



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 08:30 PM UTC

PDB ID : 5VJH / pdb_00005vjh
EMDB ID : EMD-8697
Title : Closed State CryoEM Reconstruction of Hsp104:ATPyS and FITC casein
Authors : Gates, S.N.; Yokom, A.L.; Lin, J.-B.; Jackrel, M.E.; Rizo, A.N.; Kendsersky, N.M.; Buell, C.E.; Sweeny, E.A.; Chuang, E.; Torrente, M.P.; Mack, K.L.; Su, M.; Shorter, J.; Southworth, D.R.
Deposited on : 2017-04-19
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

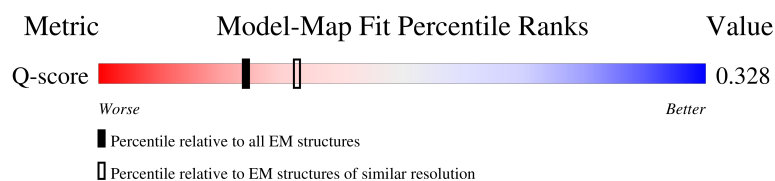
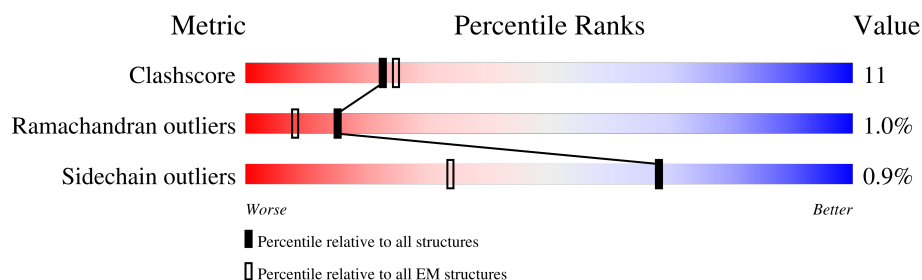
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

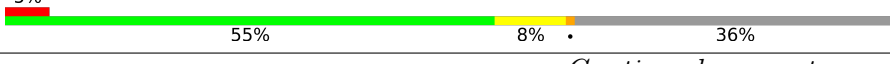
The reported resolution of this entry is 4.00 Å.

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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	908	
1	B	908	
1	C	908	
1	D	908	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	908	
1	F	908	
2	P	26	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AGS	B	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

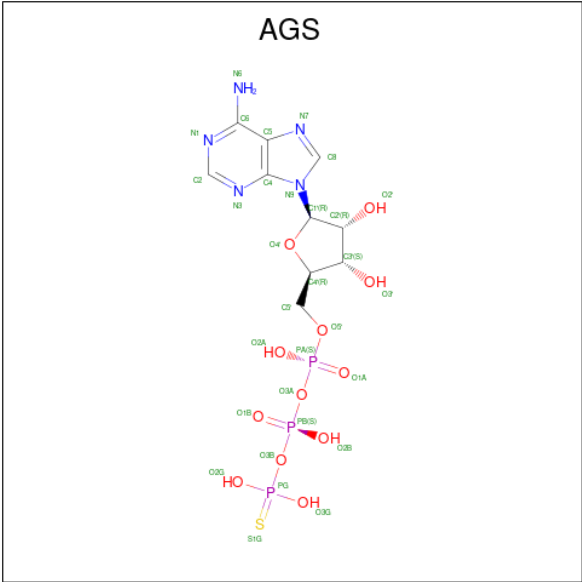
- Molecule 1 is a protein called Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	B	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	C	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	D	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	E	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	F	564	Total	C	N	O	S	0	0
			4424	2782	779	845	18		

- Molecule 2 is a protein called FITC casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	26	Total	C	N	O	0	0
			131	78	26	27		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

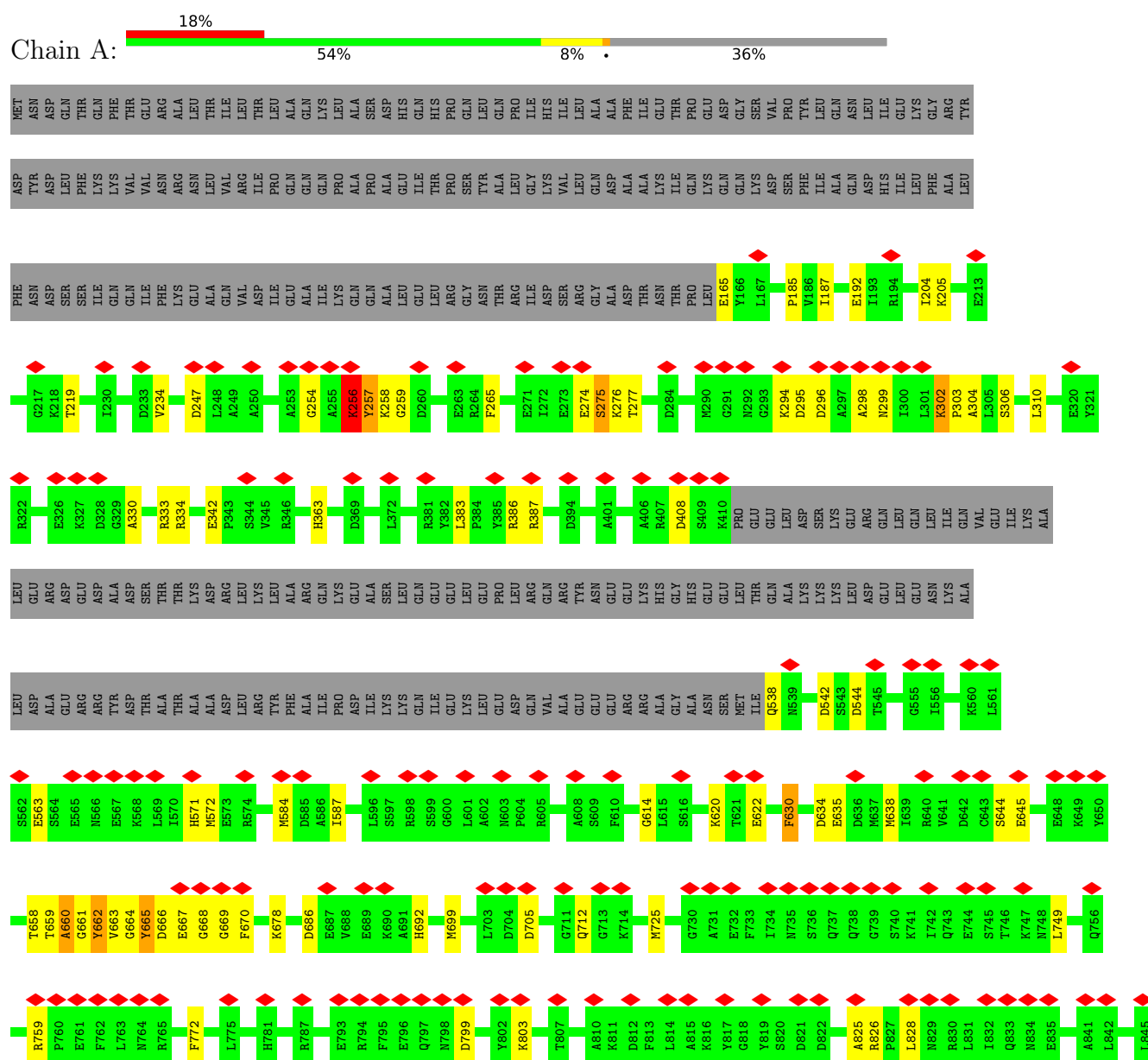


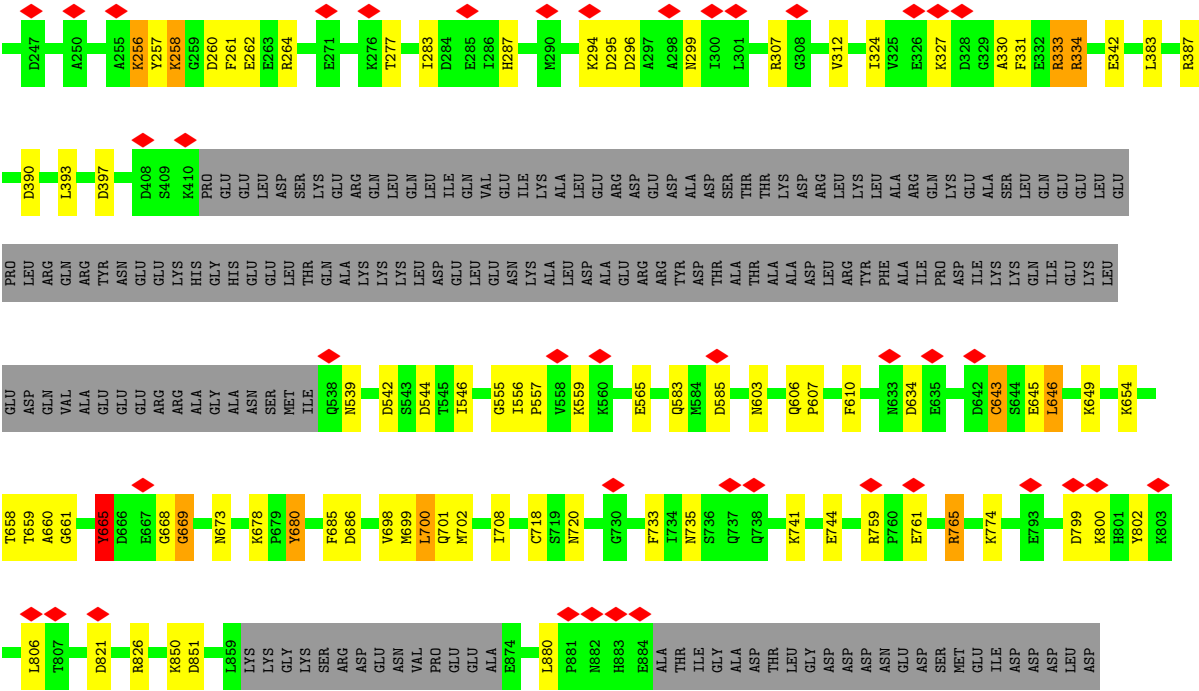
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1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

3 Residue-property plots

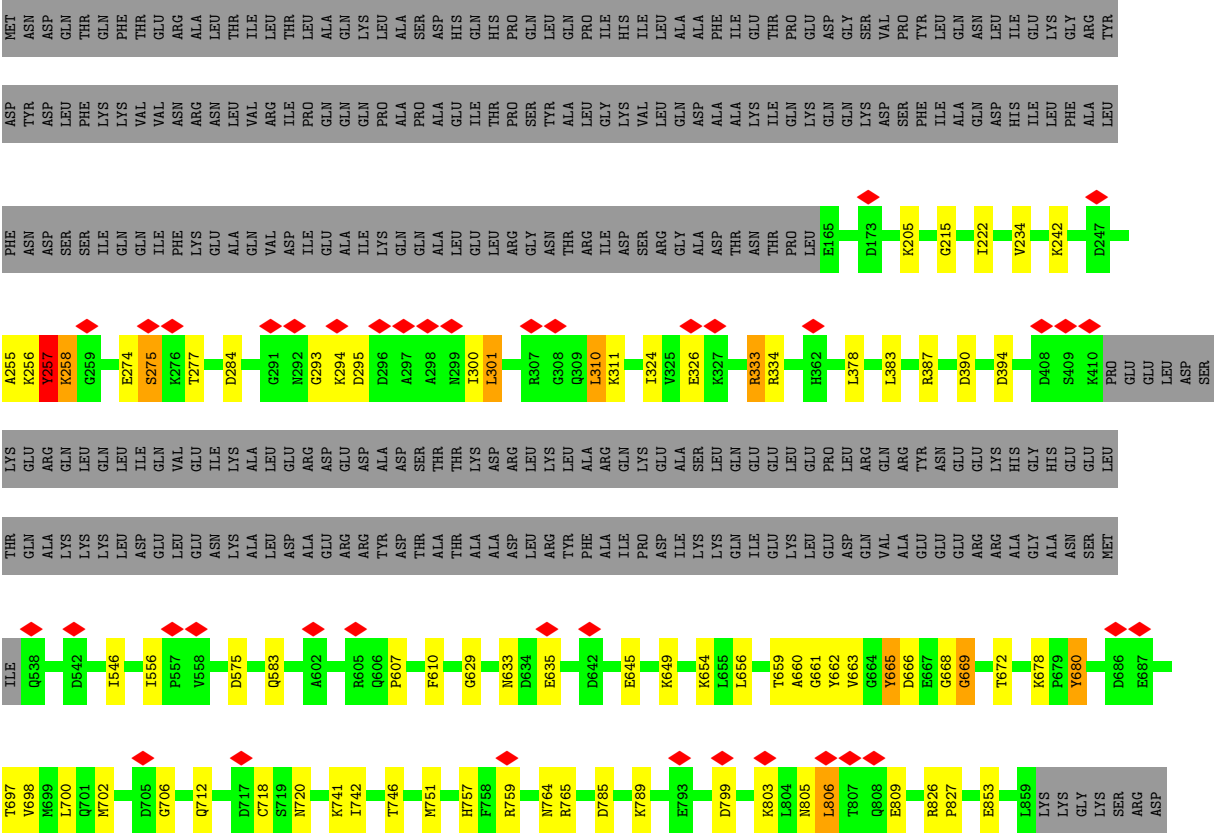
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

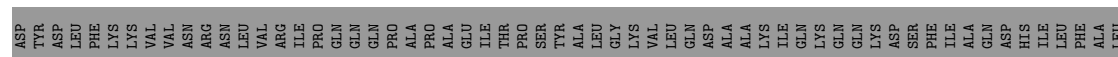
• Molecule 1: Heat shock protein 104

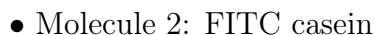




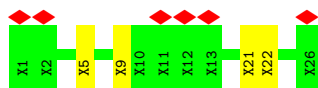
• Molecule 1: Heat shock protein 104







Response	Percentage
Current government is best	23%
A different government would be better	85%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0283	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS

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	1.15	4/4586 (0.1%)	1.29	36/6171 (0.6%)
1	B	1.31	7/4586 (0.2%)	1.30	38/6171 (0.6%)
1	C	1.36	8/4586 (0.2%)	1.32	37/6171 (0.6%)
1	D	1.34	6/4586 (0.1%)	1.30	23/6171 (0.4%)
1	E	1.26	4/4586 (0.1%)	1.29	39/6171 (0.6%)
1	F	1.14	6/4476 (0.1%)	1.33	39/6020 (0.6%)
All	All	1.26	35/27406 (0.1%)	1.31	212/36875 (0.6%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	383	LEU	CB-CG	-8.51	1.36	1.53
1	C	700	LEU	CB-CG	-7.85	1.37	1.53
1	C	287	HIS	CB-CG	-7.45	1.39	1.50
1	D	324	ILE	CB-CG1	-7.22	1.39	1.53
1	C	207	ASN	CB-CG	-7.16	1.34	1.52
1	B	700	LEU	CB-CG	-6.93	1.39	1.53
1	E	757	HIS	CB-CG	-6.82	1.40	1.50
1	D	806	LEU	CB-CG	-6.46	1.40	1.53
1	B	207	ASN	CB-CG	-6.28	1.36	1.52
1	A	363	HIS	CB-CG	-6.10	1.41	1.50
1	B	287	HIS	CB-CG	-6.10	1.41	1.50
1	F	877	LEU	CB-CG	-5.81	1.41	1.53
1	C	610	PHE	CB-CG	-5.70	1.37	1.50
1	E	610	PHE	CB-CG	-5.55	1.37	1.50
1	F	783	ILE	CB-CG1	-5.52	1.42	1.53
1	B	692	HIS	CB-CG	-5.51	1.42	1.50
1	B	569	LEU	CB-CG	-5.49	1.42	1.53
1	B	663	VAL	CA-C	-5.47	1.46	1.52
1	C	216	ILE	CB-CG1	-5.46	1.42	1.53
1	E	207	ASN	CB-CG	-5.45	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	571	HIS	CB-CG	-5.42	1.42	1.50
1	A	692	HIS	CB-CG	-5.42	1.42	1.50
1	E	670	PHE	CB-CG	-5.37	1.38	1.50
1	D	310	LEU	CB-CG	-5.34	1.42	1.53
1	F	581	VAL	CA-CB	-5.33	1.47	1.54
1	F	230	ILE	CB-CG1	-5.32	1.42	1.53
1	A	386	ARG	CD-NE	-5.26	1.38	1.46
1	F	595	ARG	NE-CZ	5.24	1.38	1.33
1	B	700	LEU	CG-CD2	-5.24	1.35	1.52
1	D	757	HIS	CB-CG	-5.15	1.43	1.50
1	C	546	ILE	CB-CG1	-5.14	1.43	1.53
1	D	610	PHE	CB-CG	-5.10	1.39	1.50
1	C	733	PHE	CB-CG	-5.08	1.39	1.50
1	C	673	ASN	CB-CG	-5.07	1.39	1.52
1	D	222	ILE	CB-CG1	-5.02	1.43	1.53

