



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:11 PM UTC

PDB ID : 5VY9 / pdb_00005vy9
EMDB ID : EMD-8745
Title : S. cerevisiae Hsp104:casein complex, Middle Domain Conformation
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 : 2017-05-24
Resolution : 6.70 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:

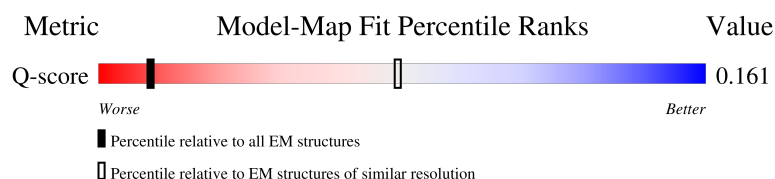
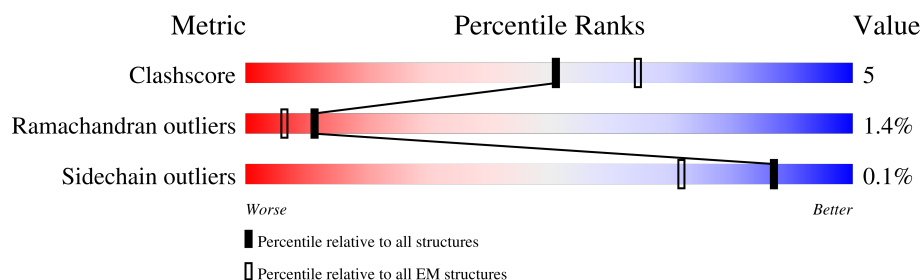
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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	523 (6.20 - 7.20)

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	44% 80% 13% 6%
1	B	908	28% 80% 11% 6%
1	C	908	21% 68% 11% 21%
1	D	908	29% 65% 13% 21%

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Mol	Chain	Length	Quality of chain
1	E	908	
1	F	908	
2	P	28	

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	D	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38737 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.

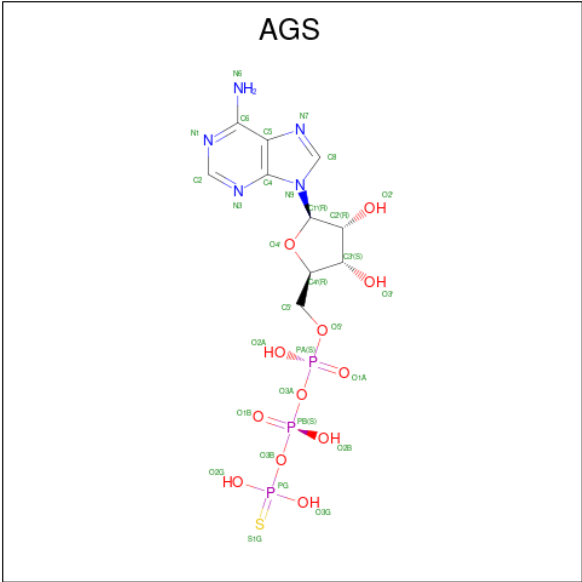
- Molecule 1 is a protein called Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	849	Total	C	N	O	S	0	0
			6722	4223	1182	1298	19		
1	B	849	Total	C	N	O	S	0	0
			6722	4223	1182	1298	19		
1	C	721	Total	C	N	O	S	0	0
			5669	3580	991	1080	18		
1	D	721	Total	C	N	O	S	0	0
			5669	3580	991	1080	18		
1	E	849	Total	C	N	O	S	0	0
			6722	4223	1182	1298	19		
1	F	849	Total	C	N	O	S	0	0
			6722	4223	1182	1298	19		

- Molecule 2 is a protein called Alpha-S1-casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	28	Total	C	N	O	0	0
			140	84	28	28		

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

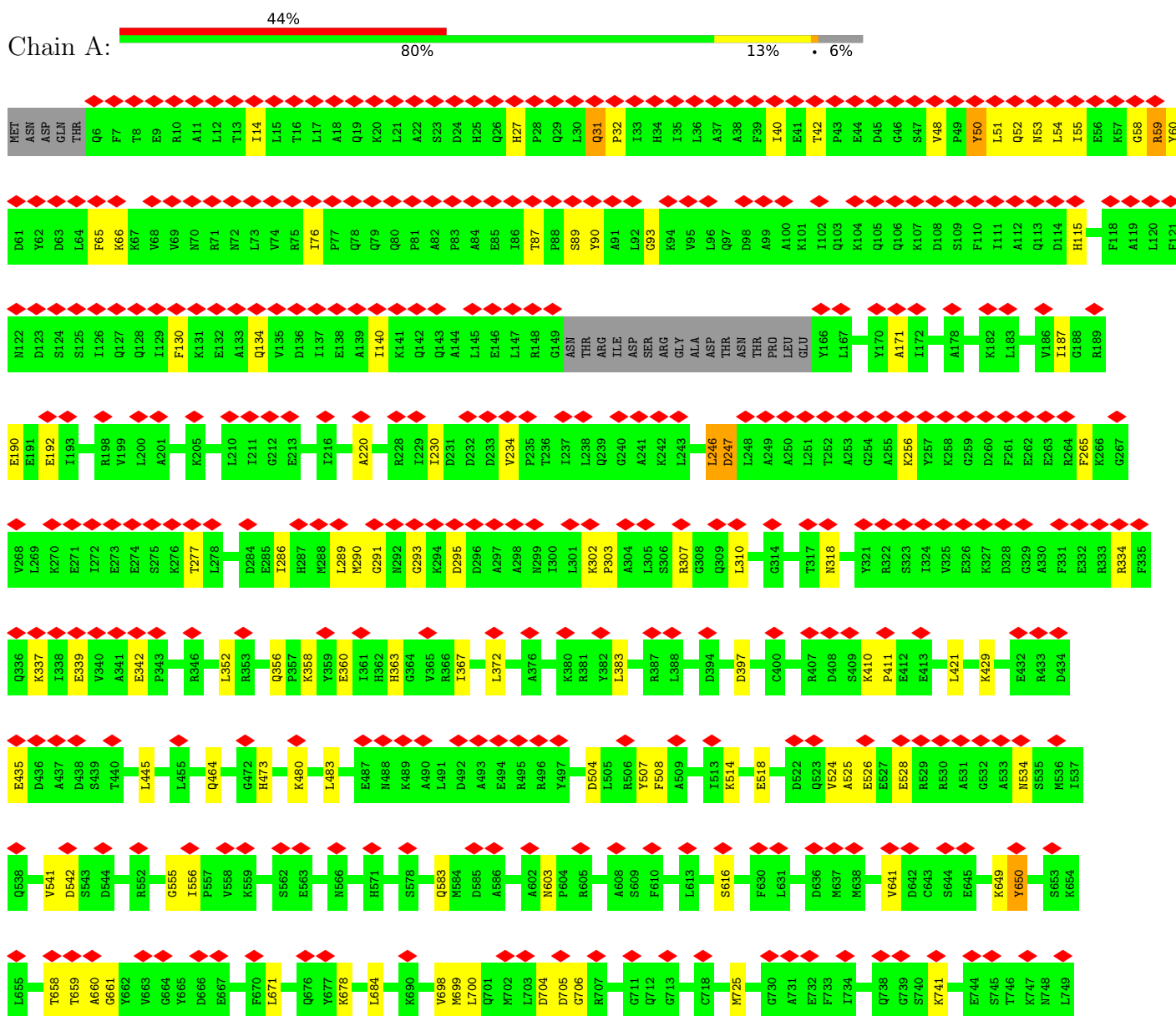


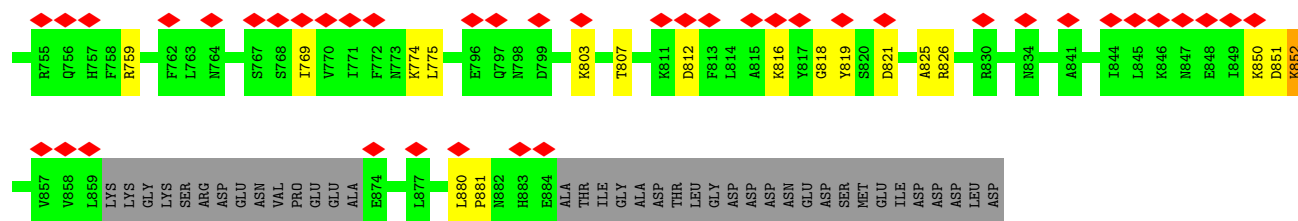
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			30	10	5	11	3	1	
3	E	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

