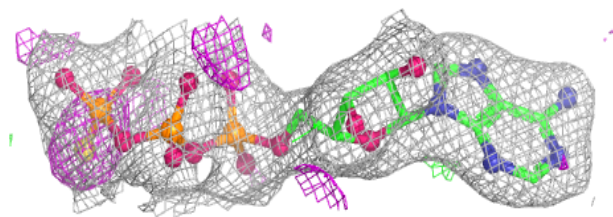
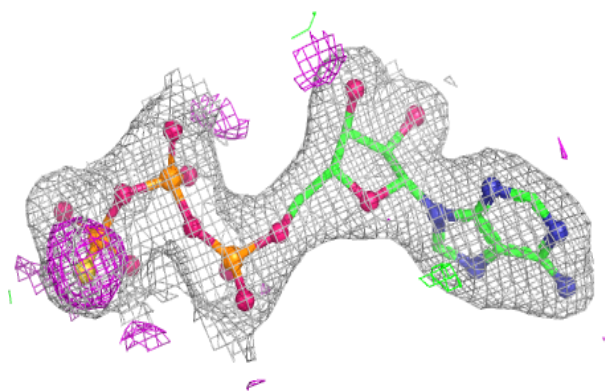


Electron density around AGS N 1:

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

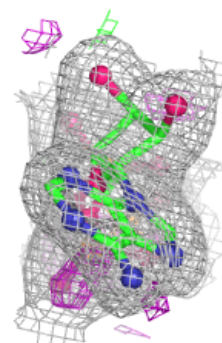
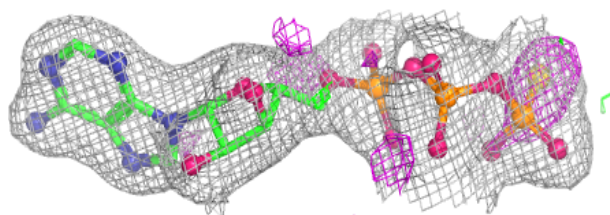
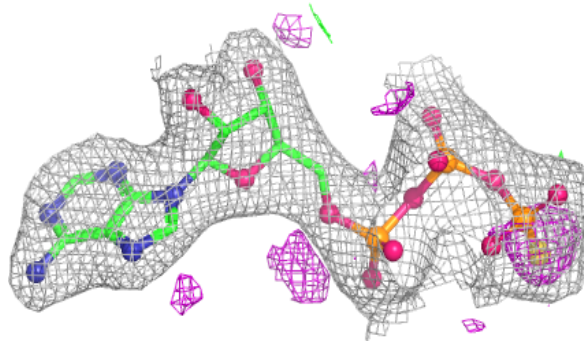
**Electron density around AGS H 1:**

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

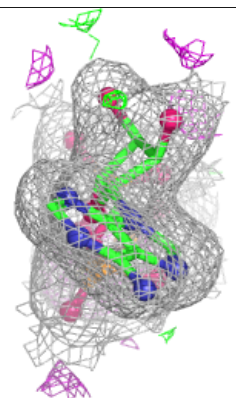
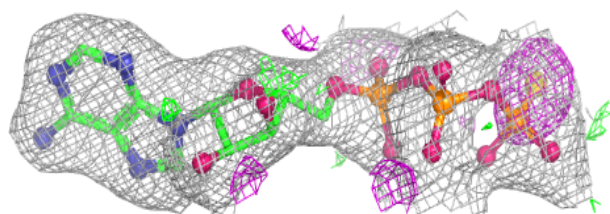
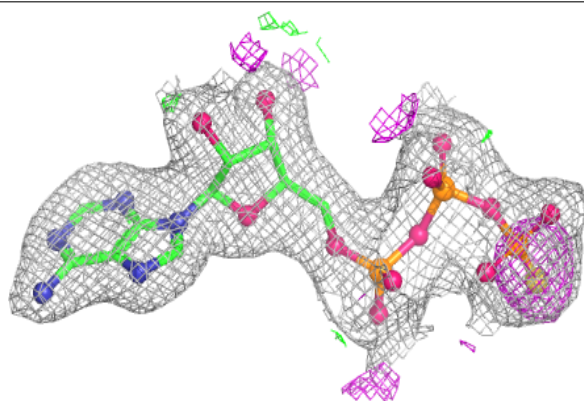


Electron density around AGS A 1:

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

**Electron density around AGS 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.