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	799	ASP	N-CA-C	-12.67	97.95	113.41
1	B	882	ASN	N-CA-C	-12.44	98.57	113.88
1	E	799	ASP	N-CA-C	-12.37	98.67	113.88
1	E	803	LYS	N-CA-C	-11.86	98.29	113.12
1	D	803	LYS	N-CA-C	-11.10	100.23	113.88
1	B	803	LYS	N-CA-C	-10.09	101.05	113.97
1	E	575	ASP	CA-CB-CG	-9.93	102.67	112.60
1	A	803	LYS	N-CA-C	-9.07	102.73	113.88
1	A	572	MET	N-CA-C	-8.49	101.53	112.23
1	B	256	LYS	N-CA-C	-8.36	98.71	110.50
1	F	769	ILE	N-CA-C	-8.36	96.55	108.58
1	E	880	LEU	CA-C-N	8.25	127.90	119.82
1	E	880	LEU	C-N-CA	8.25	127.90	119.82
1	D	556	ILE	CA-C-N	8.21	127.85	119.56
1	D	556	ILE	C-N-CA	8.21	127.85	119.56
1	F	580	VAL	N-CA-C	-8.10	96.82	108.48
1	F	351	ILE	CB-CA-C	-7.86	101.91	111.97
1	A	383	LEU	CA-C-N	7.80	127.51	119.56
1	A	383	LEU	C-N-CA	7.80	127.51	119.56
1	F	883	HIS	CA-CB-CG	7.64	121.44	113.80
1	B	556	ILE	CA-C-N	7.49	128.16	119.47
1	B	556	ILE	C-N-CA	7.49	128.16	119.47
1	C	324	ILE	CB-CA-C	-7.48	102.39	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	575	ASP	CA-CB-CG	-7.48	105.12	112.60
1	F	672	THR	N-CA-C	7.39	120.34	109.69
1	C	733	PHE	CA-CB-CG	-7.33	106.47	113.80
1	A	544	ASP	N-CA-C	7.31	119.25	111.28
1	F	187	ILE	N-CA-C	7.29	124.51	109.34
1	B	665	TYR	N-CA-C	-7.28	95.29	110.80
1	D	678	LYS	CA-C-N	7.28	127.91	119.47
1	D	678	LYS	C-N-CA	7.28	127.91	119.47
1	E	540	VAL	N-CA-C	7.26	118.57	108.12
1	F	826	ARG	CA-C-N	7.24	126.94	119.56
1	F	826	ARG	C-N-CA	7.24	126.94	119.56
1	C	698	VAL	N-CA-C	-7.23	103.74	110.53
1	B	678	LYS	CA-C-N	7.17	127.33	119.87
1	B	678	LYS	C-N-CA	7.17	127.33	119.87
1	E	808	GLN	N-CA-C	-7.04	104.69	113.55
1	B	716	ILE	N-CA-C	6.94	117.55	110.82
1	F	678	LYS	CA-C-N	6.78	126.41	119.56
1	F	678	LYS	C-N-CA	6.78	126.41	119.56
1	C	678	LYS	CA-C-N	6.78	126.92	119.87
1	C	678	LYS	C-N-CA	6.78	126.92	119.87
1	C	544	ASP	CA-CB-CG	-6.77	105.83	112.60
1	F	758	PHE	CA-CB-CG	-6.76	107.04	113.80
1	C	708	ILE	N-CA-C	-6.68	99.54	108.35
1	E	219	THR	N-CA-C	-6.68	104.08	111.36
1	E	733	PHE	CA-CB-CG	-6.62	107.18	113.80
1	C	556	ILE	CA-C-N	6.61	126.24	119.56
1	C	556	ILE	C-N-CA	6.61	126.24	119.56
1	C	234	VAL	CA-C-N	6.56	126.94	119.92
1	C	234	VAL	C-N-CA	6.56	126.94	119.92
1	C	216	ILE	N-CA-C	6.55	118.45	112.29
1	A	772	PHE	CA-CB-CG	-6.54	107.26	113.80
1	F	234	VAL	CA-C-N	6.50	126.42	119.85
1	F	234	VAL	C-N-CA	6.50	126.42	119.85
1	C	397	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	665	TYR	N-CA-C	-6.44	104.10	114.09
1	C	383	LEU	CA-C-N	6.42	126.11	119.56
1	C	383	LEU	C-N-CA	6.42	126.11	119.56
1	A	234	VAL	CA-C-N	6.38	126.41	119.90
1	A	234	VAL	C-N-CA	6.38	126.41	119.90
1	E	556	ILE	CA-C-N	6.33	125.96	119.56
1	E	556	ILE	C-N-CA	6.33	125.96	119.56
1	A	799	ASP	N-CA-C	-6.32	104.49	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	883	HIS	N-CA-C	-6.27	100.92	109.95
1	D	759	ARG	CA-C-N	6.26	126.73	119.47
1	D	759	ARG	C-N-CA	6.26	126.73	119.47
1	C	312	VAL	N-CA-C	6.19	117.40	108.48
1	E	666	ASP	CA-CB-CG	-6.15	106.45	112.60
1	B	740	SER	N-CA-C	-6.15	104.50	111.14
1	A	749	LEU	N-CA-C	-6.14	105.45	113.12
1	F	186	VAL	N-CA-C	6.12	117.51	106.61
1	E	603	ASN	CA-C-N	6.12	127.49	119.84
1	E	603	ASN	C-N-CA	6.12	127.49	119.84
1	B	383	LEU	CA-C-N	6.11	125.81	119.82
1	B	383	LEU	C-N-CA	6.11	125.81	119.82
1	E	759	ARG	CA-C-N	6.10	126.54	119.47
1	E	759	ARG	C-N-CA	6.10	126.54	119.47
1	D	274	GLU	N-CA-C	6.09	119.67	108.58
1	E	383	LEU	CA-C-N	6.07	125.75	119.56
1	E	383	LEU	C-N-CA	6.07	125.75	119.56
1	E	764	ASN	CA-CB-CG	-6.07	106.53	112.60
1	C	759	ARG	CA-C-N	6.03	126.47	119.47
1	C	759	ARG	C-N-CA	6.03	126.47	119.47
1	C	556	ILE	N-CA-C	6.03	113.05	107.56
1	A	342	GLU	CA-C-N	6.02	125.98	119.78
1	A	342	GLU	C-N-CA	6.02	125.98	119.78
1	D	324	ILE	CB-CA-C	-6.01	101.43	111.29
1	F	284	ASP	N-CA-C	-6.01	102.78	110.53
1	D	383	LEU	CA-C-N	6.00	125.68	119.56
1	D	383	LEU	C-N-CA	6.00	125.68	119.56
1	D	234	VAL	CA-C-N	6.00	125.97	120.03
1	D	234	VAL	C-N-CA	6.00	125.97	120.03
1	F	849	ILE	N-CA-C	5.99	116.64	107.77
1	A	630	PHE	CA-CB-CG	-5.98	107.82	113.80
1	A	705	ASP	N-CA-C	-5.93	103.06	111.24
1	C	207	ASN	N-CA-CB	-5.90	103.78	111.09
1	F	580	VAL	CA-C-N	-5.89	114.77	122.37
1	F	580	VAL	C-N-CA	-5.89	114.77	122.37
1	B	324	ILE	CB-CA-C	-5.89	101.63	111.29
1	F	544	ASP	CA-CB-CG	-5.88	106.72	112.60
1	E	342	GLU	CA-C-N	5.81	125.77	119.78
1	E	342	GLU	C-N-CA	5.81	125.77	119.78
1	A	571	HIS	CA-C-N	-5.81	110.81	120.68
1	A	571	HIS	C-N-CA	-5.81	110.81	120.68
1	E	234	VAL	CA-C-N	5.80	125.75	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	234	VAL	C-N-CA	5.80	125.75	119.78
1	B	603	ASN	CA-C-N	5.79	127.08	119.84
1	B	603	ASN	C-N-CA	5.79	127.08	119.84
1	E	313	ILE	CA-C-N	-5.79	116.30	122.67
1	E	313	ILE	C-N-CA	-5.79	116.30	122.67
1	B	671	LEU	N-CA-C	5.78	120.61	112.93
1	F	184	ASP	CA-C-N	5.78	125.73	119.78
1	F	184	ASP	C-N-CA	5.78	125.73	119.78
1	B	720	ASN	CA-CB-CG	-5.77	106.83	112.60
1	C	603	ASN	CA-C-N	5.74	125.42	119.56
1	C	603	ASN	C-N-CA	5.74	125.42	119.56
1	C	880	LEU	CA-C-N	5.73	127.00	119.84
1	C	880	LEU	C-N-CA	5.73	127.00	119.84
1	D	607	PRO	N-CA-C	-5.68	102.17	111.15
1	A	759	ARG	CA-C-N	5.66	126.92	119.84
1	A	759	ARG	C-N-CA	5.66	126.92	119.84
1	A	692	HIS	CA-C-N	5.65	126.02	119.47
1	A	692	HIS	C-N-CA	5.65	126.02	119.47
1	E	546	ILE	CB-CA-C	-5.63	104.53	112.14
1	B	759	ARG	CA-C-N	5.63	126.00	119.47
1	B	759	ARG	C-N-CA	5.63	126.00	119.47
1	B	234	VAL	CA-C-N	5.62	125.56	119.78
1	B	234	VAL	C-N-CA	5.62	125.56	119.78
1	C	565	GLU	N-CA-C	-5.61	105.25	111.36
1	E	184	ASP	CA-C-N	5.59	126.83	119.84
1	E	184	ASP	C-N-CA	5.59	126.83	119.84
1	C	646	LEU	N-CA-C	5.58	117.71	108.49
1	E	247	ASP	CA-CB-CG	5.58	118.19	112.60
1	E	670	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	828	LEU	N-CA-C	-5.58	104.83	111.69
1	B	853	GLU	N-CA-C	5.56	118.29	110.23
1	A	408	ASP	CA-CB-CG	-5.56	107.04	112.60
1	D	310	LEU	CB-CA-C	-5.56	103.99	111.89
1	C	283	ILE	N-CA-C	5.56	115.86	107.75
1	C	658	THR	N-CA-C	5.56	117.70	110.53
1	A	187	ILE	N-CA-C	5.53	115.85	108.11
1	F	802	TYR	N-CA-C	5.48	117.52	109.24
1	B	826	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	E	723	VAL	N-CA-C	5.47	115.74	107.80
1	F	335	PHE	N-CA-C	5.47	118.14	109.50
1	D	275	SER	N-CA-C	5.46	122.43	110.80
1	D	853	GLU	N-CA-C	5.46	118.15	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	372	LEU	N-CA-C	-5.41	105.47	111.36
1	D	706	GLY	N-CA-C	-5.40	107.52	115.30
1	F	681	SER	N-CA-C	5.39	117.04	110.41
1	C	222	ILE	CB-CA-C	-5.38	104.87	112.14
1	E	810	ALA	N-CA-C	-5.38	105.49	111.36
1	F	759	ARG	CA-C-N	5.36	126.54	119.84
1	F	759	ARG	C-N-CA	5.36	126.54	119.84
1	E	678	LYS	CA-C-N	5.35	125.06	119.82
1	E	678	LYS	C-N-CA	5.35	125.06	119.82
1	F	366	ARG	CA-C-N	-5.34	116.17	123.12
1	F	366	ARG	C-N-CA	-5.34	116.17	123.12
1	B	184	ASP	CA-C-N	5.34	125.31	120.03
1	B	184	ASP	C-N-CA	5.34	125.31	120.03
1	A	274	GLU	N-CA-C	5.32	117.78	108.52
1	B	648	GLU	N-CA-C	5.32	117.49	111.11
1	F	186	VAL	CA-C-N	5.31	131.53	121.97
1	F	186	VAL	C-N-CA	5.31	131.53	121.97
1	F	581	VAL	N-CA-C	5.31	116.23	108.58
1	C	342	GLU	CA-C-N	5.30	125.28	120.03
1	C	342	GLU	C-N-CA	5.30	125.28	120.03
1	B	657	GLY	N-CA-C	-5.29	106.02	112.68
1	B	262	GLU	N-CA-C	-5.28	105.61	111.36
1	D	284	ASP	N-CA-C	-5.27	103.73	110.53
1	F	722	ILE	CA-C-N	-5.25	116.29	123.12
1	F	722	ILE	C-N-CA	-5.25	116.29	123.12
1	A	614	GLY	N-CA-C	5.25	117.92	110.74
1	E	671	LEU	CA-C-N	-5.23	111.98	121.14
1	E	671	LEU	C-N-CA	-5.23	111.98	121.14
1	C	262	GLU	N-CA-C	-5.23	105.64	112.23
1	A	275	SER	N-CA-C	5.23	121.93	110.80
1	B	294	LYS	CB-CA-C	-5.20	110.60	116.63
1	A	678	LYS	CA-C-N	5.19	125.26	119.87
1	A	678	LYS	C-N-CA	5.19	125.26	119.87
1	B	664	GLY	N-CA-C	-5.19	106.20	112.48
1	D	746	THR	N-CA-C	-5.19	105.63	111.28
1	C	744	GLU	N-CA-C	-5.18	103.65	110.43
1	F	686	ASP	N-CA-C	5.17	117.18	108.96
1	E	187	ILE	N-CA-C	5.16	115.39	108.17
1	B	666	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	204	ILE	N-CA-C	5.13	115.36	108.17
1	A	265	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	725	MET	CA-C-N	-5.13	114.61	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	MET	C-N-CA	-5.13	114.61	122.62
1	C	555	GLY	CA-C-N	-5.13	119.11	122.60
1	C	555	GLY	C-N-CA	-5.13	119.11	122.60
1	D	546	ILE	CB-CA-C	-5.13	105.22	112.14
1	B	388	LEU	N-CA-C	5.11	119.90	113.25
1	F	795	PHE	CA-CB-CG	-5.09	108.71	113.80
1	F	358	LYS	N-CA-C	-5.08	105.44	111.69
1	A	855	VAL	N-CA-C	5.06	116.25	108.71
1	B	565	GLU	N-CA-C	-5.05	105.47	111.69
1	C	187	ILE	N-CA-C	5.05	115.18	108.11
1	E	692	HIS	CA-C-N	5.04	125.32	119.47
1	E	692	HIS	C-N-CA	5.04	125.32	119.47
1	B	397	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	587	ILE	CB-CA-C	-5.04	105.34	112.14
1	A	622	GLU	N-CA-C	-5.04	105.70	111.14
1	B	256	LYS	CA-C-O	-5.03	116.08	121.56
1	F	391	SER	N-CA-C	5.03	117.65	111.82
1	B	382	TYR	N-CA-C	5.02	120.03	113.30
1	B	648	GLU	CB-CA-C	-5.02	102.78	110.81
1	A	644	SER	N-CA-C	-5.02	106.67	112.89
1	F	805	ASN	N-CA-C	-5.01	102.86	110.28

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	4530	0	4645	129	0
1	B	4530	0	4647	149	0
1	C	4530	0	4643	121	0
1	D	4530	0	4642	168	0
1	E	4530	0	4646	114	0
1	F	4424	0	4553	51	0
2	P	131	0	40	5	0
3	A	62	0	24	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	93	0	36	20	0
3	C	31	0	12	1	0
3	D	93	0	36	11	0
3	E	31	0	12	3	0
3	F	62	0	24	5	0
All	All	27577	0	27960	625	0

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 11.