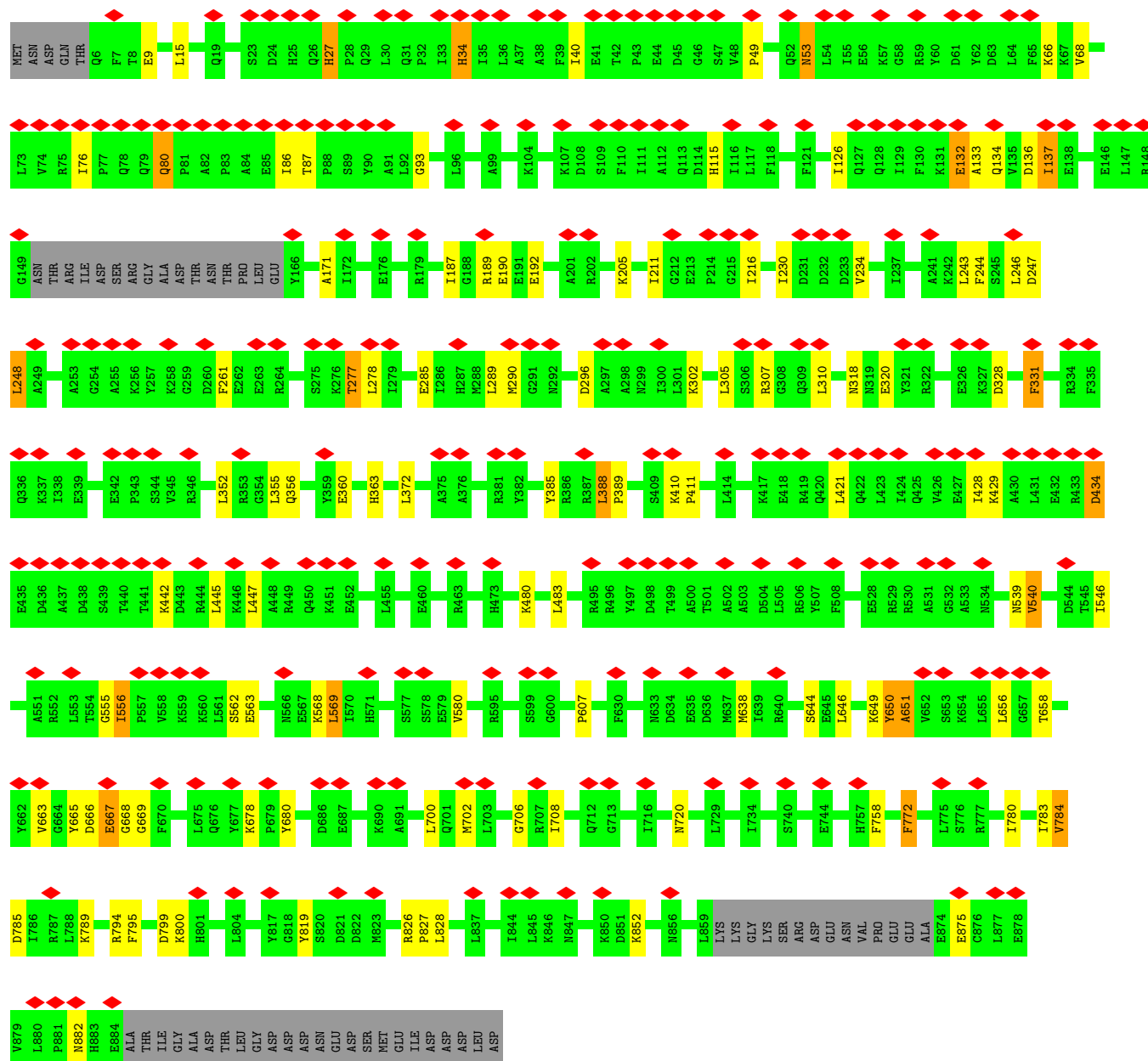
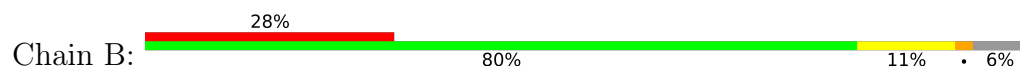
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

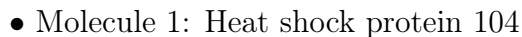


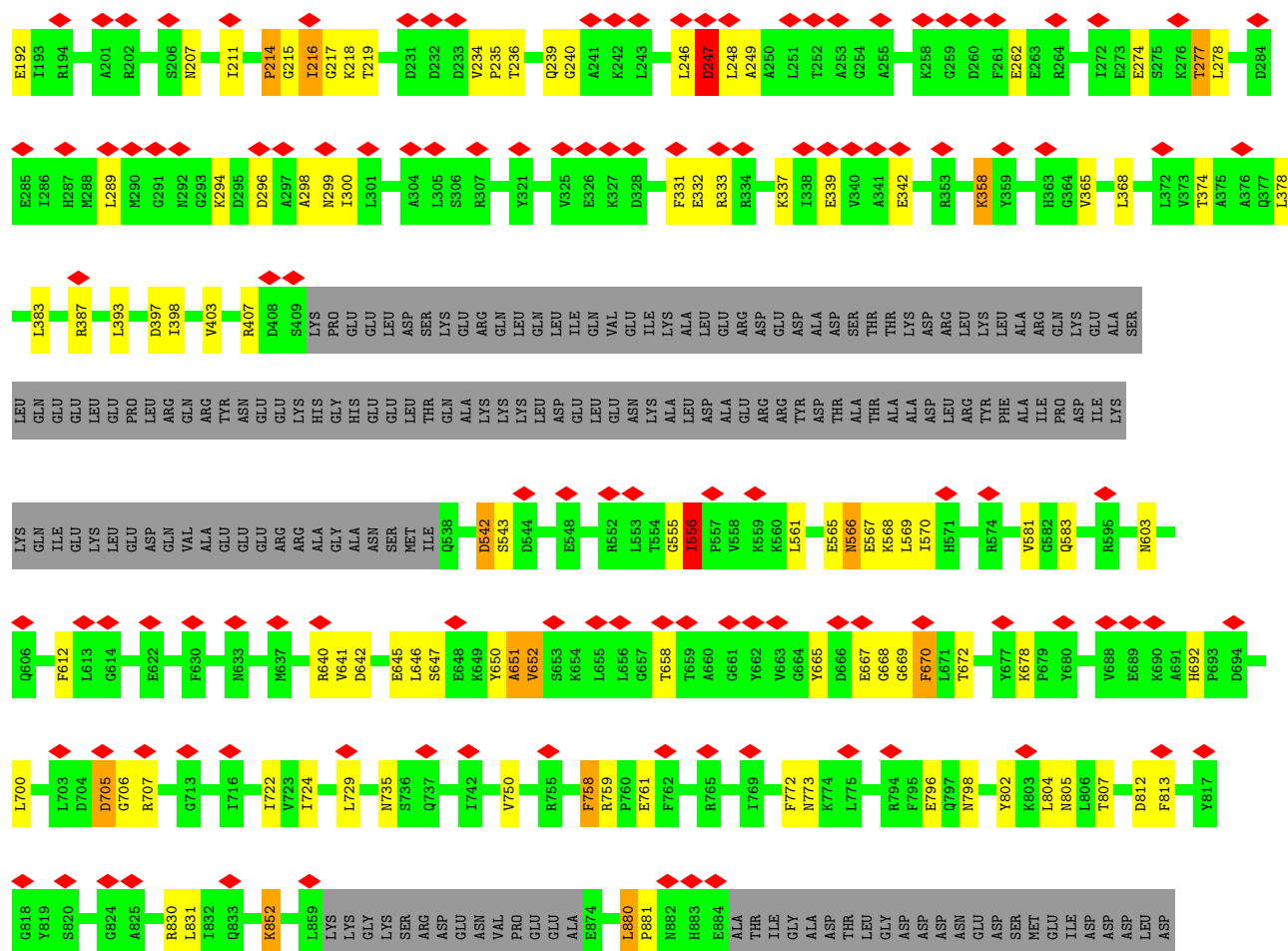


• Molecule 1: Heat shock protein 104

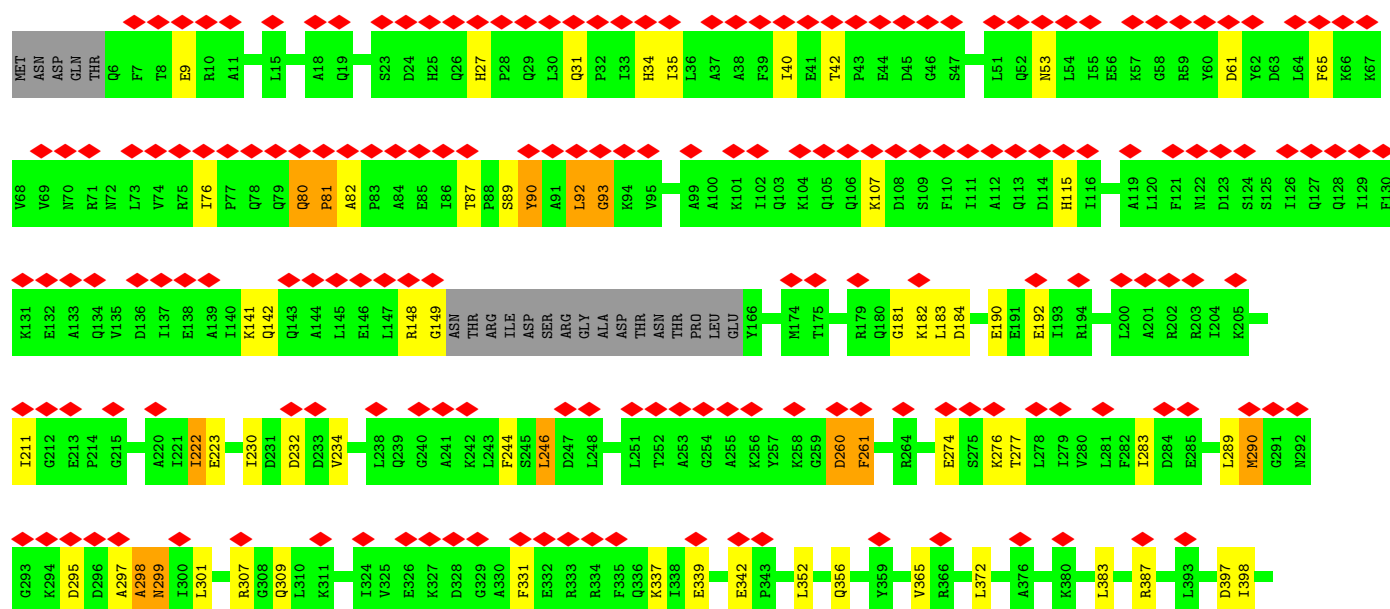
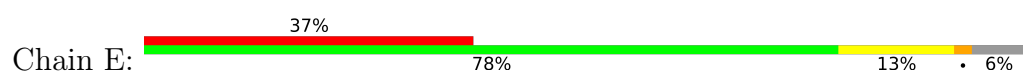