All (625) 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:A:205:LYS:HZ3	1:A:306:SER:CA	1.02	1.61
1:A:258:LYS:NZ	1:B:261:PHE:CE2	1.70	1.55
1:D:205:LYS:CE	1:D:333:ARG:HH21	1.13	1.52
1:A:205:LYS:NZ	1:A:306:SER:CB	1.78	1.44
1:A:330:ALA:HB1	1:A:334:ARG:NH1	1.32	1.44
1:A:258:LYS:NZ	1:B:261:PHE:CD2	1.84	1.44
1:D:256:LYS:O	1:D:257:TYR:CD2	1.71	1.40
1:D:205:LYS:HE2	1:D:333:ARG:NH2	1.34	1.38
1:D:765:ARG:NH1	3:E:1001:AGS:S1G	1.99	1.35
1:A:205:LYS:NZ	1:A:306:SER:CA	1.82	1.35
1:A:258:LYS:HB3	1:B:255:ALA:CB	1.54	1.34
1:A:333:ARG:NH2	3:B:1001:AGS:H5'2	1.05	1.34
1:C:765:ARG:NH2	3:D:1003:AGS:S1G	1.99	1.34
1:D:205:LYS:NZ	1:D:333:ARG:HH21	1.25	1.33
1:D:660:ALA:HB2	1:D:665:TYR:OH	1.18	1.32
1:B:330:ALA:HB1	1:B:334:ARG:NH1	1.45	1.29
1:B:660:ALA:HB2	1:B:665:TYR:OH	1.15	1.27
1:A:205:LYS:CE	1:A:306:SER:CB	2.13	1.26
1:A:333:ARG:NH2	3:B:1001:AGS:C5'	1.98	1.25
1:A:258:LYS:HB2	2:P:9:UNK:CB	1.66	1.25
1:D:765:ARG:HE	1:E:826:ARG:NH1	1.36	1.24
1:B:333:ARG:HD3	1:C:390:ASP:OD2	1.35	1.24
1:D:205:LYS:CE	1:D:333:ARG:NH2	1.91	1.20
1:B:660:ALA:CB	1:B:665:TYR:OH	1.89	1.20
1:A:205:LYS:HZ3	1:A:306:SER:CB	1.44	1.19
1:A:205:LYS:CE	1:A:306:SER:HB2	1.71	1.17
1:D:258:LYS:HD3	1:E:261:PHE:CE2	1.79	1.16
1:A:205:LYS:NZ	1:A:306:SER:HB3	1.46	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:ALA:HB2	1:C:665:TYR:OH	1.42	1.16
1:D:660:ALA:HB2	1:D:665:TYR:CZ	1.82	1.14
1:A:205:LYS:NZ	1:A:306:SER:HA	1.52	1.14
1:B:659:THR:C	1:B:665:TYR:HE1	1.54	1.13
1:B:333:ARG:CD	1:C:390:ASP:OD2	1.96	1.12
1:C:660:ALA:HA	1:C:665:TYR:CZ	1.85	1.11
1:A:205:LYS:HE2	1:A:306:SER:CB	1.77	1.10
1:D:258:LYS:CG	1:E:261:PHE:HZ	1.63	1.10
1:D:258:LYS:CG	1:E:261:PHE:CZ	2.34	1.10
1:C:660:ALA:CB	1:C:665:TYR:OH	2.02	1.07
1:D:205:LYS:NZ	1:D:333:ARG:NH2	1.99	1.07
1:A:333:ARG:HH21	3:B:1001:AGS:C5'	1.61	1.06
1:D:660:ALA:CB	1:D:665:TYR:OH	2.01	1.06
1:A:205:LYS:CE	1:A:306:SER:CA	2.32	1.05
1:A:258:LYS:HB3	1:B:255:ALA:HB3	1.07	1.04
1:B:333:ARG:HD2	1:C:390:ASP:CG	1.82	1.04
1:A:205:LYS:CE	1:A:306:SER:HA	1.86	1.04
1:A:330:ALA:CB	1:A:334:ARG:HH12	1.69	1.04
1:A:205:LYS:HE2	1:A:306:SER:HB2	1.07	1.03
1:C:660:ALA:CA	1:C:665:TYR:OH	2.06	1.03
1:D:256:LYS:C	1:D:257:TYR:CD2	2.34	1.03
1:E:643:CYS:SG	1:E:699:MET:HE1	1.98	1.03
1:F:330:ALA:O	1:F:334:ARG:HG2	1.57	1.03
1:C:205:LYS:HZ2	1:D:390:ASP:CG	1.65	1.02
1:E:662:TYR:OH	1:F:650:TYR:CE1	2.11	1.02
1:B:330:ALA:HB1	1:B:334:ARG:HH12	0.85	1.00
1:D:700:LEU:HD12	1:D:765:ARG:HD2	1.44	1.00
1:F:826:ARG:HB2	1:F:827:PRO:HD3	1.40	1.00
1:B:330:ALA:CB	1:B:334:ARG:HH12	1.76	0.99
1:D:660:ALA:N	1:D:665:TYR:CE1	2.31	0.99
1:A:333:ARG:HH22	3:B:1001:AGS:H5'2	1.26	0.98
1:D:765:ARG:NE	1:E:826:ARG:NH1	2.12	0.98
1:A:665:TYR:HE2	1:B:666:ASP:OD2	1.44	0.97
1:C:205:LYS:NZ	1:D:390:ASP:CG	2.23	0.97
1:B:660:ALA:CA	1:B:665:TYR:CZ	2.48	0.96
1:A:205:LYS:HZ3	1:A:306:SER:N	1.62	0.96
1:A:254:GLY:O	1:A:256:LYS:HD2	1.66	0.96
1:C:660:ALA:CA	1:C:665:TYR:CZ	2.48	0.96
1:C:258:LYS:HG2	1:D:255:ALA:HB3	1.47	0.95
1:B:205:LYS:HD3	1:B:333:ARG:NH1	1.80	0.95
1:B:660:ALA:HA	1:B:665:TYR:CZ	2.00	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ALA:CB	1:A:334:ARG:NH1	2.27	0.95
1:B:660:ALA:HA	1:B:665:TYR:CE1	2.01	0.95
1:A:333:ARG:NE	1:B:390:ASP:OD2	2.00	0.95
1:D:258:LYS:CD	1:E:261:PHE:CZ	2.50	0.95
1:B:660:ALA:N	1:B:665:TYR:CE1	2.35	0.95
1:A:205:LYS:HZ1	1:A:306:SER:HB3	1.04	0.94
1:B:659:THR:C	1:B:665:TYR:CE1	2.44	0.94
1:D:258:LYS:HD3	1:E:261:PHE:CZ	2.01	0.94
1:A:258:LYS:CB	1:B:255:ALA:CB	2.44	0.94
1:C:645:GLU:CD	1:C:645:GLU:O	2.10	0.94
1:E:826:ARG:HB2	1:E:827:PRO:HD3	1.50	0.94
1:A:333:ARG:CD	1:B:390:ASP:OD2	2.16	0.94
1:D:765:ARG:HE	1:E:826:ARG:HH12	1.06	0.93
1:D:256:LYS:O	1:D:257:TYR:HD2	1.22	0.93
1:D:258:LYS:HG3	1:E:261:PHE:HZ	1.31	0.92
1:D:660:ALA:CA	1:D:665:TYR:CE1	2.52	0.92
1:B:333:ARG:CD	1:C:390:ASP:CG	2.40	0.92
1:D:660:ALA:N	1:D:665:TYR:HE1	1.66	0.91
1:D:258:LYS:HD3	1:E:261:PHE:HE2	1.33	0.91
1:A:205:LYS:CD	1:A:306:SER:HA	1.99	0.91
1:B:765:ARG:HG3	1:B:765:ARG:HH11	1.36	0.91
1:E:186:VAL:O	1:E:186:VAL:HG13	1.68	0.91
1:A:205:LYS:HD3	1:A:306:SER:HA	1.52	0.91
1:E:665:TYR:OH	1:E:712:GLN:HG2	1.69	0.91
1:C:258:LYS:CG	1:D:255:ALA:CB	2.48	0.91
1:D:765:ARG:NE	1:E:826:ARG:HH12	1.66	0.90
1:D:660:ALA:CB	1:D:665:TYR:CZ	2.54	0.90
1:D:660:ALA:HA	1:D:665:TYR:CE1	2.06	0.90
1:C:257:TYR:CG	1:D:256:LYS:HG2	2.07	0.90
1:A:258:LYS:CB	1:B:255:ALA:HB3	2.00	0.90
1:B:333:ARG:HH21	1:B:334:ARG:NH2	1.70	0.90
1:D:333:ARG:HD2	1:E:215:GLY:CA	2.02	0.89
1:C:258:LYS:HG3	1:D:255:ALA:CB	2.02	0.89
1:B:660:ALA:CA	1:B:665:TYR:CE1	2.55	0.89
1:A:258:LYS:HB3	1:B:255:ALA:HB1	1.54	0.89
1:E:662:TYR:CZ	1:F:650:TYR:CE1	2.24	0.89
1:B:761:GLU:N	1:B:761:GLU:OE1	2.05	0.89
1:C:258:LYS:CG	1:D:255:ALA:HB3	2.03	0.89
1:D:660:ALA:HB2	1:D:665:TYR:HH	1.07	0.89
1:B:660:ALA:N	1:B:665:TYR:HE1	1.72	0.88
1:F:310:LEU:O	1:F:310:LEU:HG	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ALA:CA	1:B:665:TYR:OH	2.22	0.88
1:C:333:ARG:HD3	1:D:215:GLY:CA	2.03	0.88
1:E:643:CYS:HG	1:E:699:MET:HE1	1.36	0.88
1:C:333:ARG:HD3	1:D:215:GLY:HA3	1.56	0.88
1:C:645:GLU:O	1:C:645:GLU:OE1	1.90	0.87
1:D:809:GLU:OE1	1:D:809:GLU:N	2.05	0.87
1:D:256:LYS:O	1:D:257:TYR:CG	2.26	0.87
3:D:1001:AGS:O1B	3:D:1001:AGS:O2G	1.92	0.87
1:A:258:LYS:NZ	1:B:261:PHE:HE2	1.63	0.87
3:D:1002:AGS:O1A	3:D:1002:AGS:O2G	1.93	0.86
1:C:718:CYS:SG	1:C:718:CYS:O	2.32	0.86
1:E:761:GLU:OE1	1:E:761:GLU:N	2.09	0.86
1:A:333:ARG:CG	1:B:390:ASP:OD2	2.24	0.85
1:D:256:LYS:HB2	1:D:257:TYR:CE2	2.11	0.85
1:E:665:TYR:CZ	1:E:712:GLN:HG2	2.11	0.85
1:B:333:ARG:HH21	1:B:334:ARG:HH21	1.24	0.85
1:A:662:TYR:OH	1:B:649:LYS:O	1.94	0.85
1:C:205:LYS:HD3	1:C:333:ARG:NH2	1.90	0.85
1:C:660:ALA:N	1:C:665:TYR:OH	2.10	0.85
3:E:1001:AGS:O2G	3:E:1001:AGS:O1B	1.94	0.85
1:A:205:LYS:HZ3	1:A:306:SER:HA	1.07	0.84
1:A:258:LYS:CB	2:P:9:UNK:CB	2.53	0.84
1:D:258:LYS:CD	1:E:261:PHE:CE2	2.60	0.84
1:E:330:ALA:O	1:E:334:ARG:HG2	1.78	0.84
1:C:557:PRO:HG3	1:C:680:TYR:CE2	2.11	0.84
1:B:306:SER:C	1:B:307:ARG:HE	1.84	0.84
1:D:256:LYS:C	1:D:257:TYR:CG	2.51	0.83
1:D:712:GLN:NE2	1:E:666:ASP:OD2	2.11	0.83
1:A:665:TYR:OH	1:A:712:GLN:HG3	1.79	0.83
1:D:258:LYS:HG2	1:E:261:PHE:CZ	2.12	0.83
1:A:192:GLU:N	1:A:192:GLU:OE1	2.11	0.82
1:C:660:ALA:HA	1:C:665:TYR:CE1	2.13	0.82
1:C:258:LYS:HG3	1:D:255:ALA:HB2	1.59	0.82
1:B:704:ASP:OD2	1:B:765:ARG:NE	2.13	0.82
1:A:219:THR:HG21	1:F:333:ARG:HH22	1.43	0.82
1:C:761:GLU:N	1:C:761:GLU:OE1	2.13	0.82
3:A:1001:AGS:O2G	3:A:1001:AGS:O1B	1.92	0.81
1:E:333:ARG:O	1:E:333:ARG:HD3	1.79	0.81
1:B:205:LYS:HD3	1:B:333:ARG:HH12	1.41	0.81
1:A:662:TYR:CD2	1:B:650:TYR:CE2	2.69	0.81
1:C:330:ALA:HB1	1:C:334:ARG:HH12	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LYS:NZ	1:D:390:ASP:OD2	2.13	0.80
1:A:660:ALA:O	1:B:658:THR:CG2	2.29	0.80
1:D:660:ALA:CA	1:D:665:TYR:CZ	2.63	0.80
1:C:557:PRO:HG3	1:C:680:TYR:CZ	2.17	0.80
1:A:661:GLY:O	2:P:22:UNK:CB	2.30	0.80
3:F:1002:AGS:O1B	3:F:1002:AGS:O2G	1.99	0.79
1:E:809:GLU:OE1	1:E:809:GLU:N	2.16	0.79
1:B:307:ARG:HE	1:B:307:ARG:N	1.80	0.79
3:D:1002:AGS:O2G	3:D:1002:AGS:O1B	1.93	0.79
3:B:1002:AGS:S1G	3:B:1002:AGS:O2B	2.41	0.78
1:D:205:LYS:HE2	1:D:333:ARG:HH22	1.43	0.78
1:C:327:LYS:NZ	1:D:712:GLN:HE22	1.82	0.78
1:E:643:CYS:SG	1:E:699:MET:CE	2.72	0.78
1:A:712:GLN:NE2	1:B:666:ASP:OD2	2.17	0.78
1:D:205:LYS:HZ1	1:D:333:ARG:NH2	1.78	0.78
1:F:819:TYR:O	1:F:819:TYR:CD2	2.37	0.78
1:D:258:LYS:CD	1:E:261:PHE:HZ	1.91	0.77
1:B:333:ARG:HD2	1:C:390:ASP:OD1	1.84	0.77
3:B:1003:AGS:H8	3:B:1003:AGS:H5'2	1.65	0.77
1:C:333:ARG:NH1	1:D:390:ASP:CG	2.42	0.76
1:D:300:ILE:HG23	1:D:300:ILE:O	1.84	0.76
1:A:665:TYR:CE2	1:B:666:ASP:OD2	2.36	0.76
3:A:1001:AGS:O2B	3:A:1001:AGS:O1A	1.99	0.76
1:D:256:LYS:CB	1:D:257:TYR:CE2	2.69	0.76
1:D:333:ARG:HD2	1:E:215:GLY:HA3	1.66	0.76
1:A:662:TYR:CE2	1:B:650:TYR:CE2	2.73	0.76
1:D:661:GLY:HA2	1:E:662:TYR:HB3	1.68	0.76
1:D:809:GLU:H	1:D:809:GLU:CD	1.92	0.76
1:D:205:LYS:NZ	1:D:333:ARG:HE	1.83	0.75
1:B:333:ARG:NH2	1:B:334:ARG:HE	1.83	0.75
1:D:333:ARG:HD2	1:E:215:GLY:HA2	1.69	0.75
1:A:310:LEU:O	1:A:310:LEU:HG	1.85	0.74
1:E:826:ARG:HB2	1:E:827:PRO:CD	2.17	0.74
1:E:387:ARG:HA	1:E:387:ARG:NE	2.03	0.74
3:B:1003:AGS:H8	3:B:1003:AGS:C5'	2.17	0.74
1:D:205:LYS:HZ3	1:D:333:ARG:HE	1.36	0.73
1:B:660:ALA:HB2	1:B:665:TYR:CZ	2.23	0.73
1:D:258:LYS:HG3	1:E:261:PHE:CZ	2.15	0.73
1:C:659:THR:C	1:C:665:TYR:HE1	1.96	0.73
1:A:258:LYS:HD3	1:B:255:ALA:HB1	1.69	0.72
1:C:257:TYR:HB3	1:D:256:LYS:CG	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HH21	3:B:1001:AGS:H5'2	0.91	0.72
1:C:257:TYR:CD1	1:D:256:LYS:HG2	2.23	0.72
3:B:1003:AGS:C5'	3:B:1003:AGS:C8	2.67	0.72
1:B:765:ARG:HG3	1:B:765:ARG:NH1	2.04	0.72
1:E:583:GLN:HA	1:E:583:GLN:OE1	1.90	0.71
1:B:680:TYR:O	1:B:680:TYR:CD2	2.43	0.71
1:A:254:GLY:O	1:A:256:LYS:CD	2.36	0.71
1:B:310:LEU:HG	1:B:310:LEU:O	1.90	0.71
1:C:765:ARG:NH2	3:D:1003:AGS:PG	2.64	0.71
3:B:1001:AGS:O2A	3:B:1001:AGS:O1B	2.04	0.70
1:E:397:ASP:HA	1:E:400:CYS:SG	2.32	0.70
1:C:258:LYS:HG2	1:D:255:ALA:CB	2.15	0.70
1:C:257:TYR:CD2	1:D:256:LYS:HE2	2.27	0.70
1:B:759:ARG:HA	1:B:759:ARG:NE	2.06	0.70
1:E:186:VAL:O	1:E:186:VAL:CG1	2.40	0.70
1:D:205:LYS:NZ	1:D:333:ARG:CZ	2.54	0.69
1:B:660:ALA:N	1:B:665:TYR:OH	2.26	0.69
1:D:583:GLN:OE1	1:D:583:GLN:HA	1.91	0.69
1:D:765:ARG:CZ	1:E:826:ARG:HH12	2.04	0.69
1:D:680:TYR:HB2	1:D:720:ASN:O	1.92	0.69
1:B:660:ALA:CB	1:B:665:TYR:CZ	2.75	0.69
1:E:662:TYR:OH	1:F:650:TYR:CZ	2.11	0.69
1:F:819:TYR:O	1:F:819:TYR:CG	2.45	0.69
1:B:556:ILE:HG13	1:B:556:ILE:O	1.91	0.69
1:C:205:LYS:HD3	1:C:333:ARG:HH22	1.58	0.69
3:D:1003:AGS:O1B	3:D:1003:AGS:O2G	2.07	0.68
1:D:698:VAL:HG22	1:E:645:GLU:HG3	1.75	0.68
1:C:333:ARG:HD3	1:D:215:GLY:HA2	1.74	0.68
1:D:390:ASP:OD1	1:D:394:ASP:OD1	2.11	0.68
1:D:697:THR:CG2	1:E:644:SER:HB2	2.23	0.68
1:A:333:ARG:NH2	3:B:1001:AGS:O1A	2.27	0.68
1:B:333:ARG:HH21	1:B:334:ARG:CZ	2.06	0.68
1:D:205:LYS:NZ	1:D:333:ARG:NE	2.42	0.68
1:D:258:LYS:HG3	1:D:258:LYS:O	1.94	0.68
1:B:704:ASP:CG	1:B:765:ARG:HE	2.02	0.67
1:A:665:TYR:O	1:A:667:GLU:N	2.28	0.67
1:A:538:GLN:OE1	1:A:538:GLN:N	2.28	0.67
1:E:826:ARG:CB	1:E:827:PRO:HD3	2.21	0.67
1:C:330:ALA:HB1	1:C:334:ARG:NH1	2.10	0.66
3:C:1001:AGS:O2G	3:C:1001:AGS:O1B	2.11	0.66
1:E:192:GLU:OE1	1:E:192:GLU:N	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HG2	1:B:390:ASP:OD2	1.95	0.66
1:B:307:ARG:HE	1:B:307:ARG:CA	2.08	0.66
1:B:330:ALA:CB	1:B:334:ARG:NH1	2.41	0.66
1:B:330:ALA:O	1:B:334:ARG:HG2	1.95	0.66
1:C:327:LYS:HZ3	1:D:712:GLN:HE22	1.43	0.66
1:F:559:LYS:O	1:F:559:LYS:HG2	1.96	0.66
1:F:823:MET:O	1:F:826:ARG:HG2	1.96	0.66
1:D:765:ARG:NH1	1:E:826:ARG:HH12	1.94	0.66
1:D:659:THR:C	1:D:665:TYR:HE1	2.04	0.66
3:F:1001:AGS:H8	3:F:1001:AGS:H5'2	1.76	0.66
1:D:333:ARG:CD	1:E:215:GLY:CA	2.73	0.65
1:E:397:ASP:O	1:E:400:CYS:SG	2.53	0.65
1:B:333:ARG:NH2	1:B:334:ARG:NE	2.45	0.65
1:C:557:PRO:CG	1:C:680:TYR:CE2	2.80	0.65
1:D:765:ARG:HE	1:E:826:ARG:HH11	1.43	0.65
1:A:205:LYS:HE2	1:A:306:SER:CA	2.16	0.65
1:E:330:ALA:O	1:E:334:ARG:CG	2.44	0.65
1:A:258:LYS:HD3	1:B:255:ALA:CB	2.26	0.64
1:D:700:LEU:HD12	1:D:765:ARG:CD	2.25	0.64
3:D:1002:AGS:O1A	3:D:1002:AGS:O1B	2.15	0.64
1:C:257:TYR:HB3	1:D:256:LYS:HG3	1.79	0.64
1:D:668:GLY:O	1:D:669:GLY:C	2.40	0.64
1:E:680:TYR:CD1	1:E:680:TYR:N	2.64	0.64
1:A:645:GLU:O	1:A:645:GLU:HG3	1.98	0.64
1:B:638:MET:SD	1:B:638:MET:C	2.81	0.64
3:B:1003:AGS:O2A	3:B:1003:AGS:O1B	2.11	0.64
1:A:258:LYS:NZ	1:B:261:PHE:HD2	1.88	0.63
3:D:1001:AGS:O1B	3:D:1001:AGS:O1A	2.15	0.63
3:B:1003:AGS:C8	3:B:1003:AGS:H5'1	2.28	0.63
1:C:257:TYR:CB	1:D:256:LYS:CG	2.77	0.63
1:D:378:LEU:C	1:D:378:LEU:HD23	2.24	0.63
1:D:718:CYS:O	1:D:718:CYS:SG	2.55	0.63
1:D:751:MET:HA	1:D:751:MET:HE2	1.79	0.63
1:D:698:VAL:CG2	1:E:645:GLU:HG3	2.29	0.62
1:D:700:LEU:CD1	1:D:765:ARG:HD2	2.22	0.62
1:B:387:ARG:HA	1:B:387:ARG:NE	2.14	0.62
1:C:659:THR:C	1:C:665:TYR:CE1	2.76	0.62
1:C:701:GLN:OE1	1:C:701:GLN:HA	1.99	0.62
1:D:765:ARG:HH11	1:E:826:ARG:HH12	1.48	0.62
1:B:333:ARG:NH2	1:B:334:ARG:HH21	1.97	0.62
1:E:643:CYS:SG	1:E:691:ALA:HB2	2.39	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:826:ARG:CG	1:E:826:ARG:HH21	2.12	0.62
1:B:257:TYR:HB3	1:C:256:LYS:HG3	1.82	0.61
3:B:1001:AGS:O1B	3:B:1001:AGS:O2G	2.17	0.61
1:E:700:LEU:HD23	1:E:700:LEU:C	2.25	0.61
1:D:390:ASP:OD1	1:D:394:ASP:CG	2.43	0.61
1:C:257:TYR:CB	1:D:256:LYS:HG2	2.31	0.61
1:C:700:LEU:CD1	1:C:765:ARG:HD2	2.30	0.61
1:A:387:ARG:HA	1:A:387:ARG:NE	2.15	0.61
1:C:583:GLN:HA	1:C:583:GLN:OE1	1.99	0.61
1:A:205:LYS:NZ	1:A:334:ARG:HG2	2.16	0.61
1:D:698:VAL:HG22	1:E:645:GLU:HB2	1.82	0.61
1:C:334:ARG:HH11	1:C:334:ARG:CG	2.14	0.60
1:C:387:ARG:HA	1:C:387:ARG:NE	2.16	0.60
1:E:202:ARG:O	1:E:206:SER:HB3	2.01	0.60
1:A:219:THR:HG21	1:F:333:ARG:NH2	2.12	0.60
1:B:660:ALA:N	1:B:665:TYR:CZ	2.63	0.60
1:F:310:LEU:O	1:F:310:LEU:CG	2.44	0.60
1:D:256:LYS:O	1:D:257:TYR:CB	2.48	0.60
1:D:333:ARG:CD	1:E:215:GLY:HA2	2.32	0.60
1:D:698:VAL:HG22	1:E:645:GLU:CG	2.32	0.60
1:D:205:LYS:HZ1	1:D:333:ARG:CZ	2.12	0.60
1:C:258:LYS:CE	1:D:255:ALA:HB1	2.32	0.59
1:A:333:ARG:NH2	3:B:1001:AGS:PA	2.75	0.59
1:E:665:TYR:CZ	1:E:712:GLN:CG	2.85	0.59
1:B:192:GLU:N	1:B:192:GLU:OE1	2.33	0.59
1:A:330:ALA:HB1	1:A:334:ARG:HH11	1.57	0.59
1:D:702:MET:SD	1:D:702:MET:C	2.86	0.59
1:C:765:ARG:HH22	3:D:1003:AGS:PG	2.25	0.59
1:A:662:TYR:N	1:A:662:TYR:HD1	2.01	0.58
1:E:387:ARG:HA	1:E:387:ARG:HE	1.65	0.58
1:A:333:ARG:HH21	3:B:1001:AGS:PA	2.27	0.58
1:C:660:ALA:CA	1:C:665:TYR:CE1	2.82	0.58
1:B:258:LYS:NZ	1:C:296:ASP:OD2	2.36	0.58
1:E:302:LYS:NZ	1:E:328:ASP:OD1	2.37	0.58
1:C:258:LYS:HE2	1:D:255:ALA:HB1	1.86	0.58
1:A:712:GLN:HE21	1:B:666:ASP:CB	2.16	0.58
1:B:668:GLY:O	1:B:669:GLY:C	2.44	0.58
1:C:327:LYS:HZ3	1:D:712:GLN:NE2	2.01	0.58
1:C:668:GLY:O	1:C:669:GLY:C	2.47	0.57
1:A:257:TYR:HD1	1:A:257:TYR:N	2.01	0.57
1:E:202:ARG:CZ	1:F:398:ILE:CG1	2.83	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:583:GLN:OE1	1:E:583:GLN:CA	2.53	0.57
1:D:785:ASP:OD2	1:D:789:LYS:NZ	2.37	0.57
1:C:761:GLU:O	1:C:765:ARG:CG	2.53	0.57
1:D:700:LEU:CD1	1:D:765:ARG:CD	2.83	0.57
1:A:330:ALA:HB1	1:A:334:ARG:HH12	0.76	0.57
1:C:333:ARG:CD	1:D:215:GLY:HA3	2.32	0.57
1:C:645:GLU:OE1	1:C:654:LYS:NZ	2.38	0.56
1:C:802:TYR:CD1	1:C:802:TYR:C	2.83	0.56
1:D:205:LYS:HZ3	1:D:333:ARG:NE	2.00	0.56
1:D:300:ILE:O	1:D:300:ILE:CG2	2.52	0.56
1:B:306:SER:OG	1:B:307:ARG:CZ	2.54	0.56
1:C:257:TYR:CB	1:D:256:LYS:HG3	2.36	0.56
1:A:258:LYS:CB	1:B:255:ALA:HB1	2.25	0.56
1:A:662:TYR:CD2	1:B:650:TYR:HE2	2.23	0.56
1:C:542:ASP:C	1:C:542:ASP:OD1	2.47	0.56
1:F:410:LYS:O	1:F:410:LYS:HG3	2.06	0.56
1:F:735:ASN:C	1:F:735:ASN:OD1	2.45	0.56
1:A:219:THR:CB	1:F:333:ARG:HH12	2.19	0.56
1:A:257:TYR:HD1	1:A:257:TYR:H	1.54	0.56
1:C:327:LYS:NZ	1:D:712:GLN:NE2	2.53	0.56
3:A:1002:AGS:O3A	3:A:1002:AGS:O2G	2.24	0.55
1:C:643:CYS:SG	1:C:686:ASP:N	2.80	0.55
1:C:700:LEU:HD12	1:C:765:ARG:HD2	1.88	0.55
1:A:257:TYR:N	1:A:257:TYR:CD1	2.73	0.55
1:C:261:PHE:CD1	1:C:261:PHE:C	2.85	0.55
1:B:704:ASP:CG	1:B:765:ARG:NE	2.60	0.55
1:A:662:TYR:N	1:A:662:TYR:CD1	2.73	0.55
1:A:259:GLY:H	1:B:255:ALA:HB3	1.71	0.55
1:A:584:MET:HA	1:A:584:MET:HE2	1.89	0.55
1:D:583:GLN:OE1	1:D:583:GLN:CA	2.55	0.55
1:A:219:THR:HB	1:F:333:ARG:HH12	1.71	0.55
1:B:327:LYS:NZ	1:D:666:ASP:OD2	2.39	0.55
1:C:257:TYR:HB3	1:D:256:LYS:HG2	1.87	0.55
1:A:712:GLN:HE21	1:B:666:ASP:HB3	1.71	0.54
1:D:660:ALA:N	1:D:665:TYR:CZ	2.75	0.54
1:D:635:GLU:H	1:D:635:GLU:CD	2.15	0.54
1:D:660:ALA:HA	1:D:665:TYR:CZ	2.36	0.54
1:B:702:MET:SD	1:B:702:MET:C	2.90	0.54
1:D:387:ARG:NE	1:D:387:ARG:HA	2.23	0.54
1:E:809:GLU:H	1:E:809:GLU:CD	2.14	0.54
1:C:660:ALA:N	1:C:665:TYR:CE1	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LYS:HG2	1:E:261:PHE:CE2	2.41	0.54
1:E:305:LEU:HB3	1:E:334:ARG:HD3	1.89	0.54
1:E:809:GLU:N	1:E:809:GLU:CD	2.65	0.54
1:F:826:ARG:CB	1:F:827:PRO:HD3	2.19	0.54
1:B:333:ARG:HH21	1:B:334:ARG:NE	2.05	0.54
1:B:680:TYR:O	1:B:680:TYR:CG	2.61	0.54
1:D:698:VAL:HG22	1:E:645:GLU:CB	2.38	0.54
1:C:307:ARG:HA	1:C:307:ARG:NE	2.23	0.53
1:E:668:GLY:O	1:E:669:GLY:C	2.51	0.53
1:E:668:GLY:O	1:E:670:PHE:N	2.42	0.53
1:E:202:ARG:CZ	1:F:398:ILE:HG12	2.39	0.53
1:A:165:GLU:OE2	1:A:276:LYS:NZ	2.42	0.53
1:D:256:LYS:HB3	1:D:257:TYR:CE2	2.43	0.53
1:E:386:ARG:HD3	1:E:390:ASP:OD2	2.09	0.53
1:A:258:LYS:CD	1:B:255:ALA:HB1	2.37	0.53
1:E:387:ARG:NE	1:E:387:ARG:CA	2.72	0.52
1:E:761:GLU:H	1:E:761:GLU:CD	2.07	0.52
1:B:765:ARG:NE	1:C:826:ARG:NH2	2.58	0.52
1:A:668:GLY:O	1:A:670:PHE:N	2.43	0.52
1:C:257:TYR:CG	1:D:256:LYS:CG	2.88	0.52
1:D:258:LYS:CD	1:E:261:PHE:HE2	2.13	0.52
1:E:826:ARG:NH2	1:E:826:ARG:HG3	2.24	0.52
1:B:247:ASP:OD1	1:B:248:LEU:N	2.43	0.52
1:E:825:ALA:O	1:E:826:ARG:C	2.52	0.52
1:F:559:LYS:O	1:F:559:LYS:CG	2.57	0.52
1:F:826:ARG:HB2	1:F:827:PRO:CD	2.28	0.52
1:D:656:LEU:HD12	1:E:645:GLU:OE2	2.09	0.52
1:B:294:LYS:O	1:B:296:ASP:N	2.42	0.52
1:B:307:ARG:CA	1:B:307:ARG:NE	2.73	0.52
1:C:643:CYS:SG	1:C:686:ASP:O	2.67	0.52
1:F:826:ARG:NH1	3:F:1002:AGS:H5'1	2.25	0.51
1:E:700:LEU:HD23	1:E:700:LEU:O	2.09	0.51
1:A:294:LYS:O	1:A:296:ASP:N	2.43	0.51
1:A:334:ARG:NH2	3:B:1001:AGS:S1G	2.83	0.51
1:A:658:THR:OG1	1:A:664:GLY:O	2.29	0.51
1:C:660:ALA:N	1:C:665:TYR:CZ	2.75	0.51
1:E:247:ASP:OD1	1:E:248:LEU:N	2.43	0.51
1:E:644:SER:HB3	1:E:687:GLU:HB2	1.93	0.51
1:E:826:ARG:CB	1:E:827:PRO:CD	2.78	0.51
1:E:689:GLU:OE1	1:E:689:GLU:N	2.35	0.51
1:A:247:ASP:C	1:A:247:ASP:OD1	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ALA:C	1:B:658:THR:CG2	2.84	0.51
1:D:205:LYS:HZ1	1:D:333:ARG:NE	2.08	0.51
1:A:660:ALA:HB1	1:B:658:THR:HG23	1.92	0.50
1:B:805:ASN:O	1:B:806:LEU:C	2.54	0.50
1:E:238:LEU:HD23	1:E:238:LEU:H	1.75	0.50
1:A:620:LYS:NZ	1:A:686:ASP:OD1	2.44	0.50
1:A:662:TYR:CE2	1:B:650:TYR:CZ	3.00	0.50
1:E:826:ARG:CG	1:E:826:ARG:NH2	2.72	0.50
3:B:1003:AGS:C3'	3:B:1003:AGS:PA	2.98	0.50
1:C:334:ARG:NH1	1:C:334:ARG:CG	2.73	0.50
1:F:367:ILE:N	1:F:367:ILE:HD12	2.27	0.50
1:A:256:LYS:NZ	1:A:257:TYR:CE1	2.80	0.50
1:B:712:GLN:O	1:B:712:GLN:HG2	2.12	0.49
1:D:665:TYR:OH	1:D:712:GLN:HG3	2.12	0.49
1:D:751:MET:HE2	1:D:751:MET:CA	2.42	0.49
1:F:565:GLU:CD	1:F:568:LYS:HZ3	2.20	0.49
1:A:258:LYS:CG	1:B:255:ALA:CB	2.90	0.49
1:A:712:GLN:O	1:A:712:GLN:HG2	2.12	0.49
1:A:660:ALA:O	1:B:658:THR:HG22	2.08	0.49
1:B:387:ARG:HA	1:B:387:ARG:HE	1.78	0.49
1:D:258:LYS:CG	1:E:261:PHE:CE2	2.86	0.49
1:F:167:LEU:HD12	1:F:167:LEU:C	2.38	0.49
1:B:668:GLY:O	1:B:670:PHE:N	2.45	0.49
1:C:205:LYS:NZ	1:D:390:ASP:OD1	2.40	0.49
1:C:645:GLU:CD	1:C:645:GLU:C	2.81	0.49
1:E:274:GLU:O	1:E:274:GLU:HG3	2.12	0.49
1:C:583:GLN:OE1	1:C:583:GLN:CA	2.61	0.49
1:B:306:SER:C	1:B:307:ARG:NE	2.64	0.49
1:E:165:GLU:OE2	1:E:276:LYS:NZ	2.46	0.49
1:E:185:PRO:O	1:E:186:VAL:C	2.56	0.48
1:F:602:ALA:O	1:F:603:ASN:C	2.53	0.48
1:A:205:LYS:HE3	1:A:333:ARG:NH1	2.28	0.48
1:C:850:LYS:NZ	1:C:851:ASP:OD2	2.43	0.48
1:D:880:LEU:HB3	1:D:881:PRO:HD3	1.95	0.48
1:E:616:SER:OG	1:E:826:ARG:NH2	2.45	0.48
1:D:301:LEU:O	1:D:301:LEU:HG	2.13	0.48
1:E:728:ASN:C	1:E:728:ASN:OD1	2.55	0.48
1:A:333:ARG:NE	1:B:390:ASP:CG	2.72	0.48
1:F:826:ARG:HE	1:F:826:ARG:HA	1.79	0.48
1:C:559:LYS:HE2	1:C:559:LYS:HA	1.94	0.48
1:B:884:GLU:O	1:B:884:GLU:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LEU:HD23	1:E:238:LEU:N	2.28	0.48
1:E:294:LYS:O	1:E:296:ASP:N	2.46	0.48
1:F:802:TYR:CD1	1:F:802:TYR:C	2.91	0.48
1:B:883:HIS:O	1:B:884:GLU:C	2.57	0.48
1:B:666:ASP:OD1	1:B:666:ASP:N	2.40	0.48
1:B:759:ARG:HA	1:B:759:ARG:HE	1.76	0.48
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.46	0.48
1:F:672:THR:OG1	1:F:673:ASN:N	2.46	0.48
1:F:826:ARG:N	1:F:827:PRO:CD	2.77	0.48
1:A:542:ASP:N	1:A:542:ASP:OD1	2.44	0.47
1:B:629:GLY:O	1:B:633:ASN:N	2.46	0.47
1:D:645:GLU:OE1	1:D:654:LYS:NZ	2.47	0.47
1:E:202:ARG:O	1:E:206:SER:CB	2.62	0.47
1:C:806:LEU:HD12	1:C:806:LEU:C	2.39	0.47
1:D:742:ILE:HG23	1:D:742:ILE:O	2.13	0.47
1:B:555:GLY:O	1:B:556:ILE:C	2.56	0.47
1:C:333:ARG:CD	1:D:215:GLY:CA	2.84	0.47
1:A:563:GLU:H	1:A:563:GLU:CD	2.19	0.47
1:C:260:ASP:OD2	1:C:264:ARG:NH1	2.47	0.47
1:C:680:TYR:HB2	1:C:720:ASN:O	2.14	0.47
1:E:397:ASP:CA	1:E:400:CYS:SG	3.03	0.47
1:D:255:ALA:O	1:D:256:LYS:C	2.57	0.47
1:F:230:ILE:HD13	1:F:230:ILE:HA	1.70	0.47
1:F:261:PHE:CD1	1:F:261:PHE:C	2.93	0.47
1:A:665:TYR:OH	1:A:712:GLN:CG	2.58	0.47
1:E:662:TYR:CZ	1:F:650:TYR:HE1	1.85	0.47
1:B:761:GLU:O	1:B:765:ARG:NH1	2.48	0.47
1:D:805:ASN:O	1:D:806:LEU:C	2.55	0.46
1:A:333:ARG:HD3	1:A:333:ARG:O	2.15	0.46
1:D:665:TYR:CE2	1:D:712:GLN:CD	2.94	0.46
1:D:660:ALA:CA	1:D:665:TYR:OH	2.61	0.46
1:A:185:PRO:O	3:A:1001:AGS:H2	2.16	0.46
1:B:819:TYR:CD2	1:B:819:TYR:C	2.93	0.46
1:C:258:LYS:CE	1:D:255:ALA:CB	2.93	0.46
1:A:660:ALA:O	1:B:658:THR:HG23	2.15	0.46
1:C:539:ASN:OD1	1:C:539:ASN:N	2.44	0.46
1:D:378:LEU:HD23	1:D:378:LEU:O	2.14	0.46
1:B:284:ASP:O	1:B:285:GLU:C	2.59	0.46
1:C:799:ASP:OD2	1:C:800:LYS:NZ	2.48	0.46
1:F:789:LYS:NZ	1:F:793:GLU:OE2	2.45	0.46
1:A:302:LYS:HB3	1:A:303:PRO:HD3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:PHE:CD2	1:A:630:PHE:C	2.92	0.46
1:C:634:ASP:OD1	1:C:634:ASP:C	2.59	0.46
1:C:257:TYR:HA	2:P:5:UNK:O	2.16	0.45
1:E:202:ARG:CZ	1:F:398:ILE:HG13	2.46	0.45
1:E:249:ALA:O	1:E:250:ALA:C	2.59	0.45
1:F:851:ASP:OD2	1:F:852:LYS:NZ	2.44	0.45
1:B:638:MET:HE2	1:B:638:MET:HB2	1.56	0.45
1:C:387:ARG:HA	1:C:387:ARG:HE	1.80	0.45
1:C:649:LYS:HB2	1:C:649:LYS:HE2	1.78	0.45
3:E:1001:AGS:O1B	3:E:1001:AGS:O2A	2.27	0.45
1:A:634:ASP:OD1	1:A:635:GLU:N	2.50	0.45
1:D:256:LYS:CB	1:D:257:TYR:CD2	3.00	0.45
1:D:880:LEU:CB	1:D:881:PRO:CD	2.95	0.45
1:E:255:ALA:O	1:E:256:LYS:C	2.58	0.45
1:D:326:GLU:HA	1:D:326:GLU:OE1	2.16	0.45
1:D:809:GLU:N	1:D:809:GLU:CD	2.66	0.45
1:F:826:ARG:HA	1:F:826:ARG:NE	2.31	0.45
1:C:660:ALA:CB	1:C:665:TYR:CZ	2.88	0.45
1:B:761:GLU:H	1:B:761:GLU:CD	2.13	0.45
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.71	0.45
1:D:764:ASN:C	1:D:764:ASN:OD1	2.53	0.45
1:E:667:GLU:OE1	1:E:712:GLN:OE1	2.34	0.45
1:A:660:ALA:CB	1:B:658:THR:HG23	2.47	0.44
1:B:309:GLN:N	1:B:309:GLN:CD	2.75	0.44
1:B:704:ASP:OD1	1:B:765:ARG:HD3	2.17	0.44
1:B:261:PHE:CD1	1:B:261:PHE:C	2.94	0.44
1:B:820:SER:O	1:B:824:GLY:N	2.51	0.44
1:D:629:GLY:O	1:D:633:ASN:N	2.47	0.44
1:C:294:LYS:O	1:C:295:ASP:C	2.60	0.44
1:D:680:TYR:O	1:D:680:TYR:CG	2.70	0.44
1:E:568:LYS:O	1:E:572:MET:N	2.50	0.44
1:A:880:LEU:HB2	1:A:881:PRO:HD2	2.00	0.44
1:C:387:ARG:NE	1:C:387:ARG:CA	2.80	0.44
1:D:649:LYS:NZ	2:P:21:UNK:O	2.43	0.44
1:A:825:ALA:O	1:A:826:ARG:C	2.57	0.44
3:F:1001:AGS:H5'2	3:F:1001:AGS:C8	2.47	0.44
1:A:205:LYS:HZ2	1:A:334:ARG:HG2	1.83	0.43
1:A:712:GLN:NE2	1:B:666:ASP:CB	2.81	0.43
1:A:665:TYR:HD1	1:A:665:TYR:HA	1.67	0.43
1:B:307:ARG:HE	1:B:307:ARG:HA	1.78	0.43
1:B:539:ASN:OD1	1:B:539:ASN:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:774:LYS:NZ	1:E:822:ASP:OD1	2.50	0.43
1:A:299:ASN:OD1	1:A:299:ASN:C	2.60	0.43
1:A:302:LYS:O	1:A:304:ALA:N	2.52	0.43
1:F:382:TYR:CD1	1:F:383:LEU:HG	2.54	0.43
1:F:805:ASN:O	1:F:806:LEU:C	2.60	0.43
1:D:635:GLU:OE1	1:D:635:GLU:N	2.35	0.43
1:D:662:TYR:CD1	1:D:662:TYR:N	2.86	0.43
1:A:219:THR:CG2	1:F:333:ARG:HH12	2.32	0.43
1:A:880:LEU:CB	1:A:881:PRO:CD	2.97	0.43
1:B:673:ASN:OD1	1:B:674:GLN:N	2.51	0.43
1:B:772:PHE:N	1:B:772:PHE:CD1	2.87	0.43
1:C:735:ASN:OD1	1:C:735:ASN:C	2.61	0.43
1:D:702:MET:HE3	1:D:702:MET:HB3	1.86	0.43
1:A:302:LYS:HB3	1:A:303:PRO:CD	2.49	0.43
1:D:293:GLY:O	1:D:294:LYS:HB2	2.19	0.43
1:F:607:PRO:O	1:F:608:ALA:C	2.60	0.43
1:B:302:LYS:HB2	1:B:303:PRO:HD3	2.01	0.42
1:C:393:LEU:HA	1:C:393:LEU:HD23	1.79	0.42
1:E:408:ASP:OD1	1:E:409:SER:N	2.52	0.42
1:E:660:ALA:HA	1:E:665:TYR:CE1	2.54	0.42
1:E:704:ASP:O	1:E:705:ASP:CB	2.66	0.42
1:C:299:ASN:OD1	1:C:299:ASN:C	2.59	0.42
1:B:659:THR:O	1:B:665:TYR:CE1	2.71	0.42
3:D:1003:AGS:O2A	3:D:1003:AGS:O2B	2.38	0.42
1:A:258:LYS:CD	1:B:255:ALA:CB	2.95	0.42
1:B:852:LYS:HD2	1:B:852:LYS:N	2.34	0.42
1:F:588:LYS:HB2	1:F:588:LYS:HE2	1.83	0.42
1:F:218:LYS:HE2	1:F:218:LYS:HB3	1.81	0.42
1:F:583:GLN:OE1	1:F:583:GLN:HA	2.20	0.42
1:A:333:ARG:HH22	3:B:1001:AGS:C5'	1.98	0.42
3:B:1003:AGS:PA	3:B:1003:AGS:H3'	2.60	0.42
1:A:205:LYS:HZ1	1:A:334:ARG:HG2	1.85	0.42
1:B:302:LYS:CB	1:B:303:PRO:CD	2.98	0.42
1:C:660:ALA:N	1:C:665:TYR:HH	2.15	0.42
1:D:256:LYS:HB3	1:D:257:TYR:CZ	2.55	0.42
1:D:741:LYS:O	1:D:742:ILE:C	2.60	0.42
1:B:230:ILE:HA	1:B:230:ILE:HD13	1.83	0.42
1:B:307:ARG:NE	1:B:307:ARG:HA	2.33	0.42
1:C:334:ARG:NH1	1:C:334:ARG:HG2	2.35	0.42
1:C:702:MET:HE2	1:C:702:MET:HB3	1.96	0.42
1:D:665:TYR:CZ	1:D:712:GLN:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LYS:NZ	1:E:274:GLU:OE1	2.48	0.42
1:D:310:LEU:O	1:D:311:LYS:C	2.60	0.42
1:D:826:ARG:N	1:D:827:PRO:CD	2.83	0.42
3:D:1001:AGS:H5'1	3:D:1001:AGS:H8	2.01	0.42
1:A:310:LEU:O	1:A:310:LEU:CG	2.53	0.41
1:A:712:GLN:NE2	1:B:666:ASP:CG	2.78	0.41
1:B:835:GLU:OE1	1:B:839:LYS:NZ	2.53	0.41
1:C:606:GLN:O	1:C:607:PRO:C	2.63	0.41
1:D:656:LEU:CD1	1:E:645:GLU:CD	2.93	0.41
1:B:218:LYS:HB2	1:B:218:LYS:HE2	1.81	0.41
1:B:765:ARG:HE	1:C:826:ARG:NH2	2.18	0.41
1:C:761:GLU:O	1:C:765:ARG:HG3	2.21	0.41
1:C:800:LYS:HA	1:C:800:LYS:HD3	1.85	0.41
1:A:302:LYS:CB	1:A:303:PRO:CD	2.98	0.41
1:B:257:TYR:O	1:B:258:LYS:C	2.62	0.41
1:B:306:SER:O	1:B:307:ARG:NH2	2.43	0.41
1:C:699:MET:O	1:C:700:LEU:C	2.62	0.41
1:E:585:ASP:OD2	1:E:741:LYS:NZ	2.53	0.41
1:F:678:LYS:HB3	1:F:681:SER:HB3	2.01	0.41
1:B:638:MET:SD	1:B:638:MET:O	2.78	0.41
1:B:765:ARG:NH1	1:B:765:ARG:CG	2.73	0.41
1:C:333:ARG:NH1	1:D:390:ASP:OD2	2.49	0.41
1:C:643:CYS:SG	1:C:685:PHE:C	3.04	0.41
1:D:712:GLN:O	1:D:712:GLN:HG2	2.20	0.41
1:D:378:LEU:C	1:D:378:LEU:CD2	2.93	0.41
1:D:665:TYR:HD1	1:D:665:TYR:HA	1.62	0.41
1:E:603:ASN:OD1	1:E:603:ASN:C	2.62	0.41
1:A:660:ALA:C	1:B:658:THR:HG21	2.46	0.41
1:C:680:TYR:O	1:C:680:TYR:CG	2.70	0.41
1:A:665:TYR:C	1:A:667:GLU:N	2.78	0.41
1:C:643:CYS:HA	1:C:646:LEU:CD1	2.51	0.41
1:D:635:GLU:CD	1:D:635:GLU:N	2.79	0.41
1:D:668:GLY:CA	1:D:672:THR:HB	2.50	0.41
1:B:704:ASP:OD1	1:B:765:ARG:CD	2.68	0.41
1:B:759:ARG:NE	1:B:759:ARG:CA	2.77	0.41
1:C:774:LYS:NZ	1:C:821:ASP:O	2.48	0.41
1:E:302:LYS:HB2	1:E:303:PRO:CD	2.50	0.41
1:F:644:SER:HB3	1:F:687:GLU:HB3	2.03	0.41
1:B:306:SER:HB2	1:B:307:ARG:NH2	2.36	0.41
1:B:388:LEU:O	1:B:389:PRO:C	2.62	0.41
1:C:242:LYS:HE3	1:C:242:LYS:HB3	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LYS:O	1:C:296:ASP:N	2.54	0.41
1:C:661:GLY:N	1:D:663:VAL:O	2.52	0.41
1:D:660:ALA:N	1:D:665:TYR:OH	2.54	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.86	0.41
1:E:649:LYS:HA	1:E:649:LYS:HD3	1.81	0.41
1:E:805:ASN:O	1:E:806:LEU:C	2.61	0.41
1:F:172:ILE:HD12	1:F:172:ILE:N	2.36	0.41
1:A:638:MET:HE2	1:A:638:MET:HB2	1.89	0.40
1:D:242:LYS:HB3	1:D:242:LYS:HE3	1.94	0.40
1:F:568:LYS:O	1:F:572:MET:N	2.54	0.40
1:A:699:MET:SD	1:A:699:MET:C	3.04	0.40
1:B:306:SER:CB	1:B:307:ARG:NH2	2.85	0.40
1:B:634:ASP:OD1	1:B:634:ASP:C	2.63	0.40
1:B:735:ASN:OD1	1:B:735:ASN:C	2.64	0.40
1:F:881:PRO:O	1:F:882:ASN:C	2.65	0.40
1:A:665:TYR:CZ	1:A:712:GLN:CD	2.99	0.40
1:B:302:LYS:HB2	1:B:303:PRO:CD	2.52	0.40
1:B:333:ARG:HD3	1:C:215:GLY:HA2	2.03	0.40
1:E:813:PHE:CD2	1:E:813:PHE:C	2.99	0.40
1:B:583:GLN:HA	1:B:583:GLN:OE1	2.22	0.40
1:D:294:LYS:O	1:D:295:ASP:C	2.63	0.40
1:F:352:LEU:O	1:F:356:GLN:N	2.55	0.40
3:F:1001:AGS:O2G	3:F:1001:AGS:O1B	2.39	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	573/908 (63%)	533 (93%)	28 (5%)	12 (2%)	5	32
1	B	573/908 (63%)	552 (96%)	18 (3%)	3 (0%)	24	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	573/908 (63%)	548 (96%)	22 (4%)	3 (0%)	24	60
1	D	573/908 (63%)	547 (96%)	20 (4%)	6 (1%)	12	45
1	E	573/908 (63%)	544 (95%)	22 (4%)	7 (1%)	10	42
1	F	556/908 (61%)	535 (96%)	19 (3%)	2 (0%)	30	65
All	All	3421/5448 (63%)	3259 (95%)	129 (4%)	33 (1%)	15	45

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	669	GLY
1	B	302	LYS
1	E	186	VAL
1	E	274	GLU
1	E	669	GLY
1	F	187	ILE
1	F	819	TYR
1	A	256	LYS
1	A	277	THR
1	A	660	ALA
1	A	666	ASP
1	B	295	ASP
1	C	669	GLY
1	D	277	THR
1	D	669	GLY
1	E	257	TYR
1	E	277	THR
1	A	295	ASP
1	A	298	ALA
1	C	258	LYS
1	C	277	THR
1	D	275	SER
1	E	295	ASP
1	A	257	TYR
1	A	275	SER
1	D	880	LEU
1	A	880	LEU
1	D	257	TYR
1	D	301	LEU
1	A	663	VAL
1	B	556	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	705	ASP

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 PDB entries followed by that with respect to all EM entries.

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	497/783 (64%)	493 (99%)	4 (1%)	73	77
1	B	497/783 (64%)	492 (99%)	5 (1%)	68	76
1	C	497/783 (64%)	490 (99%)	7 (1%)	59	71
1	D	497/783 (64%)	491 (99%)	6 (1%)	63	73
1	E	497/783 (64%)	492 (99%)	5 (1%)	68	76
1	F	488/783 (62%)	487 (100%)	1 (0%)	87	87
All	All	2973/4698 (63%)	2945 (99%)	28 (1%)	68	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	A	659	THR
1	A	662	TYR
1	A	665	TYR
1	B	307	ARG
1	B	333	ARG
1	B	334	ARG
1	B	665	TYR
1	B	765	ARG
1	C	256	LYS
1	C	333	ARG
1	C	334	ARG
1	C	643	CYS
1	C	665	TYR
1	C	680	TYR
1	C	765	ARG
1	D	257	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	258	LYS
1	D	333	ARG
1	D	334	ARG
1	D	665	TYR
1	D	680	TYR
1	E	334	ARG
1	E	643	CYS
1	E	663	VAL
1	E	665	TYR
1	E	826	ARG
1	F	334	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	GLN
1	A	674	GLN
1	A	712	GLN
1	A	728	ASN
1	B	377	GLN
1	B	633	ASN
1	B	701	GLN
1	B	712	GLN
1	B	838	ASN
1	B	883	HIS
1	C	177	GLN
1	C	571	HIS
1	C	712	GLN
1	C	808	GLN
1	D	239	GLN
1	D	309	GLN
1	D	362	HIS
1	D	701	GLN
1	D	712	GLN
1	D	720	ASN
1	E	781	HIS
1	E	808	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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$
3	AGS	F	1002	-	32,33,33	2.18	8 (25%)	45,52,52	2.28	17 (37%)
3	AGS	B	1003	-	32,33,33	2.26	10 (31%)	45,52,52	2.08	11 (24%)
3	AGS	B	1002	-	32,33,33	2.22	10 (31%)	45,52,52	2.31	16 (35%)
3	AGS	D	1001	-	32,33,33	2.36	10 (31%)	45,52,52	2.15	13 (28%)
3	AGS	C	1001	-	32,33,33	2.28	9 (28%)	45,52,52	2.37	17 (37%)
3	AGS	E	1001	-	32,33,33	2.29	10 (31%)	45,52,52	2.32	17 (37%)
3	AGS	A	1001	-	32,33,33	2.28	10 (31%)	45,52,52	2.29	15 (33%)
3	AGS	D	1003	-	32,33,33	2.31	8 (25%)	45,52,52	2.37	16 (35%)
3	AGS	D	1002	-	32,33,33	2.35	9 (28%)	45,52,52	2.27	14 (31%)
3	AGS	A	1002	-	32,33,33	2.07	5 (15%)	45,52,52	2.10	12 (26%)
3	AGS	F	1001	-	32,33,33	1.93	6 (18%)	45,52,52	2.17	13 (28%)
3	AGS	B	1001	-	32,33,33	2.34	9 (28%)	45,52,52	2.06	14 (31%)

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
3	AGS	F	1002	-	-	7/21/38/38	0/3/3/3
3	AGS	B	1003	-	-	7/21/38/38	0/3/3/3
3	AGS	B	1002	-	-	5/21/38/38	0/3/3/3
3	AGS	D	1001	-	-	4/21/38/38	0/3/3/3
3	AGS	C	1001	-	-	7/21/38/38	0/3/3/3
3	AGS	E	1001	-	-	5/21/38/38	0/3/3/3
3	AGS	A	1001	-	-	6/21/38/38	0/3/3/3
3	AGS	D	1003	-	-	3/21/38/38	0/3/3/3
3	AGS	D	1002	-	-	3/21/38/38	0/3/3/3
3	AGS	A	1002	-	-	9/21/38/38	0/3/3/3
3	AGS	F	1001	-	-	6/21/38/38	0/3/3/3
3	AGS	B	1001	-	-	4/21/38/38	0/3/3/3

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	AGS	PG-S1G	8.02	2.08	1.90
3	F	1002	AGS	PG-S1G	7.38	2.06	1.90
3	B	1001	AGS	PG-S1G	7.36	2.06	1.90
3	D	1002	AGS	PG-S1G	7.31	2.06	1.90
3	F	1001	AGS	PG-S1G	7.21	2.06	1.90
3	A	1001	AGS	PG-S1G	7.10	2.06	1.90
3	D	1001	AGS	PG-S1G	6.98	2.05	1.90
3	B	1002	AGS	PG-S1G	6.97	2.05	1.90
3	E	1001	AGS	PG-S1G	6.47	2.04	1.90
3	B	1003	AGS	PG-S1G	6.44	2.04	1.90
3	C	1001	AGS	PG-S1G	6.41	2.04	1.90
3	D	1003	AGS	PG-S1G	6.16	2.04	1.90
3	D	1003	AGS	PB-O3A	-5.49	1.53	1.59
3	E	1001	AGS	PB-O3A	-5.45	1.53	1.59
3	C	1001	AGS	PB-O3B	-5.18	1.53	1.59
3	F	1002	AGS	C5-C4	5.08	1.48	1.39
3	D	1001	AGS	PB-O3A	-4.95	1.54	1.59
3	D	1002	AGS	PB-O3A	-4.93	1.54	1.59
3	B	1001	AGS	PA-O3A	-4.93	1.54	1.59
3	A	1001	AGS	C5-C4	4.83	1.47	1.39
3	B	1003	AGS	PB-O3A	-4.78	1.54	1.59
3	C	1001	AGS	C5-N7	-4.63	1.30	1.39
3	A	1002	AGS	C5-C4	4.59	1.47	1.39
3	F	1001	AGS	C5-C4	4.56	1.47	1.39
3	D	1001	AGS	PA-O3A	-4.55	1.54	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	AGS	PB-O3A	-4.54	1.54	1.59
3	B	1001	AGS	C5-C4	4.52	1.47	1.39
3	B	1002	AGS	C5-C4	4.44	1.47	1.39
3	D	1002	AGS	PA-O3A	-4.40	1.54	1.59
3	D	1003	AGS	PB-O3B	-4.38	1.54	1.59
3	D	1003	AGS	C5-N7	-4.37	1.31	1.39
3	D	1002	AGS	C5-C4	4.36	1.46	1.39
3	E	1001	AGS	C5-N7	-4.35	1.31	1.39
3	C	1001	AGS	C5-C4	4.30	1.46	1.39
3	D	1003	AGS	C5-C4	4.28	1.46	1.39
3	D	1001	AGS	C5-C4	4.27	1.46	1.39
3	E	1001	AGS	PA-O3A	-4.23	1.54	1.59
3	F	1002	AGS	C5-N7	-4.21	1.31	1.39
3	B	1003	AGS	C5-C4	4.08	1.46	1.39
3	B	1001	AGS	PB-O3A	-4.07	1.55	1.59
3	E	1001	AGS	C5-C4	4.03	1.46	1.39
3	A	1001	AGS	PA-O3A	-3.96	1.55	1.59
3	B	1002	AGS	C5-N7	-3.96	1.31	1.39
3	B	1002	AGS	PB-O3B	-3.92	1.55	1.59
3	B	1002	AGS	PA-O3A	-3.91	1.55	1.59
3	B	1003	AGS	C5-N7	-3.91	1.31	1.39
3	A	1002	AGS	C5-N7	-3.82	1.32	1.39
3	C	1001	AGS	PB-O3A	-3.76	1.55	1.59
3	D	1001	AGS	PB-O3B	-3.73	1.55	1.59
3	F	1002	AGS	PB-O3A	-3.70	1.55	1.59
3	D	1002	AGS	PB-O3B	-3.60	1.55	1.59
3	B	1003	AGS	PB-O3B	-3.59	1.55	1.59
3	B	1001	AGS	C5-N7	-3.54	1.32	1.39
3	D	1001	AGS	C5-N7	-3.53	1.32	1.39
3	D	1002	AGS	C5-N7	-3.51	1.32	1.39
3	F	1001	AGS	C5-N7	-3.31	1.33	1.39
3	B	1003	AGS	PA-O3A	-3.25	1.56	1.59
3	C	1001	AGS	PA-O3A	-3.24	1.56	1.59
3	A	1001	AGS	C5-N7	-3.24	1.33	1.39
3	B	1001	AGS	PB-O3B	-2.94	1.56	1.59
3	D	1003	AGS	PA-O3A	-2.93	1.56	1.59
3	B	1003	AGS	C4-N9	-2.93	1.31	1.37
3	B	1001	AGS	C4-N9	-2.92	1.31	1.37
3	E	1001	AGS	C8-N9	-2.90	1.32	1.37
3	B	1002	AGS	PB-O3A	-2.83	1.56	1.59
3	D	1001	AGS	C4-N9	-2.78	1.31	1.37
3	B	1003	AGS	C8-N9	-2.77	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1001	AGS	PB-O3B	-2.71	1.56	1.59
3	C	1001	AGS	C8-N9	-2.69	1.33	1.37
3	D	1003	AGS	PG-O3G	-2.60	1.46	1.54
3	D	1003	AGS	C8-N9	-2.56	1.33	1.37
3	B	1002	AGS	C4-N9	-2.56	1.32	1.37
3	D	1002	AGS	C4-N9	-2.50	1.32	1.37
3	B	1001	AGS	C8-N9	-2.46	1.33	1.37
3	B	1002	AGS	C8-N9	-2.46	1.33	1.37
3	D	1001	AGS	C8-N9	-2.40	1.33	1.37
3	F	1002	AGS	C8-N9	-2.39	1.33	1.37
3	A	1002	AGS	PG-O2G	2.39	1.62	1.54
3	A	1001	AGS	PG-O2G	2.39	1.62	1.54
3	F	1002	AGS	PG-O2G	2.38	1.62	1.54
3	A	1001	AGS	PB-O3B	-2.36	1.56	1.59
3	B	1003	AGS	PG-O3G	-2.34	1.47	1.54
3	A	1001	AGS	C5-C6	2.32	1.47	1.41
3	F	1001	AGS	PG-O2G	2.32	1.62	1.54
3	D	1001	AGS	PG-O3G	-2.31	1.47	1.54
3	A	1001	AGS	C8-N9	-2.30	1.33	1.37
3	C	1001	AGS	C4-N9	-2.28	1.32	1.37
3	D	1002	AGS	PG-O3G	-2.21	1.47	1.54
3	E	1001	AGS	C4-N9	-2.19	1.33	1.37
3	E	1001	AGS	PG-O3G	-2.19	1.47	1.54
3	B	1001	AGS	PG-O2G	2.18	1.61	1.54
3	A	1001	AGS	C4-N9	-2.18	1.33	1.37
3	F	1002	AGS	PB-O3B	-2.16	1.57	1.59
3	C	1001	AGS	PG-O3G	-2.15	1.47	1.54
3	B	1002	AGS	PG-O2G	2.15	1.61	1.54
3	B	1002	AGS	PG-O3G	-2.14	1.47	1.54
3	F	1002	AGS	PG-O3G	-2.12	1.47	1.54
3	A	1002	AGS	C4-N9	-2.09	1.33	1.37
3	B	1003	AGS	PG-O2G	2.09	1.61	1.54
3	D	1002	AGS	PG-O2G	2.06	1.61	1.54
3	D	1001	AGS	PG-O2G	2.05	1.61	1.54
3	F	1001	AGS	PB-O3A	-2.05	1.57	1.59
3	E	1001	AGS	PG-O2G	2.02	1.61	1.54
3	F	1001	AGS	PG-O3G	-2.00	1.48	1.54