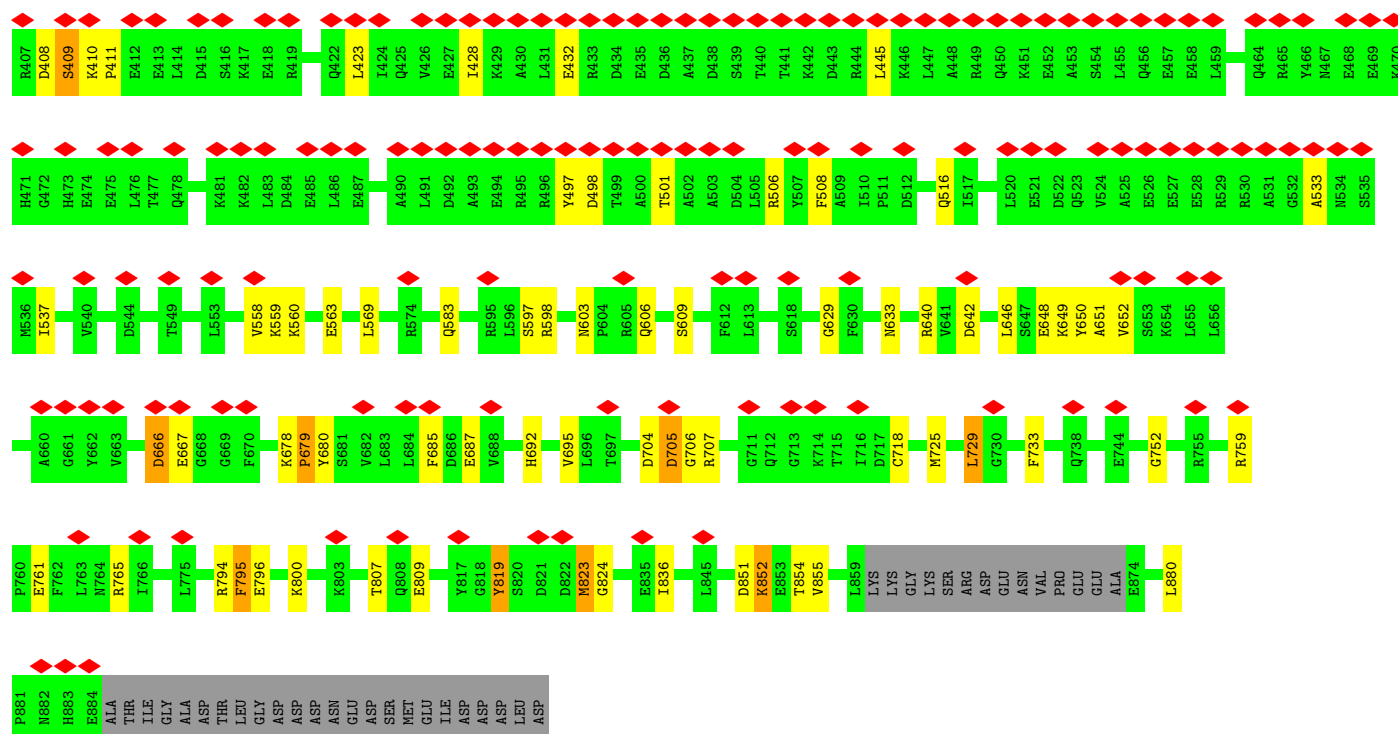
• Molecule 1: Heat shock protein 104



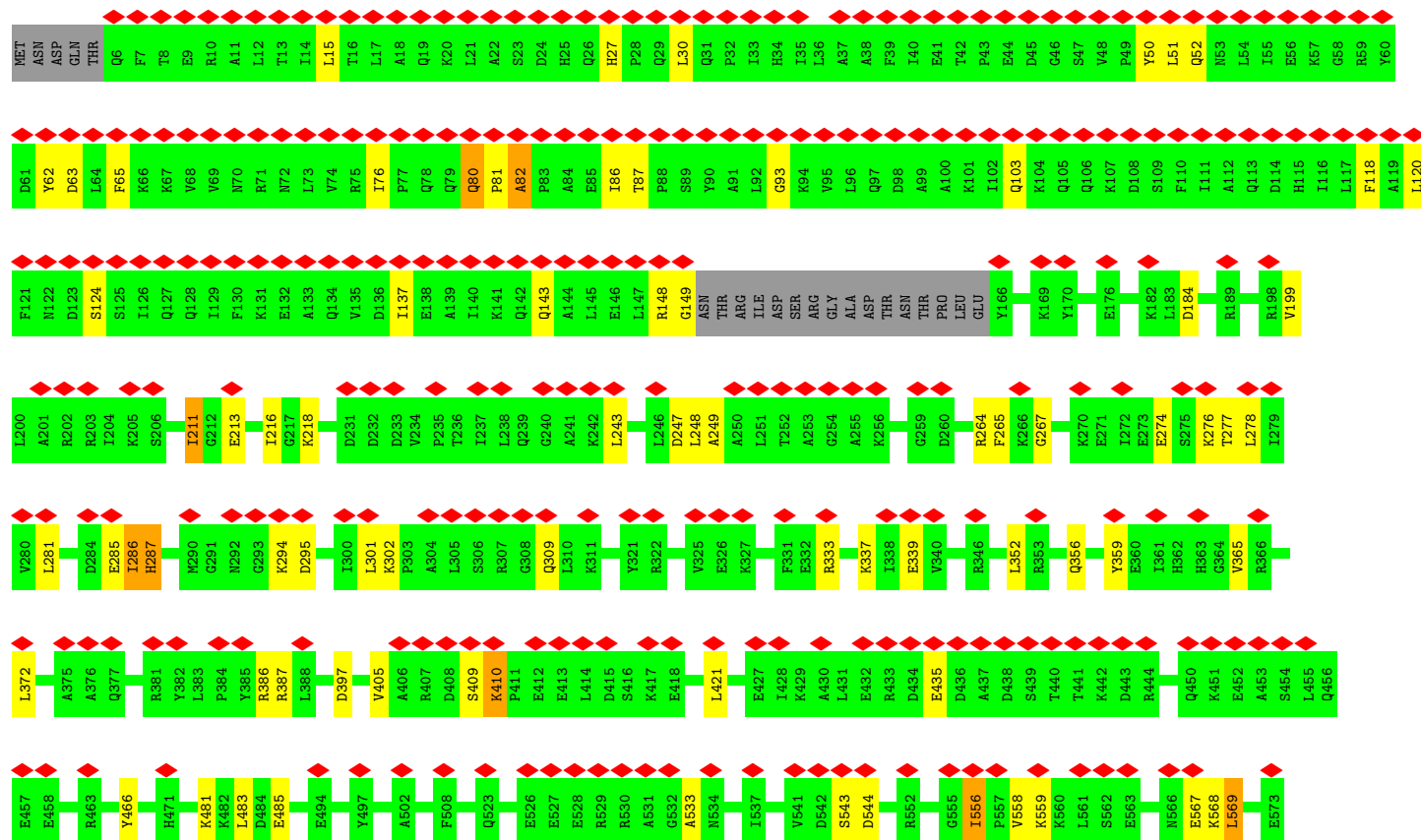
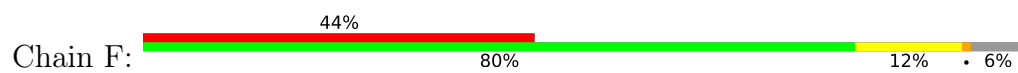


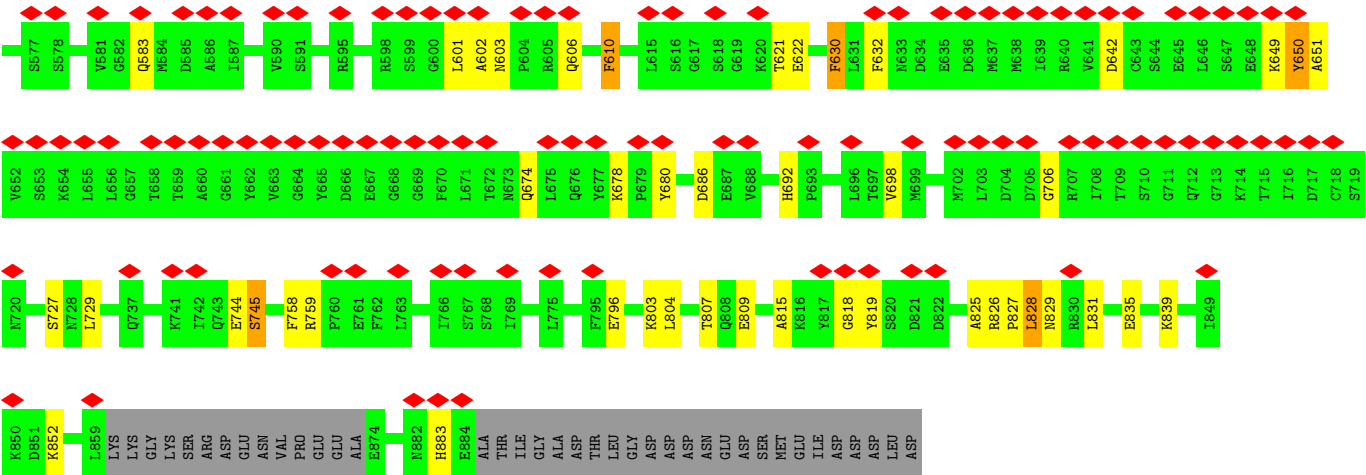
• Molecule 1: Heat shock protein 104



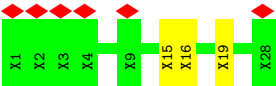
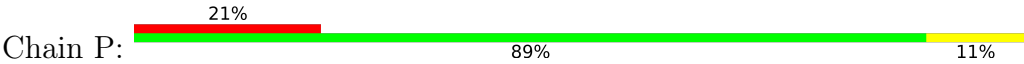


• Molecule 1: Heat shock protein 104





● Molecule 2: Alpha-S1-casein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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	0.083	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0222	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 ⓘ

5.1 Standard geometry ⓘ

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	1.04	9/6810 (0.1%)	1.28	61/9169 (0.7%)
1	B	1.10	5/6811 (0.1%)	1.32	54/9172 (0.6%)
1	C	1.10	3/5747 (0.1%)	1.32	51/7745 (0.7%)
1	D	1.10	7/5747 (0.1%)	1.31	54/7745 (0.7%)
1	E	1.12	9/6810 (0.1%)	1.34	70/9169 (0.8%)
1	F	1.07	9/6810 (0.1%)	1.28	59/9169 (0.6%)
All	All	1.09	42/38735 (0.1%)	1.31	349/52169 (0.7%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	216	ILE	CB-CG1	-6.96	1.39	1.53
1	E	646	LEU	CB-CG	-6.83	1.39	1.53
1	B	34	HIS	CB-CG	-6.82	1.40	1.50
1	F	397	ASP	CB-CG	6.55	1.68	1.52
1	E	729	LEU	CB-CG	-6.49	1.40	1.53
1	C	646	LEU	CB-CG	-6.25	1.41	1.53
1	D	216	ILE	CB-CG1	-6.20	1.41	1.53
1	E	823	MET	CG-SD	-6.17	1.65	1.80
1	E	695	VAL	CA-CB	-6.14	1.46	1.54
1	E	397	ASP	CB-CG	6.09	1.67	1.52
1	A	397	ASP	CB-CG	5.89	1.66	1.52
1	F	387	ARG	CD-NE	-5.86	1.38	1.46
1	D	652	VAL	CB-CG1	-5.82	1.33	1.52
1	E	222	ILE	CA-CB	-5.71	1.47	1.54
1	C	652	VAL	CB-CG1	-5.66	1.33	1.52
1	E	34	HIS	CB-CG	-5.65	1.42	1.50
1	B	569	LEU	CB-CG	-5.61	1.42	1.53
1	A	671	LEU	CB-CG	-5.59	1.42	1.53
1	A	246	LEU	CB-CG	-5.55	1.42	1.53
1	A	445	LEU	CB-CG	-5.55	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	VAL	CA-C	-5.50	1.48	1.53
1	E	92	LEU	CB-CG	-5.47	1.42	1.53
1	F	281	LEU	CB-CG	-5.46	1.42	1.53
1	C	671	LEU	CB-CG	-5.42	1.42	1.53
1	D	758	PHE	CB-CG	-5.41	1.38	1.50
1	D	670	PHE	CB-CG	-5.39	1.38	1.50
1	D	802	TYR	CB-CG	-5.36	1.39	1.51
1	A	230	ILE	CB-CG1	-5.36	1.42	1.53
1	E	230	ILE	CB-CG1	-5.33	1.42	1.53
1	F	30	LEU	CB-CG	-5.33	1.42	1.53
1	D	646	LEU	CB-CG	-5.29	1.42	1.53
1	F	828	LEU	CB-CG	-5.22	1.43	1.53
1	A	684	LEU	CB-CG	-5.16	1.43	1.53
1	F	610	PHE	CB-CG	-5.14	1.38	1.50
1	B	189	ARG	CZ-NH2	-5.13	1.26	1.33
1	B	363	HIS	CB-CG	-5.13	1.43	1.50
1	F	199	VAL	CA-CB	-5.09	1.48	1.54
1	A	14	ILE	CB-CG1	-5.05	1.43	1.53
1	F	630	PHE	CB-CG	-5.04	1.39	1.50
1	A	363	HIS	CB-CG	-5.03	1.43	1.50
1	D	640	ARG	CD-NE	-5.00	1.39	1.46
1	B	248	LEU	CB-CG	-5.00	1.43	1.53