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1003	AGS	PB-O3B-PG	-7.47	105.85	133.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	PB-O3B-PG	-7.29	106.48	133.17
3	B	1002	AGS	PB-O3B-PG	-7.13	107.09	133.17
3	C	1001	AGS	PB-O3B-PG	-7.07	107.31	133.17
3	D	1003	AGS	C5-C4-N3	-6.79	117.37	126.72
3	A	1001	AGS	PB-O3B-PG	-6.64	108.87	133.17
3	F	1002	AGS	C5-C4-N3	-6.59	117.65	126.72
3	E	1001	AGS	C5-C4-N3	-6.53	117.72	126.72
3	A	1001	AGS	C5-C4-N3	-6.45	117.84	126.72
3	C	1001	AGS	C5-C4-N3	-6.34	117.99	126.72
3	D	1001	AGS	PB-O3B-PG	-6.31	110.06	133.17
3	A	1002	AGS	C5-C4-N3	-6.24	118.12	126.72
3	F	1001	AGS	C5-C4-N3	-6.20	118.18	126.72
3	B	1002	AGS	C5-C4-N3	-6.13	118.28	126.72
3	B	1003	AGS	C5-C4-N3	-6.12	118.29	126.72
3	E	1001	AGS	PB-O3B-PG	-6.11	110.82	133.17
3	C	1001	AGS	N3-C4-N9	6.08	137.51	127.17
3	D	1003	AGS	N3-C4-N9	6.01	137.38	127.17
3	D	1002	AGS	C5-C4-N3	-5.94	118.53	126.72
3	F	1002	AGS	N3-C4-N9	5.92	137.24	127.17
3	B	1001	AGS	C5-C4-N3	-5.91	118.58	126.72
3	D	1001	AGS	C5-C4-N3	-5.88	118.61	126.72
3	E	1001	AGS	N3-C4-N9	5.87	137.15	127.17
3	B	1003	AGS	PB-O3B-PG	-5.86	111.71	133.17
3	F	1001	AGS	N3-C4-N9	5.68	136.83	127.17
3	F	1001	AGS	PB-O3B-PG	-5.61	112.63	133.17
3	B	1002	AGS	N3-C4-N9	5.52	136.56	127.17
3	A	1002	AGS	N3-C4-N9	5.48	136.48	127.17
3	B	1001	AGS	PB-O3B-PG	-5.35	113.59	133.17
3	F	1002	AGS	PB-O3B-PG	-5.32	113.69	133.17
3	A	1001	AGS	N3-C4-N9	5.20	136.01	127.17
3	D	1002	AGS	N3-C4-N9	5.06	135.78	127.17
3	B	1001	AGS	N3-C4-N9	4.98	135.64	127.17
3	D	1001	AGS	N3-C4-N9	4.92	135.54	127.17
3	B	1003	AGS	N3-C4-N9	4.71	135.18	127.17
3	A	1002	AGS	PB-O3B-PG	-4.31	117.41	133.17
3	C	1001	AGS	N6-C6-N1	3.72	126.67	118.38
3	A	1001	AGS	C4-C5-N7	-3.65	106.41	110.58
3	A	1002	AGS	O2G-PG-O3B	3.48	116.25	104.64
3	F	1001	AGS	O2G-PG-O3B	3.44	116.13	104.64
3	E	1001	AGS	O3A-PA-O1A	-3.40	100.48	110.70
3	F	1002	AGS	O2G-PG-O3B	3.35	115.82	104.64
3	B	1002	AGS	N6-C6-N1	3.34	125.81	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1003	AGS	N6-C6-N1	3.31	125.74	118.38
3	B	1002	AGS	O2G-PG-O3B	3.30	115.65	104.64
3	B	1003	AGS	C4-C5-N7	-3.28	106.83	110.58
3	E	1001	AGS	C2-N3-C4	3.27	119.81	111.83
3	D	1001	AGS	O3A-PA-O1A	-3.26	100.90	110.70
3	D	1003	AGS	C2-N3-C4	3.26	119.79	111.83
3	F	1001	AGS	C2-N3-C4	3.25	119.78	111.83
3	A	1001	AGS	C2-N3-C4	3.25	119.77	111.83
3	E	1001	AGS	N6-C6-N1	3.25	125.61	118.38
3	D	1002	AGS	C2-N3-C4	3.25	119.76	111.83
3	D	1002	AGS	O3A-PA-O1A	-3.24	100.97	110.70
3	A	1002	AGS	C2-N3-C4	3.22	119.70	111.83
3	B	1003	AGS	C2-N3-C4	3.20	119.64	111.83
3	B	1002	AGS	C2-N3-C4	3.16	119.54	111.83
3	B	1001	AGS	C2-N3-C4	3.15	119.53	111.83
3	D	1001	AGS	C2-N3-C4	3.11	119.43	111.83
3	F	1002	AGS	N6-C6-N1	3.08	125.23	118.38
3	B	1003	AGS	O2G-PG-O3B	3.05	114.81	104.64
3	D	1001	AGS	O2G-PG-O3B	3.05	114.81	104.64
3	F	1002	AGS	C2-N3-C4	3.04	119.25	111.83
3	F	1001	AGS	N6-C6-N1	3.00	125.05	118.38
3	F	1002	AGS	C1'-N9-C8	-3.00	120.45	127.09
3	A	1002	AGS	N6-C6-N1	2.99	125.03	118.38
3	C	1001	AGS	C2-N3-C4	2.99	119.12	111.83
3	B	1001	AGS	C4-C5-N7	-2.96	107.20	110.58
3	D	1001	AGS	N6-C6-N1	2.95	124.94	118.38
3	D	1001	AGS	C4-C5-N7	-2.94	107.22	110.58
3	A	1002	AGS	O3B-PB-O1B	-2.92	101.93	110.70
3	F	1002	AGS	C4-C5-N7	-2.90	107.26	110.58
3	A	1001	AGS	O2G-PG-O3B	2.88	114.24	104.64
3	B	1002	AGS	O3A-PA-O1A	-2.84	102.16	110.70
3	C	1001	AGS	O2G-PG-O3B	2.79	113.96	104.64
3	F	1001	AGS	N3-C2-N1	-2.79	124.36	128.58
3	C	1001	AGS	C4-N9-C8	2.78	108.66	105.74
3	D	1002	AGS	N3-C2-N1	-2.78	124.38	128.58
3	E	1001	AGS	C4-C5-N7	-2.77	107.41	110.58
3	E	1001	AGS	O2G-PG-O3B	2.77	113.87	104.64
3	A	1002	AGS	C5'-C4'-C3'	-2.76	105.28	115.21
3	C	1001	AGS	C1'-N9-C8	-2.74	121.01	127.09
3	A	1002	AGS	C4-C5-N7	-2.73	107.46	110.58
3	D	1001	AGS	C4-N9-C8	2.72	108.59	105.74
3	B	1001	AGS	C4-N9-C8	2.67	108.54	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	N6-C6-N1	2.66	124.31	118.38
3	D	1002	AGS	C4-C5-N7	-2.65	107.55	110.58
3	A	1001	AGS	N6-C6-N1	2.65	124.28	118.38
3	F	1002	AGS	C5-N7-C8	2.64	107.59	103.45
3	F	1002	AGS	O3A-PA-O1A	-2.63	102.78	110.70
3	E	1001	AGS	C5'-C4'-C3'	-2.63	105.73	115.21
3	A	1001	AGS	C5-N7-C8	2.63	107.59	103.45
3	B	1002	AGS	C4-C5-N7	-2.62	107.59	110.58
3	B	1002	AGS	N3-C2-N1	-2.62	124.62	128.58
3	D	1003	AGS	O2G-PG-O3B	2.61	113.37	104.64
3	B	1002	AGS	C4-N9-C8	2.61	108.48	105.74
3	A	1001	AGS	O2B-PB-O1B	2.60	124.52	112.44
3	C	1001	AGS	O3A-PA-O1A	-2.59	102.92	110.70
3	E	1001	AGS	C5-N7-C8	2.58	107.50	103.45
3	B	1002	AGS	O2B-PB-O1B	2.57	124.39	112.44
3	F	1002	AGS	O2B-PB-O1B	2.56	124.36	112.44
3	B	1003	AGS	N6-C6-N1	2.56	124.08	118.38
3	F	1001	AGS	O3B-PB-O1B	-2.56	103.01	110.70
3	C	1001	AGS	C5-N7-C8	2.55	107.45	103.45
3	E	1001	AGS	N3-C2-N1	-2.55	124.73	128.58
3	D	1002	AGS	C4-N9-C8	2.53	108.40	105.74
3	E	1001	AGS	C4-N9-C8	2.49	108.36	105.74
3	C	1001	AGS	C6-C5-C4	2.49	120.58	117.18
3	F	1001	AGS	C4-N9-C8	2.49	108.35	105.74
3	B	1001	AGS	O2G-PG-O3B	2.49	112.94	104.64
3	A	1002	AGS	C5-N7-C8	2.48	107.35	103.45
3	B	1001	AGS	N6-C6-N1	2.48	123.90	118.38
3	D	1001	AGS	O2B-PB-O1B	2.46	123.90	112.44
3	A	1001	AGS	O3A-PA-O1A	-2.45	103.34	110.70
3	C	1001	AGS	N3-C2-N1	-2.44	124.88	128.58
3	A	1002	AGS	N3-C2-N1	-2.44	124.89	128.58
3	B	1003	AGS	O2A-PA-O1A	2.43	123.73	112.44
3	B	1001	AGS	O3A-PA-O1A	-2.42	103.42	110.70
3	D	1003	AGS	C4-C5-N7	-2.41	107.83	110.58
3	D	1003	AGS	N3-C2-N1	-2.40	124.95	128.58
3	F	1002	AGS	C6-C5-C4	2.40	120.45	117.18
3	A	1002	AGS	C4-N9-C8	2.39	108.25	105.74
3	C	1001	AGS	C5-C6-N6	-2.39	117.37	123.29
3	A	1001	AGS	C4-N9-C8	2.38	108.24	105.74
3	C	1001	AGS	C4-C5-N7	-2.38	107.86	110.58
3	B	1002	AGS	O3B-PB-O1B	-2.36	103.61	110.70
3	B	1001	AGS	N3-C2-N1	-2.36	125.01	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	O2B-PB-O1B	2.36	123.41	112.44
3	A	1001	AGS	C2'-C3'-C4'	2.35	107.16	102.61
3	F	1002	AGS	N3-C2-N1	-2.35	125.03	128.58
3	D	1003	AGS	O2B-PB-O1B	2.34	123.33	112.44
3	D	1002	AGS	O2G-PG-O3B	2.33	112.44	104.64
3	F	1001	AGS	C5-C6-N6	-2.32	117.53	123.29
3	F	1001	AGS	O2B-PB-O1B	2.31	123.21	112.44
3	D	1003	AGS	O3A-PA-O1A	-2.31	103.77	110.70
3	D	1003	AGS	C5-C6-N6	-2.30	117.58	123.29
3	A	1001	AGS	O5'-C5'-C4'	-2.28	101.22	108.99
3	B	1001	AGS	C2'-C3'-C4'	2.27	107.00	102.61
3	D	1003	AGS	C5'-C4'-C3'	-2.26	107.07	115.21
3	F	1001	AGS	C5-N7-C8	2.25	106.99	103.45
3	F	1002	AGS	C4-N9-C1'	2.24	131.88	126.63
3	D	1003	AGS	C5-N7-C8	2.24	106.97	103.45
3	D	1002	AGS	O5'-C5'-C4'	-2.22	101.42	108.99
3	E	1001	AGS	C5-C6-N6	-2.22	117.78	123.29
3	D	1003	AGS	C6-C5-C4	2.22	120.21	117.18
3	B	1002	AGS	C5-C6-N6	-2.22	117.79	123.29
3	B	1002	AGS	C5-N7-C8	2.21	106.92	103.45
3	B	1001	AGS	O2B-PB-O1B	2.21	122.72	112.44
3	B	1002	AGS	C2'-C3'-C4'	2.20	106.86	102.61
3	E	1001	AGS	O2B-PB-O1B	2.20	122.66	112.44
3	F	1002	AGS	O4'-C4'-C5'	2.19	116.36	109.33
3	F	1001	AGS	C4-C5-N7	-2.17	108.10	110.58
3	D	1001	AGS	C5-N7-C8	2.16	106.84	103.45
3	B	1003	AGS	C5-N7-C8	2.14	106.81	103.45
3	E	1001	AGS	O2B-PB-O3B	2.14	113.05	107.27
3	B	1003	AGS	O3A-PA-O1A	-2.14	104.28	110.70
3	C	1001	AGS	O2B-PB-O1B	2.13	122.37	112.44
3	A	1001	AGS	C5'-C4'-C3'	-2.13	107.54	115.21
3	D	1002	AGS	C5-N7-C8	2.13	106.80	103.45
3	D	1003	AGS	O3B-PB-O1B	-2.13	104.30	110.70
3	E	1001	AGS	C6-C5-C4	2.12	120.07	117.18
3	F	1002	AGS	C2-N1-C6	2.11	122.20	118.73
3	C	1001	AGS	O3B-PB-O1B	-2.10	104.39	110.70
3	B	1001	AGS	O2A-PA-O1A	2.09	122.17	112.44
3	D	1001	AGS	C5-C6-N6	-2.09	118.12	123.29
3	A	1001	AGS	O3B-PB-O1B	-2.08	104.43	110.70
3	B	1003	AGS	C5'-C4'-C3'	-2.08	107.73	115.21
3	D	1002	AGS	C5'-C4'-C3'	-2.07	107.75	115.21
3	F	1002	AGS	O3B-PB-O1B	-2.07	104.49	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1003	AGS	C1'-N9-C8	-2.06	122.53	127.09
3	D	1001	AGS	N3-C2-N1	-2.06	125.47	128.58
3	B	1001	AGS	C5-N7-C8	2.04	106.66	103.45
3	E	1001	AGS	C1'-N9-C8	-2.03	122.60	127.09
3	C	1001	AGS	C5'-C4'-C3'	-2.01	107.98	115.21
3	B	1002	AGS	O4'-C4'-C5'	2.00	115.74	109.33

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	PB-O3B-PG-O2G
3	A	1001	AGS	PB-O3B-PG-O3G
3	A	1001	AGS	C5'-O5'-PA-O3A
3	A	1002	AGS	PB-O3B-PG-O2G
3	A	1002	AGS	PB-O3B-PG-O3G
3	A	1002	AGS	C5'-O5'-PA-O1A
3	B	1002	AGS	C5'-O5'-PA-O1A
3	B	1002	AGS	C5'-O5'-PA-O2A
3	B	1002	AGS	C5'-O5'-PA-O3A
3	B	1002	AGS	O4'-C4'-C5'-O5'
3	B	1003	AGS	C5'-O5'-PA-O2A
3	B	1003	AGS	C5'-O5'-PA-O3A
3	B	1003	AGS	C4'-C5'-O5'-PA
3	C	1001	AGS	C5'-O5'-PA-O2A
3	C	1001	AGS	C5'-O5'-PA-O3A
3	D	1002	AGS	PB-O3B-PG-O2G
3	D	1003	AGS	C5'-O5'-PA-O2A
3	D	1003	AGS	C5'-O5'-PA-O3A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	E	1001	AGS	C5'-O5'-PA-O3A
3	E	1001	AGS	O4'-C4'-C5'-O5'
3	F	1001	AGS	C5'-O5'-PA-O3A
3	F	1001	AGS	O4'-C4'-C5'-O5'
3	F	1002	AGS	PB-O3B-PG-O2G
3	F	1002	AGS	PB-O3B-PG-O3G
3	F	1002	AGS	C5'-O5'-PA-O1A
3	F	1002	AGS	C5'-O5'-PA-O3A
3	F	1002	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	1001	AGS	C3'-C4'-C5'-O5'
3	D	1001	AGS	O4'-C4'-C5'-O5'
3	B	1002	AGS	C3'-C4'-C5'-O5'
3	F	1002	AGS	C3'-C4'-C5'-O5'
3	D	1002	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	C3'-C4'-C5'-O5'
3	D	1001	AGS	C3'-C4'-C5'-O5'
3	A	1002	AGS	PG-O3B-PB-O3A
3	A	1002	AGS	C2'-C1'-N9-C4
3	B	1003	AGS	C3'-C4'-C5'-O5'
3	A	1001	AGS	C5'-O5'-PA-O1A
3	F	1001	AGS	C5'-O5'-PA-O1A
3	F	1002	AGS	C5'-O5'-PA-O2A
3	D	1001	AGS	PG-O3B-PB-O1B
3	A	1002	AGS	C2'-C1'-N9-C8
3	B	1003	AGS	O4'-C4'-C5'-O5'
3	A	1001	AGS	PA-O3A-PB-O1B
3	A	1001	AGS	PA-O3A-PB-O2B
3	A	1002	AGS	PB-O3A-PA-O1A
3	B	1003	AGS	PB-O3A-PA-O1A
3	F	1001	AGS	PB-O3A-PA-O2A
3	C	1001	AGS	PB-O3B-PG-O2G
3	D	1003	AGS	C4'-C5'-O5'-PA
3	A	1002	AGS	PG-O3B-PB-O2B
3	B	1001	AGS	PG-O3B-PB-O2B
3	E	1001	AGS	PG-O3B-PB-O2B
3	B	1003	AGS	PB-O3A-PA-O2A
3	C	1001	AGS	PB-O3A-PA-O1A
3	F	1001	AGS	PB-O3A-PA-O1A
3	A	1002	AGS	PB-O3A-PA-O2A
3	B	1001	AGS	PA-O3A-PB-O2B
3	C	1001	AGS	PB-O3A-PA-O2A
3	D	1001	AGS	PA-O3A-PB-O2B
3	D	1002	AGS	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 44 short contacts:

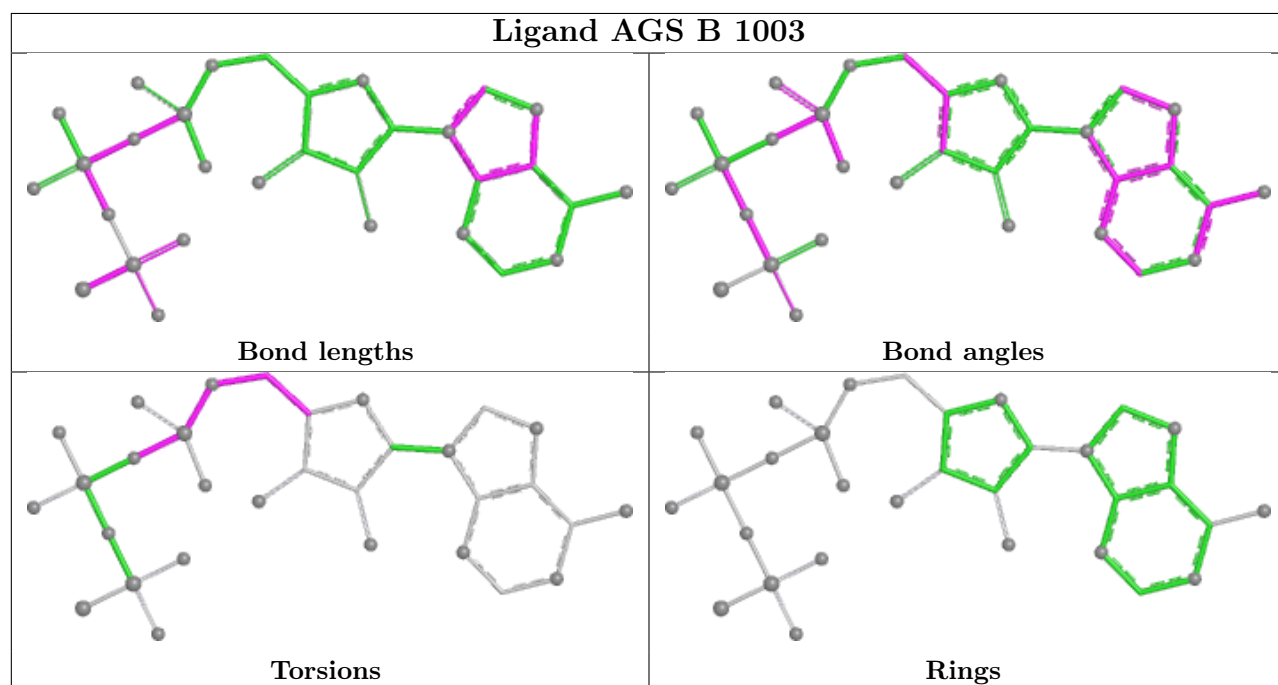
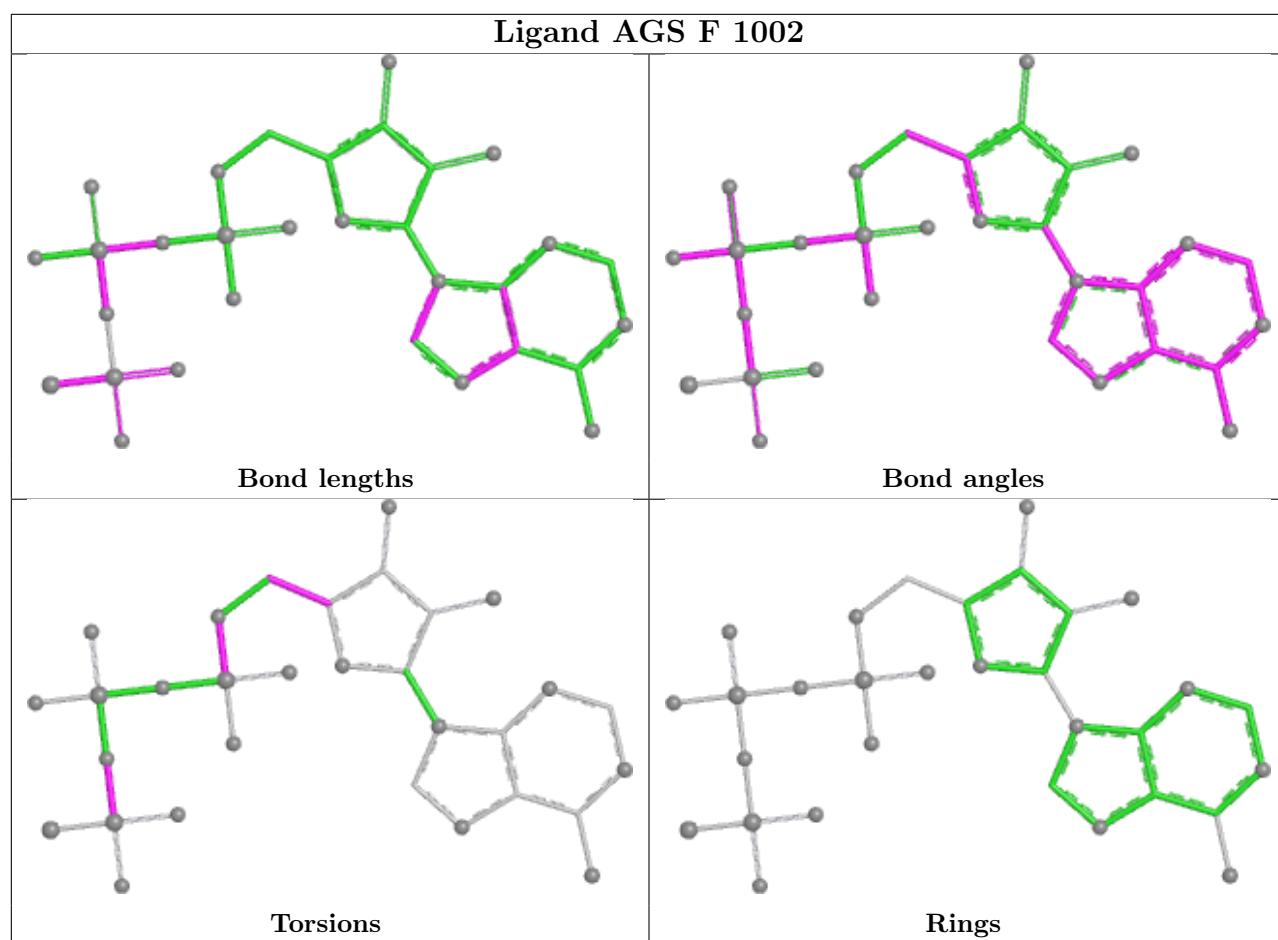
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1002	AGS	2	0
3	B	1003	AGS	7	0

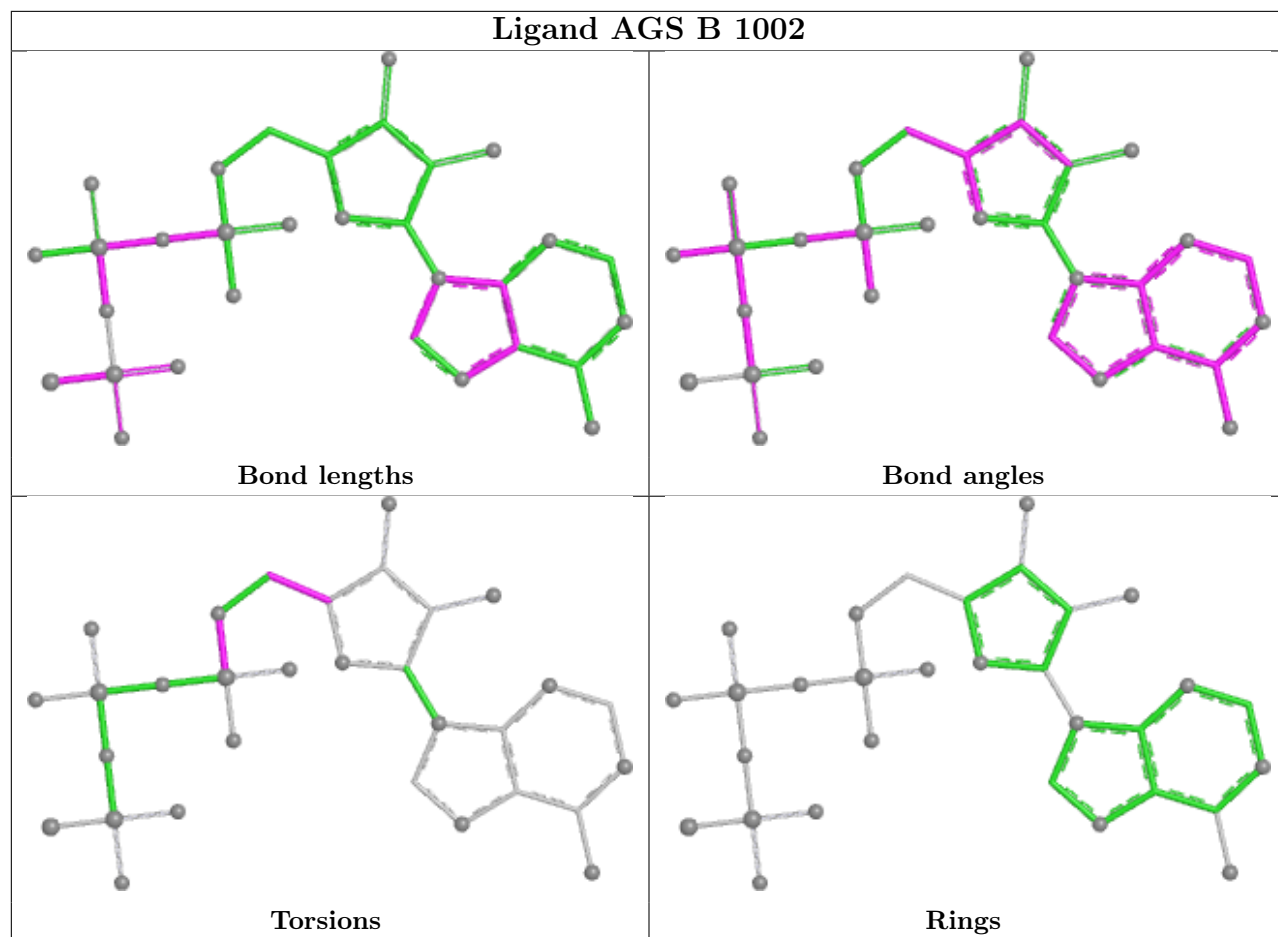
Continued on next page...

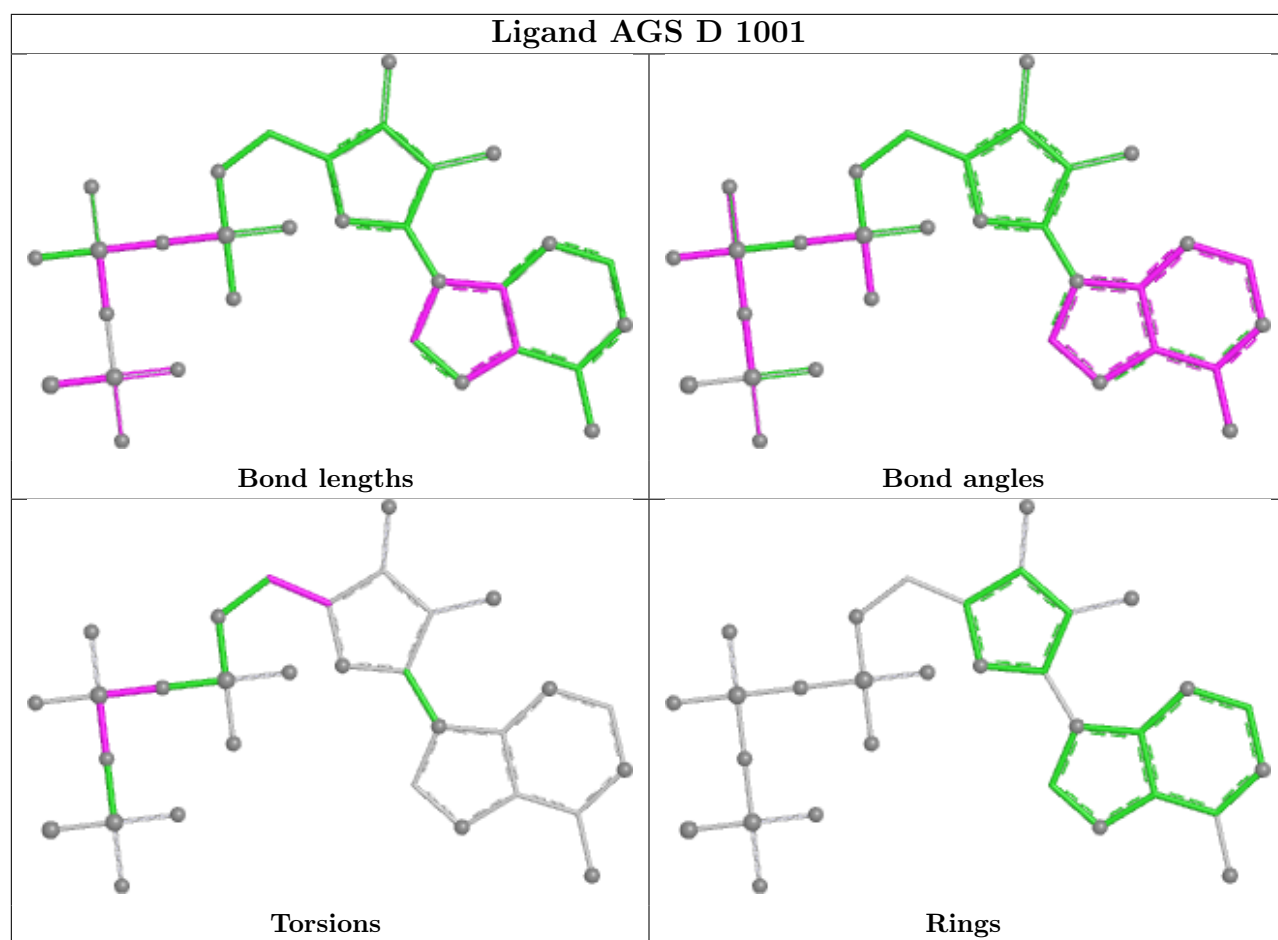
Continued from previous page...

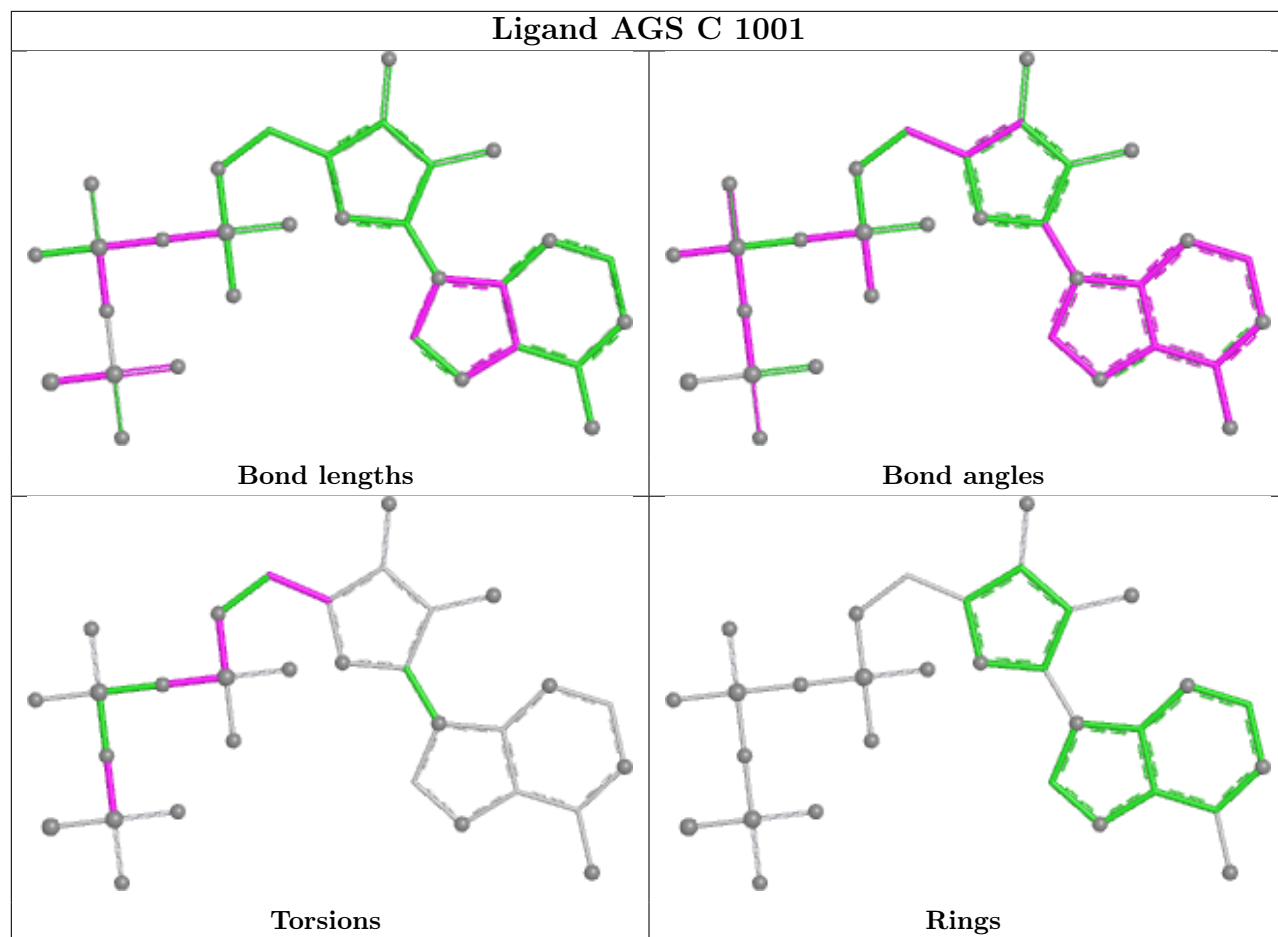
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	AGS	1	0
3	D	1001	AGS	3	0
3	C	1001	AGS	1	0
3	E	1001	AGS	3	0
3	A	1001	AGS	3	0
3	D	1003	AGS	5	0
3	D	1002	AGS	3	0
3	A	1002	AGS	1	0
3	F	1001	AGS	3	0
3	B	1001	AGS	12	0

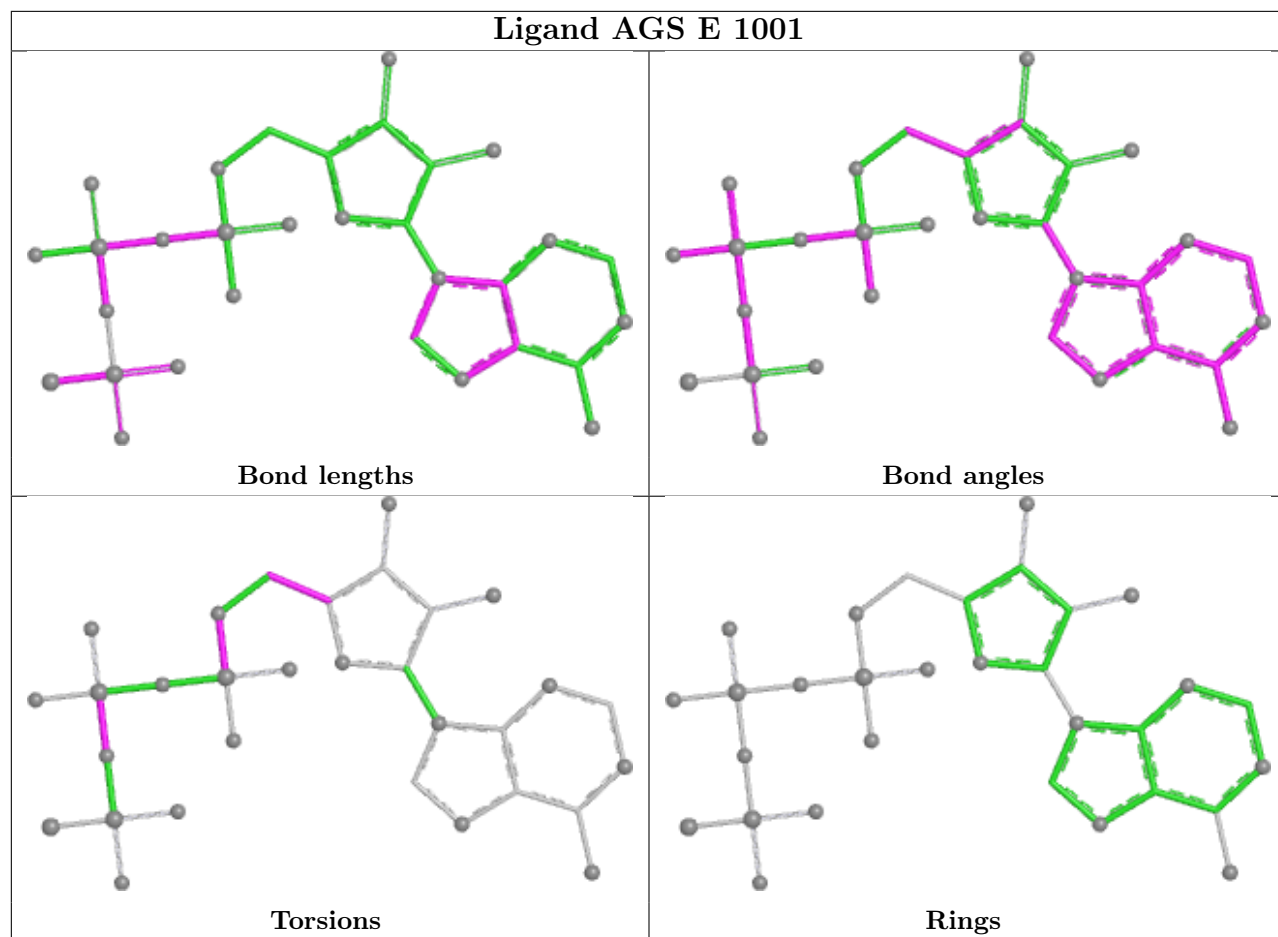
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