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	HIS	CA-CB-CG	-9.28	104.52	113.80
1	E	397	ASP	CA-CB-CG	9.13	121.73	112.60
1	E	342	GLU	CA-C-N	8.92	129.35	120.52
1	E	342	GLU	C-N-CA	8.92	129.35	120.52
1	D	670	PHE	CA-CB-CG	-8.80	105.00	113.80
1	B	882	ASN	N-CA-C	-8.79	102.97	114.31
1	D	646	LEU	N-CA-C	8.60	122.57	109.23
1	C	556	ILE	CA-C-N	8.60	128.25	119.82
1	C	556	ILE	C-N-CA	8.60	128.25	119.82
1	E	880	LEU	CA-C-N	8.58	128.23	119.82
1	E	880	LEU	C-N-CA	8.58	128.23	119.82
1	C	93	GLY	N-CA-C	-8.48	102.66	112.50
1	A	65	PHE	CA-CB-CG	8.41	122.21	113.80
1	A	87	THR	CA-C-N	8.04	127.69	119.56
1	A	87	THR	C-N-CA	8.04	127.69	119.56
1	D	658	THR	N-CA-C	-7.95	100.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	HIS	CA-CB-CG	-7.94	105.86	113.80
1	F	27	HIS	CA-C-N	7.91	128.09	119.87
1	F	27	HIS	C-N-CA	7.91	128.09	119.87
1	E	27	HIS	CA-C-N	7.74	127.46	119.56
1	E	27	HIS	C-N-CA	7.74	127.46	119.56
1	B	772	PHE	CA-CB-CG	-7.71	106.09	113.80
1	D	556	ILE	CA-C-N	7.68	127.85	119.87
1	D	556	ILE	C-N-CA	7.68	127.85	119.87
1	C	246	LEU	N-CA-C	7.64	122.26	110.42
1	B	784	VAL	N-CA-C	-7.59	101.64	110.21
1	E	823	MET	N-CA-C	7.49	121.67	112.23
1	C	219	THR	N-CA-C	-7.36	103.34	111.36
1	B	247	ASP	N-CA-C	7.34	120.52	109.95
1	A	307	ARG	N-CA-C	-7.10	105.54	114.56
1	A	678	LYS	CA-C-N	7.09	126.79	119.56
1	A	678	LYS	C-N-CA	7.09	126.79	119.56
1	B	663	VAL	N-CA-C	7.03	118.09	109.30
1	E	234	VAL	CA-C-N	6.98	126.91	120.21
1	E	234	VAL	C-N-CA	6.98	126.91	120.21
1	D	7	PHE	CA-CB-CG	6.95	120.75	113.80
1	F	610	PHE	CA-CB-CG	-6.94	106.86	113.80
1	D	397	ASP	CA-CB-CG	6.93	119.53	112.60
1	C	53	ASN	CA-CB-CG	-6.90	105.70	112.60
1	B	234	VAL	CA-C-N	6.87	126.89	119.89
1	B	234	VAL	C-N-CA	6.87	126.89	119.89
1	E	409	SER	N-CA-C	-6.87	104.87	113.18
1	B	87	THR	CA-C-N	6.85	126.55	119.56
1	B	87	THR	C-N-CA	6.85	126.55	119.56
1	C	184	ASP	CA-C-N	6.85	126.83	119.78
1	C	184	ASP	C-N-CA	6.85	126.83	119.78
1	E	115	HIS	CA-CB-CG	-6.83	106.97	113.80
1	B	702	MET	N-CA-C	-6.81	105.51	113.88
1	E	107	LYS	N-CA-C	6.80	120.46	111.28
1	E	646	LEU	N-CA-C	6.78	119.44	108.32
1	B	320	GLU	N-CA-C	-6.75	103.99	111.82
1	D	53	ASN	CA-CB-CG	6.74	119.34	112.60
1	A	850	LYS	N-CA-C	-6.73	104.71	113.12
1	F	692	HIS	CA-C-N	6.72	127.26	119.47
1	F	692	HIS	C-N-CA	6.72	127.26	119.47
1	B	678	LYS	CA-C-N	6.70	128.22	119.84
1	B	678	LYS	C-N-CA	6.70	128.22	119.84
1	E	42	THR	CA-C-N	6.70	126.39	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	THR	C-N-CA	6.70	126.39	119.82
1	E	383	LEU	CA-C-N	6.61	126.30	119.56
1	E	383	LEU	C-N-CA	6.61	126.30	119.56
1	F	556	ILE	N-CA-C	6.61	114.09	107.55
1	F	678	LYS	CA-C-N	6.58	128.06	119.84
1	F	678	LYS	C-N-CA	6.58	128.06	119.84
1	F	533	ALA	CA-C-N	6.57	130.04	120.71
1	F	533	ALA	C-N-CA	6.57	130.04	120.71
1	C	76	ILE	CA-C-N	6.55	126.24	119.56
1	C	76	ILE	C-N-CA	6.55	126.24	119.56
1	E	733	PHE	CA-CB-CG	-6.55	107.25	113.80
1	B	668	GLY	N-CA-C	-6.54	106.20	115.30
1	B	93	GLY	N-CA-C	-6.53	104.89	112.73
1	B	171	ALA	N-CA-C	6.52	118.76	108.79
1	B	580	VAL	CA-C-N	-6.50	113.98	122.37
1	B	580	VAL	C-N-CA	-6.50	113.98	122.37
1	A	42	THR	CA-C-N	6.50	126.19	119.82
1	A	42	THR	C-N-CA	6.50	126.19	119.82
1	E	606	GLN	CA-C-N	6.48	126.45	120.03
1	E	606	GLN	C-N-CA	6.48	126.45	120.03
1	B	307	ARG	N-CA-C	-6.48	104.06	112.68
1	C	802	TYR	N-CA-C	6.45	119.59	110.50
1	E	90	TYR	N-CA-C	-6.44	105.24	113.23
1	A	342	GLU	CA-C-N	6.44	126.36	119.85
1	A	342	GLU	C-N-CA	6.44	126.36	119.85
1	C	293	GLY	N-CA-C	-6.43	103.81	114.48
1	C	880	LEU	CA-C-N	6.40	126.53	119.87
1	C	880	LEU	C-N-CA	6.40	126.53	119.87
1	D	705	ASP	N-CA-C	-6.38	102.67	111.28
1	E	40	ILE	N-CA-C	-6.37	104.83	111.58
1	C	274	GLU	N-CA-C	6.35	118.72	109.07
1	B	331	PHE	N-CA-C	-6.33	103.67	111.33
1	A	293	GLY	N-CA-C	-6.32	104.02	114.76
1	C	261	PHE	N-CA-C	-6.32	103.69	111.40
1	A	556	ILE	CA-C-N	6.29	126.75	120.52
1	A	556	ILE	C-N-CA	6.29	126.75	120.52
1	D	299	ASN	N-CA-C	6.29	119.81	111.75
1	F	52	GLN	N-CA-C	-6.29	105.19	112.92
1	C	247	ASP	N-CA-C	6.26	117.27	108.00
1	E	372	LEU	N-CA-C	-6.26	103.99	111.69
1	E	652	VAL	N-CA-C	6.24	116.99	110.62
1	B	246	LEU	N-CA-C	6.21	120.45	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	GLU	N-CA-C	6.21	118.61	109.24
1	F	698	VAL	N-CA-C	-6.21	105.77	111.67
1	A	541	VAL	N-CA-C	6.19	115.53	106.55
1	D	342	GLU	CA-C-N	6.18	126.15	120.03
1	D	342	GLU	C-N-CA	6.18	126.15	120.03
1	C	704	ASP	N-CA-C	-6.14	101.38	110.46
1	C	313	ILE	CA-C-N	-6.12	116.72	122.17
1	C	313	ILE	C-N-CA	-6.12	116.72	122.17
1	D	383	LEU	CA-C-N	6.08	125.71	119.56
1	D	383	LEU	C-N-CA	6.08	125.71	119.56
1	A	27	HIS	CA-C-N	6.08	126.19	119.87
1	A	27	HIS	C-N-CA	6.08	126.19	119.87
1	F	211	ILE	N-CA-C	6.07	116.61	108.11
1	E	759	ARG	CA-C-N	6.06	126.50	119.47
1	E	759	ARG	C-N-CA	6.06	126.50	119.47
1	F	103	GLN	CB-CA-C	-6.04	101.14	110.81
1	E	819	TYR	N-CA-C	6.04	119.00	109.39
1	A	383	LEU	N-CA-C	6.03	119.55	108.94
1	D	234	VAL	CA-C-N	6.02	126.03	119.89
1	D	234	VAL	C-N-CA	6.02	126.03	119.89
1	A	50	TYR	N-CA-C	6.02	120.38	112.13
1	F	372	LEU	N-CA-C	-6.02	104.08	112.45
1	B	261	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	244	PHE	N-CA-C	6.00	119.32	109.72
1	C	603	ASN	CA-C-N	5.99	125.69	119.82
1	C	603	ASN	C-N-CA	5.99	125.69	119.82
1	E	61	ASP	N-CA-C	5.97	117.75	109.15
1	A	658	THR	N-CA-C	-5.94	101.97	110.59
1	A	641	VAL	N-CA-C	5.94	116.42	107.75
1	B	302	LYS	CA-C-N	5.93	126.36	119.47
1	B	302	LYS	C-N-CA	5.93	126.36	119.47
1	B	546	ILE	N-CA-C	5.93	116.58	110.82
1	B	580	VAL	N-CA-C	-5.93	99.72	108.85
1	D	570	ILE	N-CA-C	-5.93	106.04	111.67
1	A	372	LEU	N-CA-C	-5.92	104.41	111.69
1	B	27	HIS	CA-C-N	5.91	125.59	119.56
1	B	27	HIS	C-N-CA	5.91	125.59	119.56
1	B	667	GLU	N-CA-C	5.90	118.26	108.99
1	A	603	ASN	CA-C-N	5.90	127.21	119.84
1	A	603	ASN	C-N-CA	5.90	127.21	119.84
1	C	692	HIS	CA-C-N	5.89	125.57	119.56
1	C	692	HIS	C-N-CA	5.89	125.57	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	667	GLU	N-CA-C	5.88	118.31	108.02
1	F	803	LYS	N-CA-C	-5.88	105.37	112.54
1	D	207	ASN	N-CA-C	5.87	119.25	108.69
1	F	265	PHE	CA-CB-CG	5.86	119.66	113.80
1	C	544	ASP	N-CA-C	5.83	117.64	111.28
1	A	265	PHE	CA-CB-CG	5.82	119.62	113.80
1	E	87	THR	CA-C-N	5.82	126.33	120.04
1	E	87	THR	C-N-CA	5.82	126.33	120.04
1	E	692	HIS	CA-C-N	5.81	126.21	119.47
1	E	692	HIS	C-N-CA	5.81	126.21	119.47
1	D	398	ILE	CB-CA-C	-5.80	104.42	112.02
1	F	803	LYS	CA-C-N	5.80	130.37	122.19
1	F	803	LYS	C-N-CA	5.80	130.37	122.19
1	A	508	PHE	CA-C-N	-5.80	112.90	120.44
1	A	508	PHE	C-N-CA	-5.80	112.90	120.44
1	E	76	ILE	CA-C-N	5.79	125.80	119.90
1	E	76	ILE	C-N-CA	5.79	125.80	119.90
1	D	358	LYS	N-CA-C	-5.78	105.06	111.36
1	F	309	GLN	CA-C-N	-5.78	112.92	121.24
1	F	309	GLN	C-N-CA	-5.78	112.92	121.24
1	D	93	GLY	N-CA-C	-5.77	105.80	112.50
1	D	68	VAL	CB-CA-C	-5.76	104.60	111.97
1	B	132	GLU	N-CA-C	-5.75	104.80	113.89
1	B	556	ILE	CA-C-N	5.75	127.03	119.84
1	B	556	ILE	C-N-CA	5.75	127.03	119.84
1	A	524	VAL	N-CA-C	-5.74	104.77	110.62
1	A	803	LYS	N-CA-C	-5.74	97.56	108.17
1	A	358	LYS	N-CA-C	-5.74	104.64	111.69
1	A	542	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	667	GLU	N-CA-C	5.73	117.99	108.99
1	E	80	GLN	CA-C-N	5.72	126.99	119.84
1	E	80	GLN	C-N-CA	5.72	126.99	119.84
1	D	64	LEU	N-CA-C	-5.70	104.97	111.07