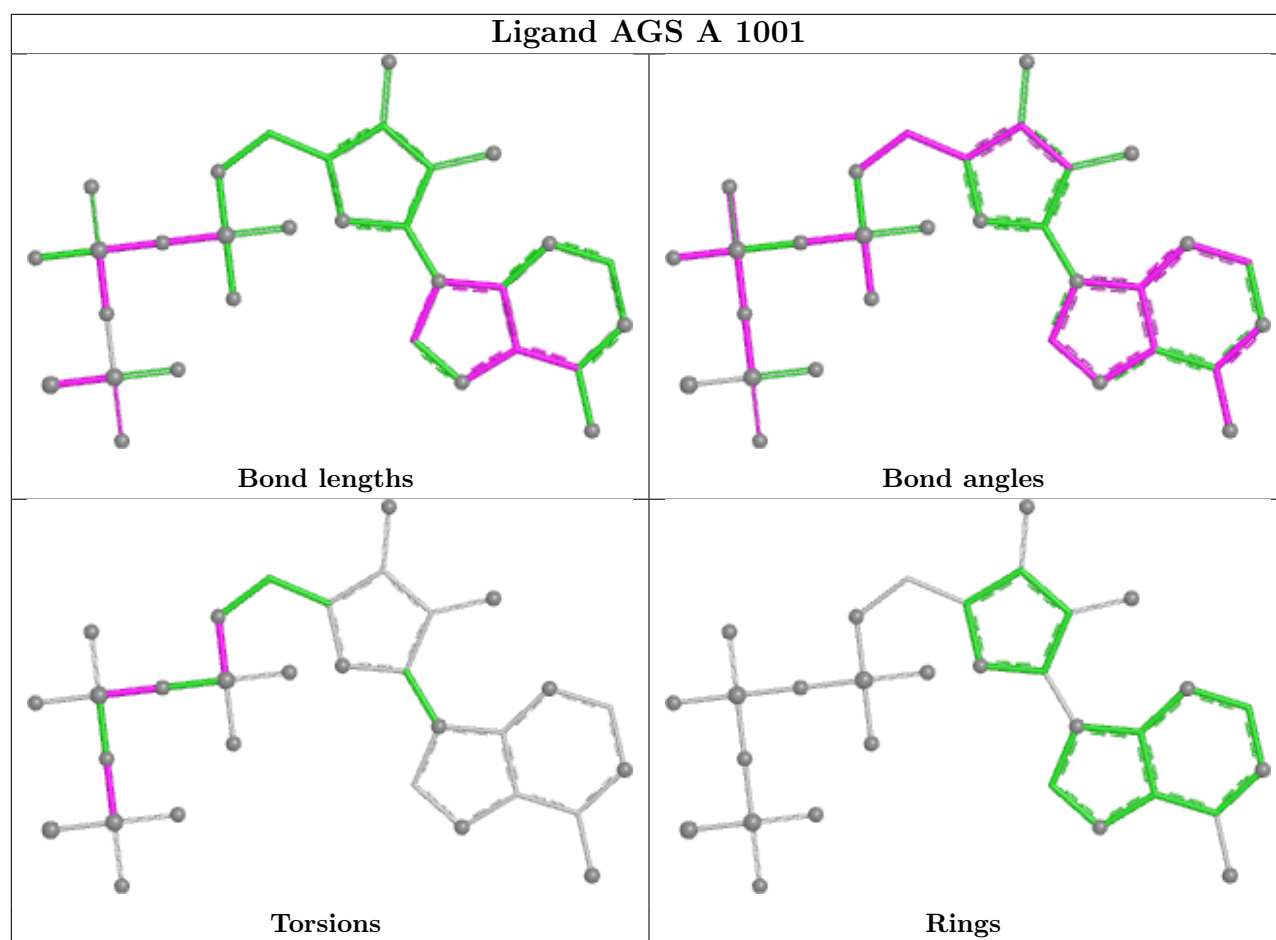


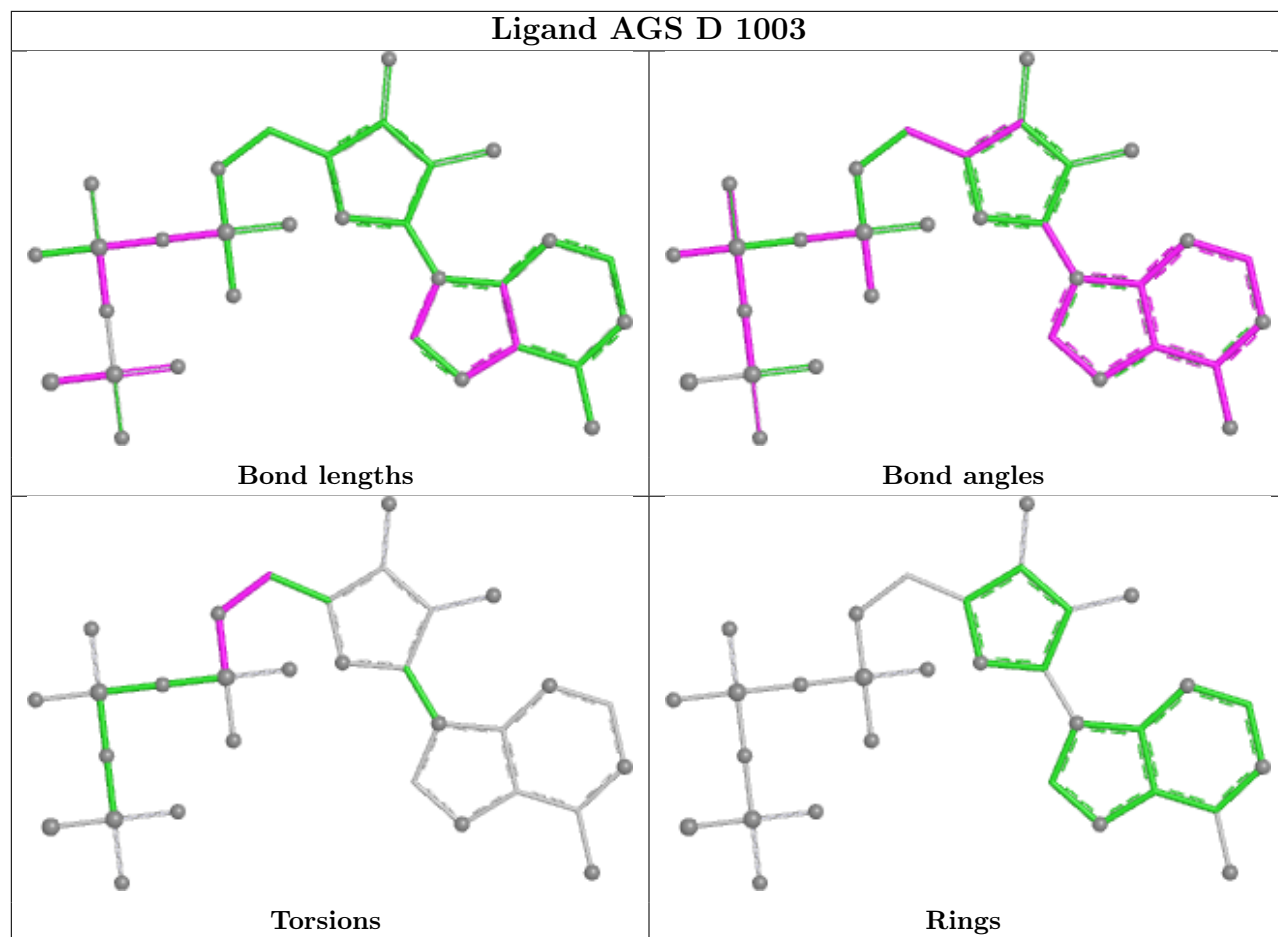


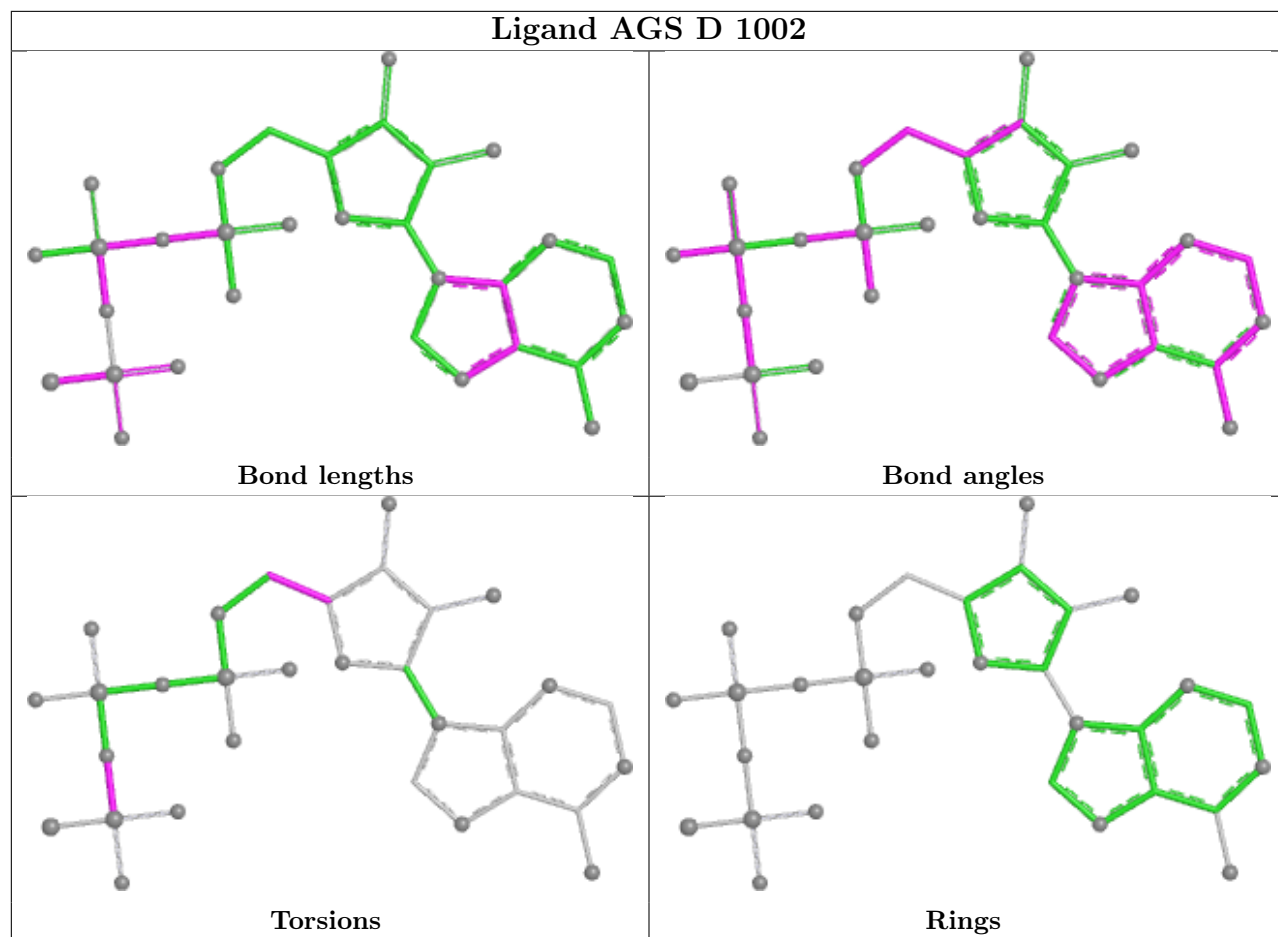


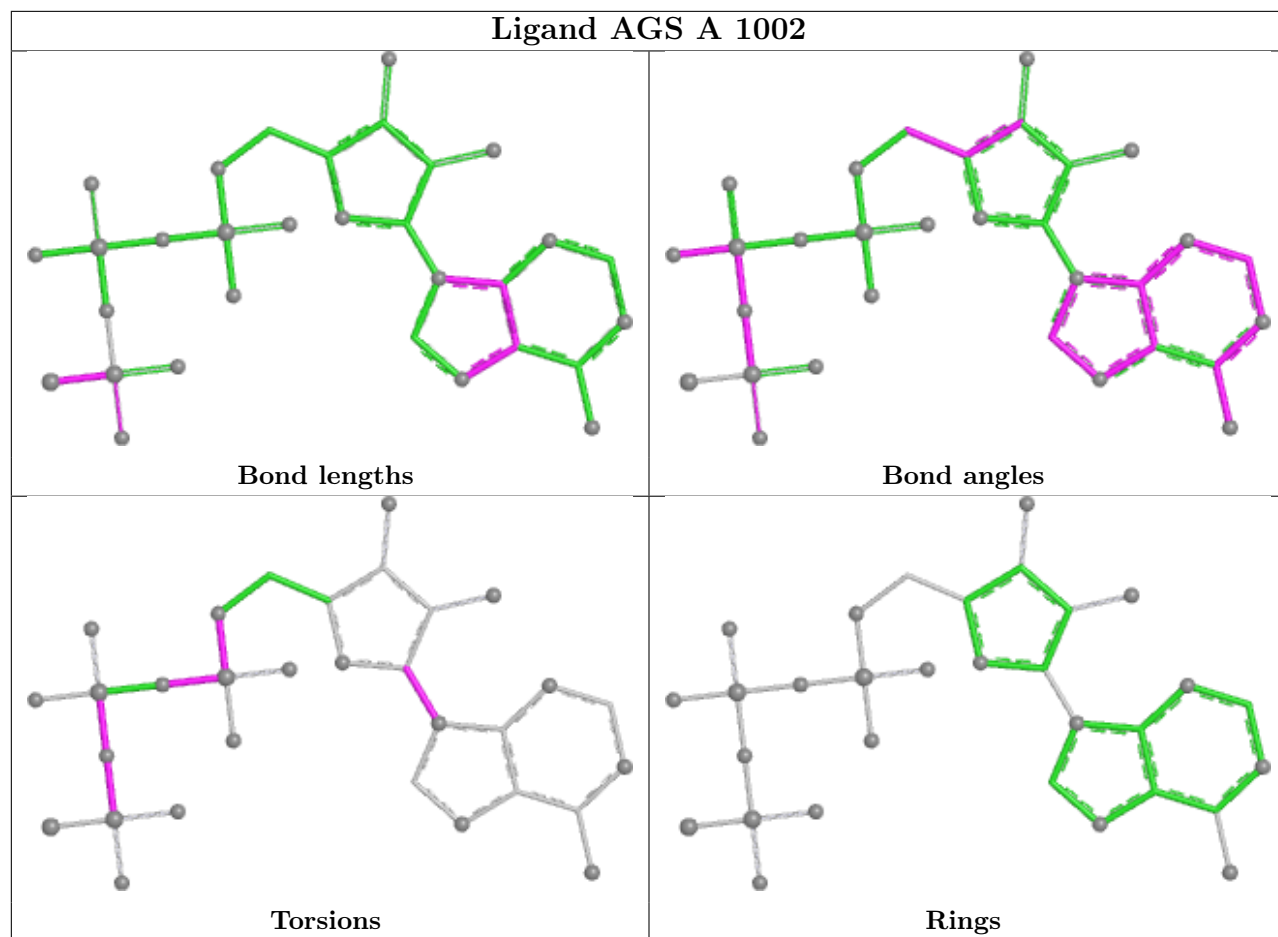


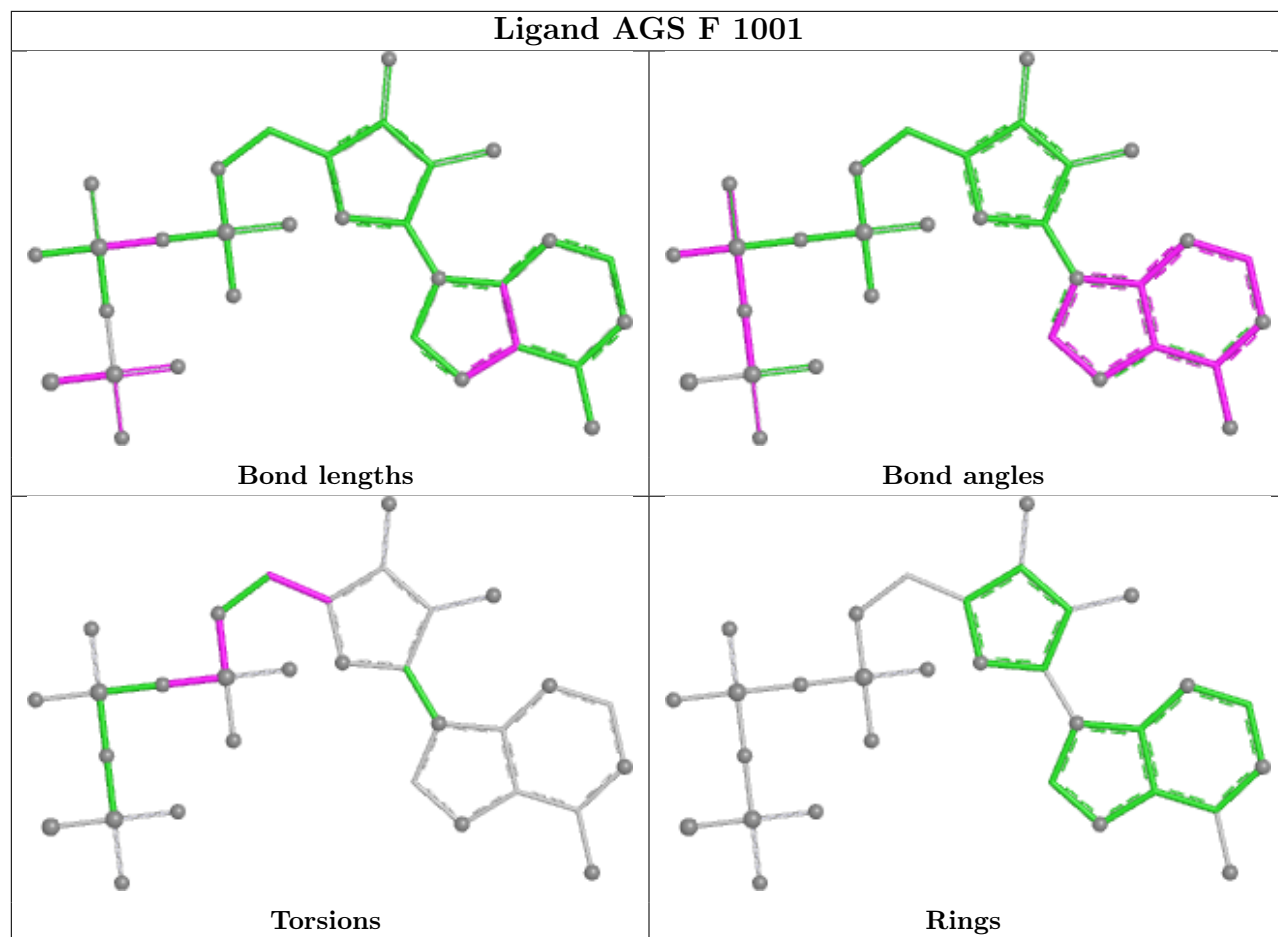


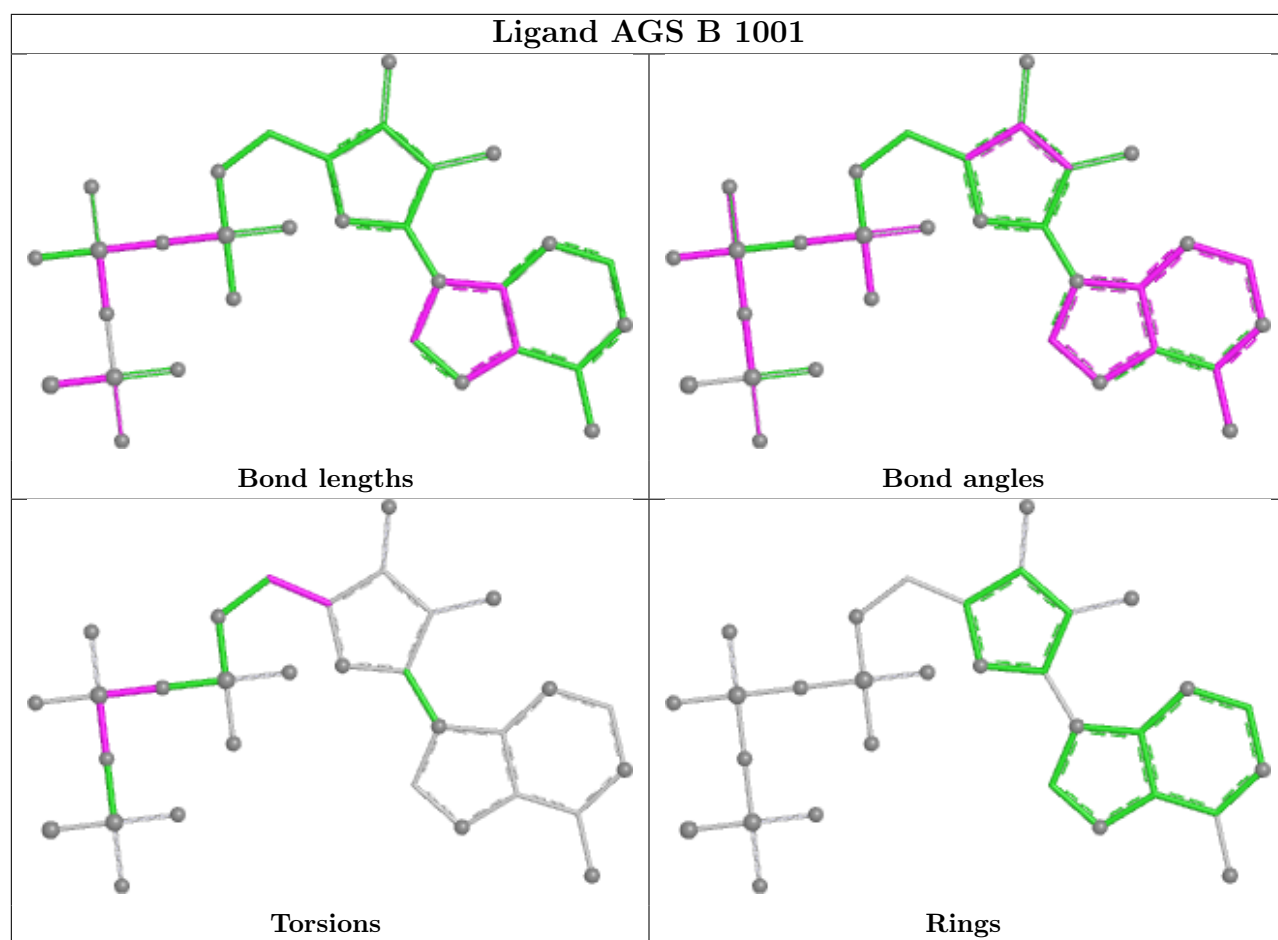












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

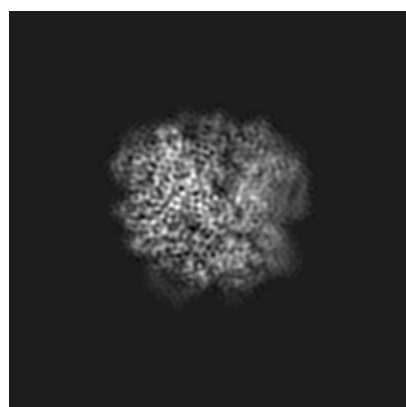
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8697. These allow visual inspection of the internal detail of the map and identification of artifacts.

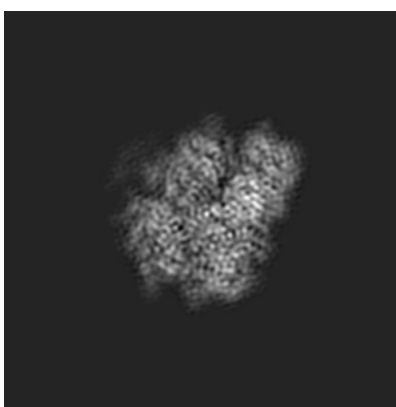
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

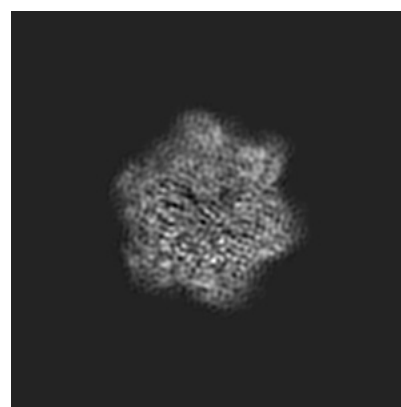
6.1.1 Primary map



X



Y

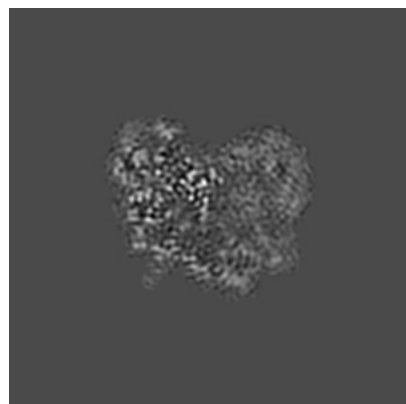


Z

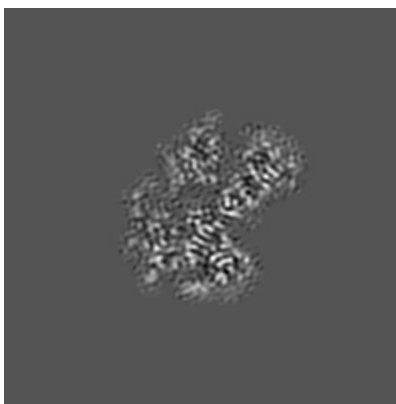
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

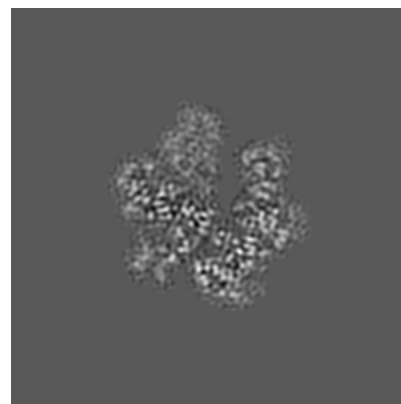
6.2.1 Primary map



X Index: 128



Y Index: 128

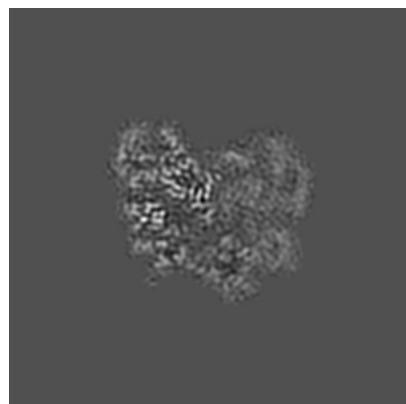


Z Index: 128

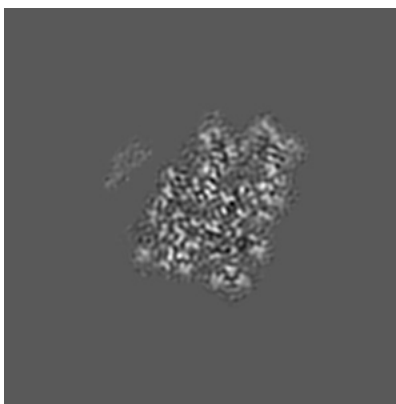
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