1	E	93	GLY	N-CA-C	-5.70	105.87	112.83
1	D	27	HIS	CA-C-N	5.70	126.97	119.84
1	D	27	HIS	C-N-CA	5.70	126.97	119.84
1	C	207	ASN	N-CA-C	5.69	119.74	108.59
1	C	382	TYR	N-CA-C	5.69	118.34	111.40
1	F	286	ILE	N-CA-C	5.68	121.17	109.34
1	A	31	GLN	CA-C-N	5.67	126.05	119.47
1	A	31	GLN	C-N-CA	5.67	126.05	119.47
1	A	661	GLY	N-CA-C	-5.67	106.83	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	87	THR	CA-C-N	5.66	127.56	121.00
1	F	87	THR	C-N-CA	5.66	127.56	121.00
1	F	727	SER	N-CA-C	5.65	117.11	108.52
1	F	184	ASP	CA-CB-CG	-5.65	106.95	112.60
1	D	87	THR	CA-C-N	5.64	125.25	119.56
1	D	87	THR	C-N-CA	5.64	125.25	119.56
1	F	93	GLY	N-CA-C	-5.64	105.96	112.50
1	A	555	GLY	N-CA-C	-5.63	106.39	112.08
1	C	641	VAL	N-CA-C	5.63	116.23	108.12
1	B	644	SER	N-CA-C	-5.63	105.53	112.90
1	E	809	GLU	N-CA-C	5.61	117.48	111.36
1	B	80	GLN	CA-C-N	5.61	125.98	119.47
1	B	80	GLN	C-N-CA	5.61	125.98	119.47
1	E	261	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	115	HIS	N-CA-C	-5.61	105.25	111.36
1	B	243	LEU	N-CA-C	5.60	118.03	108.90
1	E	609	SER	N-CA-C	5.60	117.56	108.26
1	F	80	GLN	CA-C-N	5.60	126.84	119.84
1	F	80	GLN	C-N-CA	5.60	126.84	119.84
1	D	647	SER	N-CA-C	-5.59	101.02	108.74
1	F	397	ASP	CA-CB-CG	5.59	118.19	112.60
1	E	533	ALA	N-CA-C	-5.59	105.28	111.71
1	D	645	GLU	CB-CA-C	-5.58	103.01	112.00
1	D	247	ASP	CA-CB-CG	5.57	118.17	112.60
1	F	264	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	76	ILE	CA-C-N	5.55	125.56	119.90
1	B	76	ILE	C-N-CA	5.55	125.56	119.90
1	E	506	ARG	N-CA-C	-5.55	105.23	111.28
1	C	87	THR	CA-C-N	5.55	125.64	119.87
1	C	87	THR	C-N-CA	5.55	125.64	119.87
1	B	783	ILE	CB-CA-C	-5.55	104.87	111.97
1	C	372	LEU	N-CA-C	-5.55	105.31	111.36
1	C	681	SER	N-CA-C	5.54	115.15	107.73
1	D	42	THR	CA-C-N	5.54	125.63	119.87
1	D	42	THR	C-N-CA	5.54	125.63	119.87
1	E	232	ASP	N-CA-C	5.53	119.05	111.54
1	E	331	PHE	CA-CB-CG	-5.53	108.28	113.80
1	F	622	GLU	N-CA-C	-5.52	105.34	111.36
1	B	137	ILE	N-CA-C	5.52	118.78	111.17
1	C	640	ARG	N-CA-C	-5.52	102.31	110.48
1	A	769	ILE	N-CA-C	-5.51	100.64	108.58
1	E	31	GLN	CA-C-N	5.51	125.87	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	GLN	C-N-CA	5.51	125.87	119.47
1	A	48	VAL	CA-C-N	5.51	125.18	119.56
1	A	48	VAL	C-N-CA	5.51	125.18	119.56
1	A	741	LYS	N-CA-C	-5.51	99.31	108.34
1	B	187	ILE	N-CA-C	5.50	115.81	108.11
1	B	562	SER	N-CA-C	5.50	118.26	110.50
1	D	581	VAL	N-CA-C	5.50	116.22	108.36
1	F	52	GLN	CA-C-N	5.50	129.05	120.75
1	F	52	GLN	C-N-CA	5.50	129.05	120.75
1	F	287	HIS	CA-C-N	5.49	129.47	120.63
1	F	287	HIS	C-N-CA	5.49	129.47	120.63
1	F	63	ASP	N-CA-C	-5.48	105.39	111.36
1	D	207	ASN	CA-C-N	5.47	126.63	120.66
1	D	207	ASN	C-N-CA	5.47	126.63	120.66
1	D	115	HIS	N-CA-C	-5.47	105.40	111.36
1	E	65	PHE	CA-CB-CG	-5.46	108.34	113.80
1	F	118	PHE	CA-CB-CG	5.46	119.26	113.80
1	D	692	HIS	CA-C-N	5.45	125.12	119.56
1	D	692	HIS	C-N-CA	5.45	125.12	119.56
1	C	260	ASP	CA-CB-CG	5.45	118.05	112.60
1	E	423	LEU	N-CA-C	-5.45	105.34	111.28
1	D	750	VAL	CB-CA-C	-5.44	105.01	111.97
1	F	274	GLU	N-CA-C	5.43	118.09	109.50
1	F	410	LYS	CA-C-N	5.42	125.09	119.56
1	F	410	LYS	C-N-CA	5.42	125.09	119.56
1	F	243	LEU	N-CA-C	5.41	118.05	109.24
1	B	447	LEU	N-CA-C	-5.40	104.94	112.45
1	D	678	LYS	CA-C-N	5.40	125.07	119.56
1	D	678	LYS	C-N-CA	5.40	125.07	119.56
1	C	82	ALA	CA-C-N	5.39	125.06	119.56
1	C	82	ALA	C-N-CA	5.39	125.06	119.56
1	E	666	ASP	CA-CB-CG	-5.39	107.21	112.60
1	E	260	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	53	ASN	N-CA-C	5.38	117.78	110.35
1	A	93	GLY	N-CA-C	-5.38	106.26	112.50
1	F	809	GLU	N-CA-C	5.38	117.22	111.36
1	A	220	ALA	N-CA-C	-5.36	105.44	111.28
1	E	223	GLU	N-CA-C	-5.36	105.44	111.28
1	E	642	ASP	CA-CB-CG	-5.36	107.25	112.60
1	B	216	ILE	N-CA-C	5.35	116.13	110.72
1	C	605	ARG	CA-C-N	-5.35	116.38	122.26
1	C	605	ARG	C-N-CA	-5.35	116.38	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	667	GLU	N-CA-C	5.35	119.04	107.49
1	E	705	ASP	N-CA-C	-5.34	103.87	111.24
1	F	567	GLU	N-CA-C	-5.34	106.44	113.12
1	A	55	ILE	N-CA-C	5.34	115.55	110.42
1	E	603	ASN	CA-C-N	5.33	126.50	119.84
1	E	603	ASN	C-N-CA	5.33	126.50	119.84
1	E	398	ILE	CB-CA-C	-5.32	105.06	112.02
1	A	435	GLU	N-CA-C	-5.31	106.93	113.41
1	F	333	ARG	N-CA-C	-5.31	107.35	113.88
1	F	405	VAL	CB-CA-C	-5.30	105.18	111.97
1	A	363	HIS	CA-CB-CG	-5.30	108.50	113.80
1	F	86	ILE	N-CA-C	-5.29	105.37	110.72
1	F	621	THR	N-CA-C	-5.29	106.67	113.23
1	E	81	PRO	N-CA-C	5.29	123.37	112.47
1	B	607	PRO	N-CA-C	-5.28	102.98	111.38
1	E	244	PHE	N-CA-C	5.27	118.15	109.72
1	B	546	ILE	CB-CA-C	-5.25	105.16	112.04
1	D	603	ASN	CA-C-N	5.25	124.92	119.56
1	D	603	ASN	C-N-CA	5.25	124.92	119.56
1	A	187	ILE	N-CA-C	5.25	115.46	108.11
1	A	234	VAL	CA-C-N	5.24	125.24	119.90
1	A	234	VAL	C-N-CA	5.24	125.24	119.90
1	C	716	ILE	CB-CA-C	-5.23	106.47	111.44
1	E	408	ASP	N-CA-C	-5.22	106.69	113.16
1	A	76	ILE	CA-C-N	5.22	125.22	119.90
1	A	76	ILE	C-N-CA	5.22	125.22	119.90
1	C	321	TYR	N-CA-C	-5.21	104.86	111.11
1	B	646	LEU	N-CA-C	5.21	116.86	108.32
1	B	68	VAL	CB-CA-C	-5.20	105.04	112.22
1	B	758	PHE	CA-C-N	-5.20	113.57	120.65
1	B	758	PHE	C-N-CA	-5.20	113.57	120.65
1	A	367	ILE	N-CA-C	5.20	115.61	108.12
1	D	555	GLY	N-CA-C	-5.20	103.23	112.58
1	E	274	GLU	N-CA-C	5.19	118.52	110.17
1	F	603	ASN	CA-C-N	5.19	126.32	119.84
1	F	603	ASN	C-N-CA	5.19	126.32	119.84
1	F	632	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	334	ARG	N-CA-C	-5.17	106.92	113.43
1	A	616	SER	N-CA-C	-5.17	103.21	110.50
1	E	800	LYS	N-CA-C	-5.16	102.14	110.14
1	D	804	LEU	N-CA-C	5.16	118.24	111.28
1	E	246	LEU	N-CA-C	5.15	117.24	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	THR	N-CA-C	-5.14	105.76	111.36
1	F	606	GLN	CA-C-N	5.14	125.05	119.76
1	F	606	GLN	C-N-CA	5.14	125.05	119.76
1	A	52	GLN	CA-C-N	5.13	131.34	121.54
1	A	52	GLN	C-N-CA	5.13	131.34	121.54
1	A	65	PHE	CB-CA-C	-5.13	102.27	110.79
1	B	434	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	298	ALA	CA-C-N	5.12	127.86	120.38
1	D	298	ALA	C-N-CA	5.12	127.86	120.38
1	E	184	ASP	CA-C-N	5.12	125.03	119.76
1	E	184	ASP	C-N-CA	5.12	125.03	119.76
1	E	752	GLY	N-CA-C	-5.11	106.57	112.50
1	D	569	LEU	N-CA-C	5.11	120.66	113.56
1	A	698	VAL	N-CA-C	-5.11	105.56	110.72
1	C	706	GLY	N-CA-C	-5.10	108.28	115.32
1	C	883	HIS	N-CA-C	5.10	115.78	108.74
1	C	712	GLN	N-CA-C	-5.10	106.65	112.92
1	A	759	ARG	CA-C-N	5.10	125.38	119.47
1	A	759	ARG	C-N-CA	5.10	125.38	119.47
1	D	214	PRO	N-CA-C	-5.08	103.21	111.19
1	F	82	ALA	CA-C-N	5.08	125.76	120.12
1	F	82	ALA	C-N-CA	5.08	125.76	120.12
1	D	722	ILE	CA-C-N	-5.08	116.54	123.10
1	D	722	ILE	C-N-CA	-5.08	116.54	123.10
1	E	836	ILE	CB-CA-C	-5.08	105.94	110.91
1	A	171	ALA	N-CA-C	5.07	116.77	109.07
1	F	435	GLU	N-CA-C	-5.06	106.27	112.90
1	C	652	VAL	N-CA-C	5.06	119.18	111.89
1	B	87	THR	N-CA-C	5.04	116.40	108.23
1	E	560	LYS	N-CA-C	5.04	116.85	111.36
1	C	27	HIS	CA-C-N	5.03	125.31	119.47
1	C	27	HIS	C-N-CA	5.03	125.31	119.47
1	C	564	SER	CA-C-N	5.02	128.63	120.60
1	C	564	SER	C-N-CA	5.02	128.63	120.60
1	C	668	GLY	N-CA-C	-5.02	106.52	114.10
1	E	35	ILE	N-CA-C	-5.02	105.65	110.72
1	F	76	ILE	CA-C-N	5.02	124.92	119.85
1	F	76	ILE	C-N-CA	5.02	124.92	119.85
1	F	883	HIS	CA-CB-CG	5.00	118.81	113.80

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	6722	0	6854	53	0
1	B	6722	0	6855	67	0
1	C	5669	0	5802	64	0
1	D	5669	0	5802	96	0
1	E	6722	0	6854	76	0
1	F	6722	0	6854	56	0
2	P	140	0	33	2	0
3	A	62	0	24	3	0
3	B	62	0	24	8	0
3	C	62	0	24	3	0
3	D	61	0	24	23	0
3	E	62	0	24	5	0
3	F	62	0	24	3	0
All	All	38737	0	39198	428	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 5.

All (428) 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:D:186:VAL:HG12	3:D:1001:AGS:C2	1.67	1.25
1:E:794:ARG:O	1:E:794:ARG:NE	1.90	1.04
3:D:1002:AGS:O1B	3:D:1002:AGS:S1G	2.18	1.01
1:D:218:LYS:NZ	3:D:1001:AGS:O2G	1.94	1.01
1:D:186:VAL:HB	3:D:1001:AGS:N1	1.78	0.97
3:E:1001:AGS:O1B	3:E:1001:AGS:S1G	2.23	0.97
1:C:650:TYR:O	1:C:650:TYR:CD1	2.21	0.94
1:C:650:TYR:O	1:C:650:TYR:HD1	1.50	0.94
1:D:217:GLY:HA2	3:D:1001:AGS:O2A	1.66	0.94
3:B:1001:AGS:H5'1	3:B:1001:AGS:H8	1.50	0.93
1:D:186:VAL:CG1	3:D:1001:AGS:C2	2.50	0.89
1:C:332:GLU:OE1	1:C:332:GLU:N	2.07	0.88
3:B:1001:AGS:O2G	3:B:1001:AGS:O1A	1.93	0.87
3:E:1001:AGS:S1G	3:E:1001:AGS:O2A	2.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1002:AGS:O1B	3:F:1002:AGS:O3G	1.89	0.86
1:D:186:VAL:CB	3:D:1001:AGS:N1	2.39	0.85
1:D:761:GLU:N	1:D:761:GLU:OE1	2.08	0.85
1:D:186:VAL:HG12	3:D:1001:AGS:H2	1.58	0.84
1:E:192:GLU:N	1:E:192:GLU:OE1	2.09	0.84
1:D:217:GLY:CA	3:D:1001:AGS:O2A	2.29	0.80
1:B:650:TYR:CD2	1:B:650:TYR:O	2.36	0.79
1:D:214:PRO:HA	3:D:1001:AGS:O3G	1.82	0.78
1:D:192:GLU:N	1:D:192:GLU:OE1	2.14	0.78
1:B:192:GLU:N	1:B:192:GLU:OE1	2.16	0.78
3:C:1001:AGS:O2G	3:C:1001:AGS:O1A	2.01	0.78
1:F:674:GLN:N	1:F:674:GLN:OE1	2.20	0.74
1:B:310:LEU:HG	1:B:310:LEU:O	1.87	0.74
3:A:1002:AGS:O1A	3:A:1002:AGS:O1B	2.06	0.73
1:C:565:GLU:OE1	1:C:565:GLU:N	2.22	0.72
1:D:556:ILE:O	1:D:556:ILE:HG22	1.91	0.70
1:E:563:GLU:OE1	1:E:563:GLU:N	2.20	0.70
1:C:53:ASN:C	1:C:53:ASN:OD1	2.32	0.69
1:A:310:LEU:O	1:A:310:LEU:HG	1.93	0.68
1:E:794:ARG:HE	1:E:794:ARG:C	1.97	0.68
3:B:1001:AGS:O2G	3:B:1001:AGS:O1B	2.12	0.67
1:B:563:GLU:N	1:B:563:GLU:OE1	2.27	0.66
1:E:387:ARG:HA	1:E:387:ARG:NE	2.11	0.66
1:E:795:PHE:CG	1:E:795:PHE:O	2.46	0.66
1:E:648:GLU:OE1	1:E:648:GLU:N	2.20	0.66
1:E:819:TYR:CD1	1:E:819:TYR:C	2.69	0.66
1:D:831:LEU:C	1:D:831:LEU:HD13	2.22	0.65
1:B:556:ILE:HG13	1:B:556:ILE:O	1.95	0.65
1:F:650:TYR:O	1:F:650:TYR:CD1	2.49	0.65
3:B:1001:AGS:H8	3:B:1001:AGS:C5'	2.26	0.65
1:B:80:GLN:OE1	1:B:80:GLN:N	2.27	0.65
1:D:217:GLY:N	3:D:1001:AGS:O2A	2.30	0.64
1:D:186:VAL:HA	3:D:1001:AGS:H2	1.79	0.64
1:E:718:CYS:O	1:E:718:CYS:SG	2.55	0.64
1:D:852:LYS:HD2	1:D:852:LYS:N	2.11	0.64
1:C:207:ASN:OD1	1:C:207:ASN:C	2.40	0.64
3:B:1002:AGS:O2B	3:B:1002:AGS:O2G	2.15	0.64
1:C:563:GLU:OE1	1:C:563:GLU:N	2.27	0.63
1:B:875:GLU:HG3	1:B:875:GLU:O	1.99	0.63
1:C:556:ILE:O	1:C:556:ILE:HG13	1.97	0.62
3:E:1001:AGS:O1B	3:E:1001:AGS:O1A	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1001:AGS:O2G	3:F:1001:AGS:O1B	2.17	0.62
1:D:652:VAL:O	1:D:652:VAL:HG22	1.98	0.62
1:C:642:ASP:OD1	1:C:642:ASP:N	2.33	0.61
1:F:386:ARG:HA	1:F:386:ARG:NE	2.14	0.61
3:C:1001:AGS:O1A	3:C:1001:AGS:O1B	2.18	0.61
1:A:507:TYR:O	1:A:507:TYR:CD2	2.54	0.61
1:D:729:LEU:C	1:D:729:LEU:HD23	2.26	0.60
3:B:1002:AGS:O1B	3:B:1002:AGS:O2A	2.18	0.60
1:C:650:TYR:CD1	1:C:650:TYR:C	2.79	0.59
1:F:831:LEU:HD23	1:F:831:LEU:C	2.26	0.59
1:A:650:TYR:O	1:A:650:TYR:CD2	2.56	0.59
1:D:387:ARG:NE	1:D:387:ARG:HA	2.18	0.59
1:D:700:LEU:O	1:D:700:LEU:HD23	2.03	0.58
3:E:1001:AGS:S1G	3:E:1001:AGS:PA	3.01	0.58
1:A:483:LEU:C	1:A:483:LEU:HD23	2.29	0.58
1:D:378:LEU:C	1:D:378:LEU:HD23	2.29	0.58
1:F:278:LEU:C	1:F:278:LEU:HD23	2.28	0.58
1:A:246:LEU:N	1:A:246:LEU:HD12	2.19	0.58
1:B:40:ILE:HG22	1:B:40:ILE:O	2.03	0.57
1:B:136:ASP:OD1	1:B:136:ASP:C	2.46	0.57
1:E:819:TYR:C	1:E:819:TYR:HD1	2.13	0.57
1:C:702:MET:SD	1:C:702:MET:N	2.78	0.57
1:A:192:GLU:OE1	1:A:192:GLU:N	2.29	0.57
1:D:650:TYR:CD1	1:D:650:TYR:C	2.82	0.57
3:C:1002:AGS:C8	3:C:1002:AGS:H5'2	2.35	0.57
1:D:186:VAL:HA	3:D:1001:AGS:C2	2.35	0.57
1:F:386:ARG:HA	1:F:386:ARG:HE	1.69	0.56
1:B:649:LYS:O	1:B:651:ALA:N	2.39	0.56
1:D:772:PHE:CD1	1:D:772:PHE:N	2.71	0.56
1:B:285:GLU:HG2	1:B:285:GLU:O	2.06	0.56
1:D:126:ILE:H	1:D:126:ILE:HD12	1.70	0.55
1:C:641:VAL:N	1:C:684:LEU:O	2.39	0.55
1:D:186:VAL:CB	3:D:1001:AGS:C2	2.82	0.55
1:B:539:ASN:O	1:B:540:VAL:C	2.50	0.55
1:D:700:LEU:HD23	1:D:700:LEU:C	2.30	0.55
1:C:262:GLU:OE1	1:C:262:GLU:N	2.31	0.55
1:B:708:ILE:O	1:B:708:ILE:CG2	2.54	0.55
1:E:508:PHE:N	1:E:508:PHE:CD1	2.74	0.55
1:C:337:LYS:NZ	1:C:339:GLU:OE2	2.40	0.55
1:A:50:TYR:CD1	1:A:50:TYR:C	2.81	0.54
1:A:504:ASP:OD1	1:B:429:LYS:NZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:NH1	3:D:1001:AGS:S1G	2.80	0.54
1:D:772:PHE:N	1:D:772:PHE:HD1	2.05	0.54
1:F:337:LYS:NZ	1:F:339:GLU:OE2	2.40	0.54
1:B:328:ASP:OD2	1:B:331:PHE:N	2.40	0.54
3:D:1001:AGS:O1B	3:D:1001:AGS:O1A	2.24	0.54
1:F:483:LEU:C	1:F:483:LEU:HD23	2.32	0.54
1:D:262:GLU:OE1	1:D:262:GLU:N	2.41	0.54
1:C:559:LYS:NZ	1:D:796:GLU:OE2	2.41	0.54
1:F:148:ARG:O	1:F:149:GLY:C	2.51	0.54
1:C:187:ILE:C	1:C:187:ILE:HD12	2.33	0.54
1:D:805:ASN:OD1	1:D:805:ASN:N	2.27	0.53
1:D:670:PHE:CD2	1:D:670:PHE:C	2.87	0.53
1:E:559:LYS:NZ	1:F:796:GLU:OE2	2.42	0.53
1:B:650:TYR:O	1:B:650:TYR:CG	2.60	0.53
1:C:655:LEU:N	1:C:655:LEU:HD23	2.24	0.53
1:F:649:LYS:O	1:F:651:ALA:N	2.41	0.53
1:E:583:GLN:HA	1:E:583:GLN:OE1	2.07	0.53