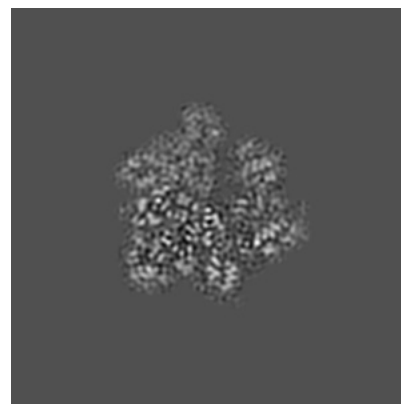
6.3.1 Primary map



X Index: 125



Y Index: 108

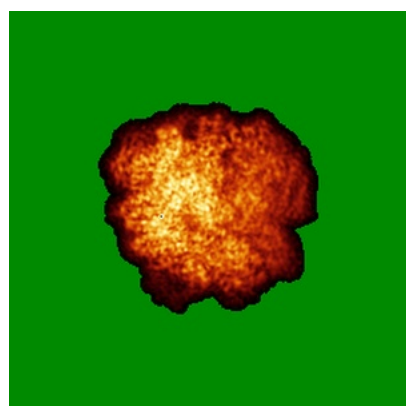


Z Index: 136

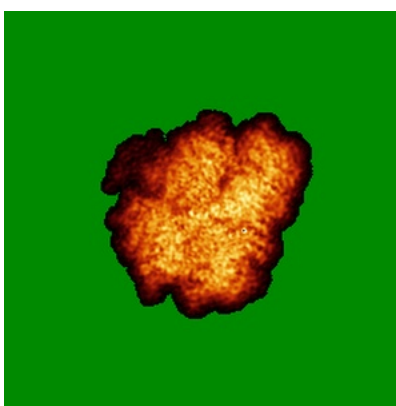
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

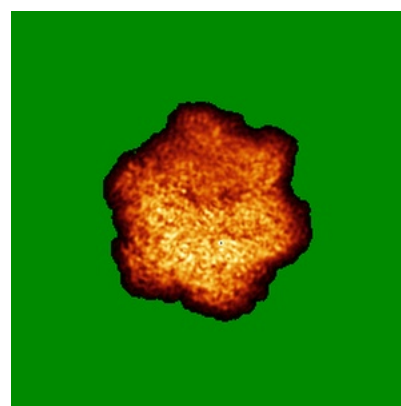
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0283. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

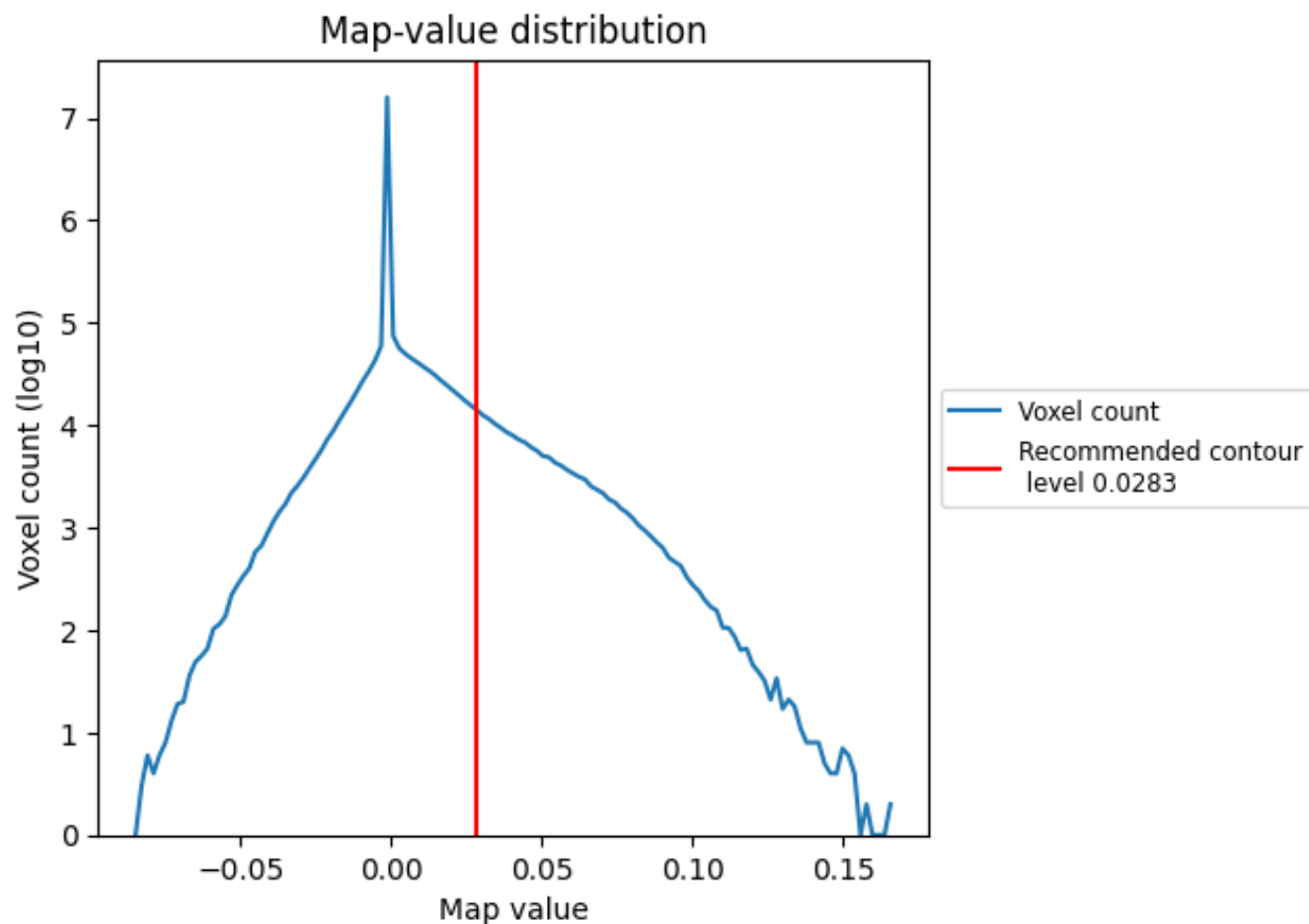
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

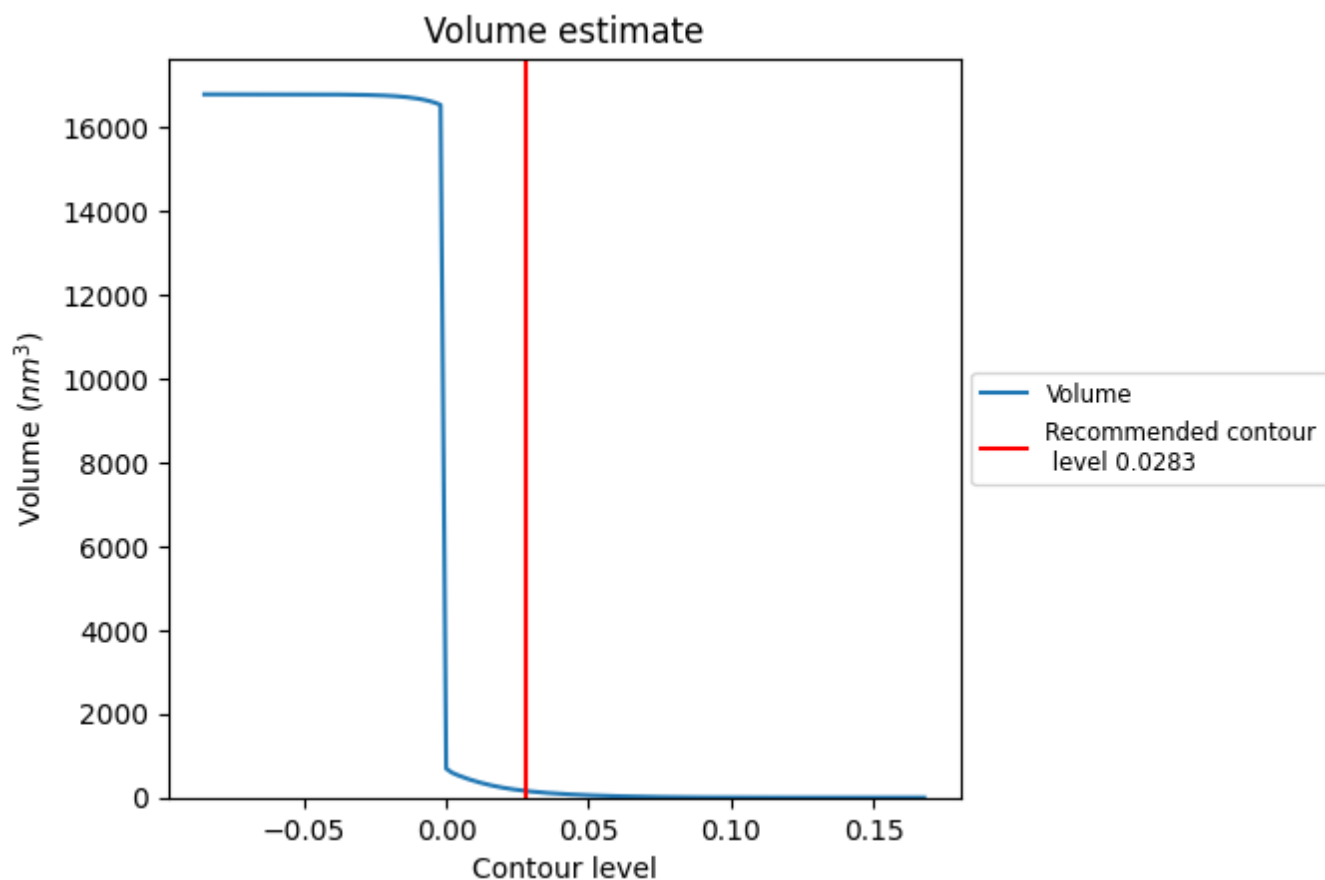
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

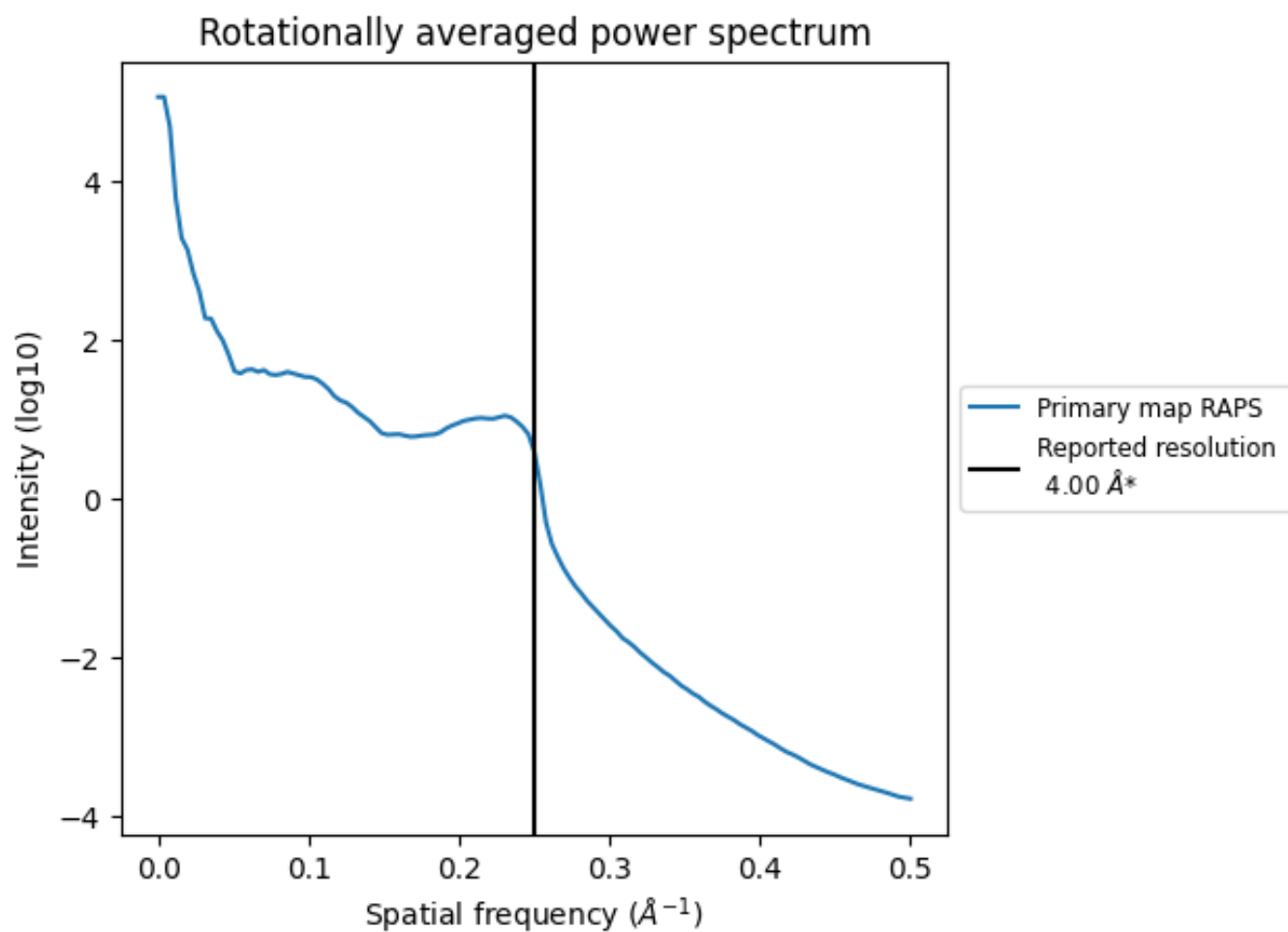
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm^3 ; this corresponds to an approximate mass of 141 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

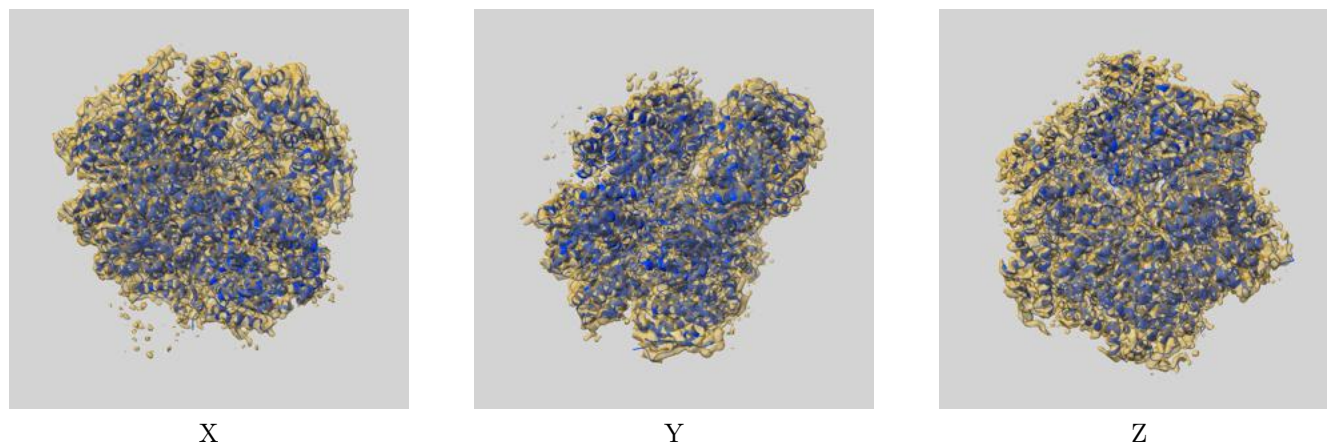
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

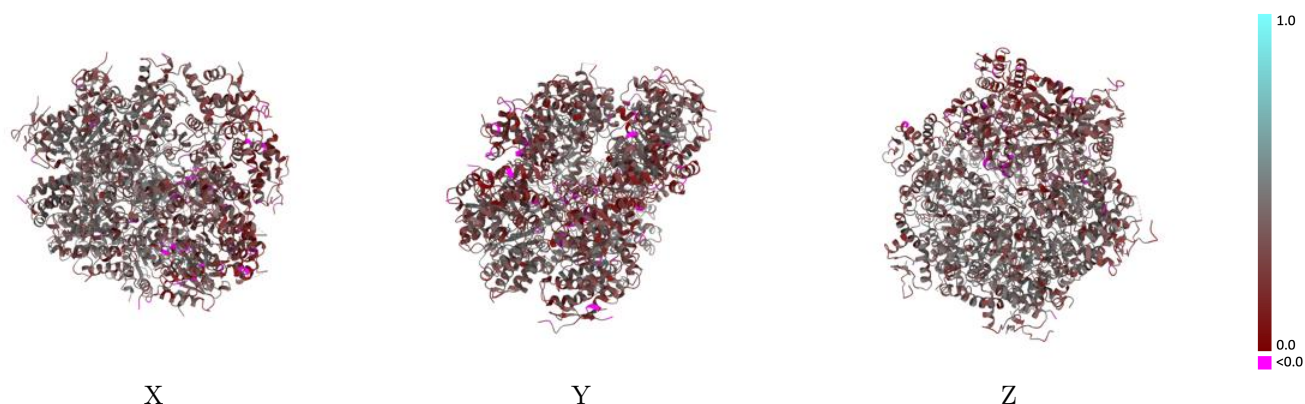
This section contains information regarding the fit between EMDB map EMD-8697 and PDB model 5VJH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



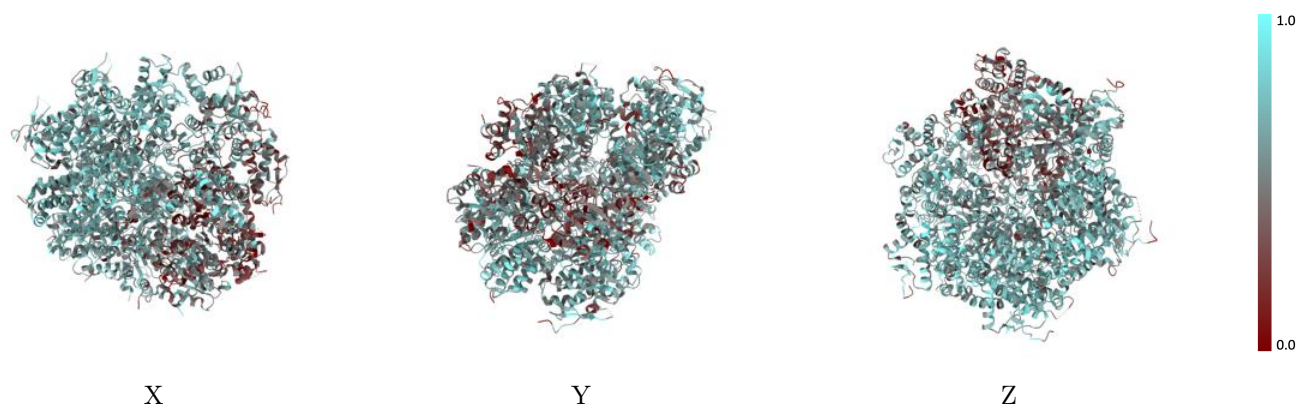
The images above show the 3D surface view of the map at the recommended contour level 0.0283 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



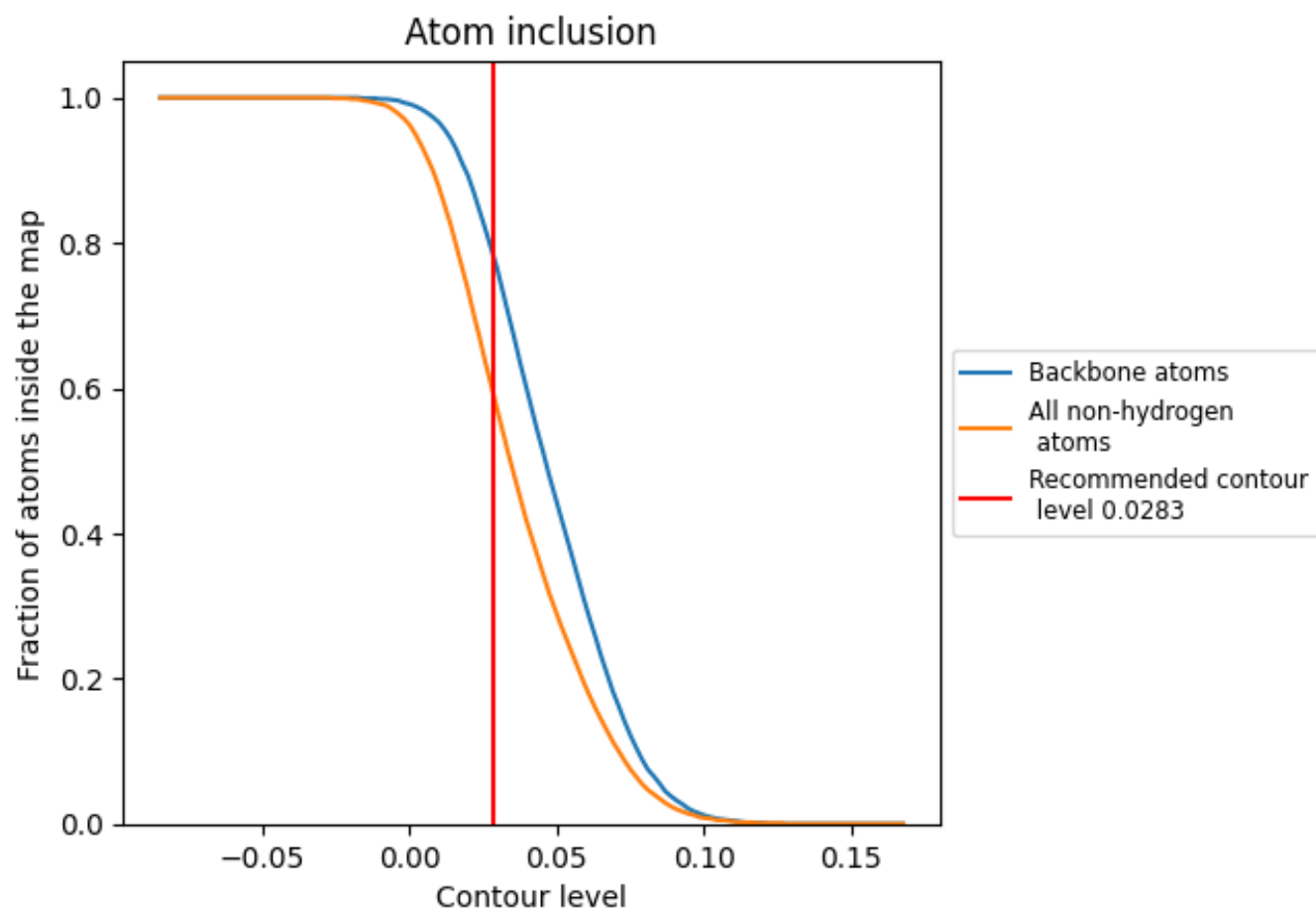
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0283).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0283) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5950	0.3280
A	0.5280	0.2820
B	0.6580	0.3570
C	0.6750	0.3690
D	0.6790	0.3790
E	0.6300	0.3430
F	0.3930	0.2310
P	0.6640	0.3860

1.0

0.0

<0.0