1:D:15:LEU:HD13	1:D:15:LEU:C	2.34	0.53
1:D:365:VAL:HG23	1:D:365:VAL:O	2.09	0.53
1:D:240:GLY:O	1:D:277:THR:OG1	2.22	0.52
1:B:126:ILE:O	1:B:126:ILE:HG22	2.07	0.52
1:E:649:LYS:NZ	2:P:19:UNK:O	2.40	0.52
3:E:1002:AGS:O1A	3:E:1002:AGS:O1B	2.24	0.52
3:B:1002:AGS:H3'	3:B:1002:AGS:N3	2.25	0.52
1:D:403:VAL:O	1:D:407:ARG:N	2.42	0.52
1:A:58:GLY:O	1:A:59:ARG:HB3	2.10	0.52
1:A:289:LEU:O	1:A:291:GLY:N	2.43	0.52
1:F:831:LEU:HD23	1:F:831:LEU:O	2.10	0.52
1:E:309:GLN:N	1:E:309:GLN:OE1	2.42	0.51
1:A:130:PHE:O	1:A:130:PHE:CD1	2.63	0.51
1:B:388:LEU:O	1:B:389:PRO:C	2.53	0.51
1:D:852:LYS:HD2	1:D:852:LYS:H	1.75	0.51
1:F:556:ILE:O	1:F:680:TYR:OH	2.29	0.51
1:C:40:ILE:HG22	1:C:40:ILE:O	2.10	0.51
1:D:831:LEU:HD13	1:D:831:LEU:O	2.10	0.51
1:D:296:ASP:O	1:D:296:ASP:CG	2.53	0.51
1:A:302:LYS:N	1:A:303:PRO:HD2	2.26	0.51
1:B:289:LEU:O	1:B:290:MET:HB2	2.10	0.51
1:C:761:GLU:OE1	1:C:761:GLU:N	2.35	0.51
1:D:215:GLY:N	3:D:1001:AGS:O2B	2.43	0.51
1:B:9:GLU:OE1	1:B:9:GLU:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLN:OE1	1:B:134:GLN:N	2.27	0.51
1:B:421:LEU:C	1:B:421:LEU:HD23	2.35	0.50
1:D:650:TYR:O	1:D:651:ALA:C	2.53	0.50
1:A:725:MET:SD	1:A:725:MET:N	2.84	0.50
1:D:393:LEU:CD1	3:D:1001:AGS:HI'	2.42	0.50
1:D:186:VAL:CA	3:D:1001:AGS:N1	2.74	0.50
1:F:294:LYS:HG3	1:F:295:ASP:H	1.76	0.50
1:E:148:ARG:O	1:E:149:GLY:C	2.53	0.50
1:B:53:ASN:OD1	1:B:53:ASN:C	2.53	0.49
1:E:794:ARG:O	1:E:796:GLU:N	2.45	0.49
1:D:9:GLU:OE1	1:D:9:GLU:N	2.29	0.49
1:E:794:ARG:O	1:E:794:ARG:HG3	2.12	0.49
1:C:763:LEU:O	1:D:830:ARG:NH2	2.45	0.49
1:F:120:LEU:O	1:F:124:SER:N	2.45	0.49
1:A:58:GLY:O	1:A:59:ARG:CB	2.60	0.49
1:E:211:ILE:HD12	1:E:211:ILE:N	2.27	0.49
1:C:555:GLY:O	1:C:556:ILE:C	2.55	0.49
1:E:678:LYS:O	1:E:679:PRO:C	2.55	0.49
1:F:729:LEU:HD23	1:F:729:LEU:C	2.38	0.49
1:E:852:LYS:N	1:E:852:LYS:HD2	2.28	0.49
1:A:134:GLN:HA	1:A:134:GLN:OE1	2.11	0.49
1:F:276:LYS:O	1:F:277:THR:OG1	2.28	0.49
1:F:410:LYS:O	1:F:410:LYS:HG3	2.11	0.49
1:E:794:ARG:O	1:E:794:ARG:CG	2.61	0.49
1:B:772:PHE:CD1	1:B:772:PHE:N	2.81	0.48
1:B:651:ALA:HA	1:B:656:LEU:HB3	1.94	0.48
1:B:785:ASP:OD1	1:B:789:LYS:NZ	2.44	0.48
1:B:819:TYR:CD1	1:B:819:TYR:N	2.81	0.48
1:E:705:ASP:O	1:E:707:ARG:N	2.46	0.48
1:A:528:GLU:H	1:A:528:GLU:CD	2.21	0.48
1:D:378:LEU:HD23	1:D:378:LEU:O	2.14	0.48
1:C:647:SER:OG	1:C:648:GLU:N	2.46	0.48
1:F:213:GLU:O	1:F:218:LYS:NZ	2.47	0.48
1:D:184:ASP:OD1	1:D:358:LYS:NZ	2.42	0.48
1:E:537:ILE:HG22	1:E:537:ILE:O	2.13	0.48
1:B:205:LYS:NZ	1:C:390:ASP:OD1	2.47	0.48
1:F:15:LEU:HD23	1:F:15:LEU:C	2.39	0.48
1:A:246:LEU:O	1:A:247:ASP:CB	2.61	0.48
1:B:483:LEU:HD23	1:B:483:LEU:C	2.38	0.48
1:F:365:VAL:HG13	1:F:365:VAL:O	2.13	0.48
1:A:50:TYR:CD1	1:A:50:TYR:O	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:ASP:CG	1:D:543:SER:H	2.20	0.48
1:A:318:ASN:OD1	1:A:318:ASN:N	2.44	0.47
1:C:668:GLY:O	1:C:672:THR:N	2.47	0.47
1:E:508:PHE:N	1:E:508:PHE:HD1	2.12	0.47
1:C:187:ILE:HD12	1:C:187:ILE:O	2.14	0.47
1:E:445:LEU:C	1:E:445:LEU:HD12	2.39	0.47
1:A:421:LEU:HD23	1:A:421:LEU:C	2.39	0.47
1:B:799:ASP:OD2	1:B:800:LYS:NZ	2.47	0.47
1:C:649:LYS:O	1:C:651:ALA:N	2.47	0.47
1:A:31:GLN:HB2	1:A:32:PRO:HD2	1.95	0.47
1:A:130:PHE:O	1:A:130:PHE:HD1	1.98	0.47
1:E:289:LEU:O	1:E:290:MET:HB2	2.15	0.47
1:F:278:LEU:HD23	1:F:278:LEU:O	2.14	0.47
1:C:655:LEU:HD23	1:C:655:LEU:H	1.79	0.47
1:D:565:GLU:O	1:D:566:ASN:C	2.58	0.47
1:E:53:ASN:C	1:E:53:ASN:OD1	2.57	0.47
1:E:725:MET:N	1:E:725:MET:SD	2.88	0.47
1:F:211:ILE:HD12	1:F:211:ILE:N	2.30	0.47
1:F:466:TYR:CD1	1:F:466:TYR:N	2.75	0.47
1:D:665:TYR:CD2	1:D:665:TYR:O	2.68	0.47
1:D:831:LEU:C	1:D:831:LEU:CD1	2.88	0.47
1:B:819:TYR:N	1:B:819:TYR:HD1	2.13	0.46
1:E:9:GLU:H	1:E:9:GLU:CD	2.14	0.46
1:B:410:LYS:N	1:B:411:PRO:CD	2.78	0.46
1:D:542:ASP:OD1	1:D:543:SER:N	2.48	0.46
1:D:668:GLY:O	1:D:672:THR:N	2.48	0.46
1:A:256:LYS:NZ	1:E:295:ASP:OD2	2.48	0.46
1:A:429:LYS:HA	1:A:429:LYS:HD3	1.74	0.46
1:E:246:LEU:N	1:E:246:LEU:HD12	2.30	0.46
1:E:823:MET:HG3	1:E:824:GLY:O	2.15	0.46
1:F:601:LEU:O	1:F:602:ALA:C	2.59	0.46
1:B:190:GLU:H	1:B:190:GLU:CD	2.21	0.46
1:C:53:ASN:OD1	1:C:53:ASN:O	2.32	0.46
1:D:289:LEU:HD22	1:D:289:LEU:N	2.31	0.46
1:D:880:LEU:CB	1:D:881:PRO:CD	2.94	0.46
1:E:685:PHE:CD1	1:E:685:PHE:N	2.83	0.46
1:F:559:LYS:O	1:F:559:LYS:HG2	2.16	0.46
1:C:632:PHE:N	1:C:632:PHE:CD1	2.84	0.46
1:E:409:SER:O	1:E:410:LYS:C	2.59	0.46
1:F:143:GLN:HA	1:F:143:GLN:OE1	2.16	0.46
3:A:1001:AGS:O2G	3:A:1001:AGS:O1B	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:HIS:ND1	1:B:34:HIS:NE2	2.54	0.46
1:E:854:THR:OG1	1:E:855:VAL:N	2.47	0.46
1:A:534:ASN:C	1:A:534:ASN:OD1	2.59	0.46
1:C:327:LYS:NZ	1:E:666:ASP:OD2	2.36	0.46
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.36	0.46
1:F:642:ASP:C	1:F:642:ASP:OD1	2.59	0.46
1:E:337:LYS:NZ	1:E:339:GLU:OE2	2.49	0.46
1:A:60:TYR:CD1	1:A:60:TYR:C	2.93	0.46
1:A:812:ASP:O	1:A:816:LYS:N	2.49	0.46
1:B:700:LEU:HD12	1:B:700:LEU:C	2.40	0.46
1:D:652:VAL:O	1:D:652:VAL:CG2	2.62	0.46
1:D:211:ILE:N	1:D:211:ILE:HD12	2.31	0.45
1:B:132:GLU:O	1:B:133:ALA:C	2.59	0.45
1:C:183:LEU:C	1:C:183:LEU:HD23	2.42	0.45
1:D:149:GLY:O	1:D:169:LYS:NZ	2.48	0.45
1:D:705:ASP:O	1:D:707:ARG:N	2.49	0.45
1:F:278:LEU:O	1:F:278:LEU:CD2	2.64	0.45
3:F:1001:AGS:O1B	3:F:1001:AGS:O2A	2.34	0.45
1:C:652:VAL:O	1:C:652:VAL:HG22	2.17	0.45
1:E:516:GLN:OE1	1:E:516:GLN:HA	2.16	0.45
1:F:409:SER:O	1:F:410:LYS:C	2.57	0.45
1:E:80:GLN:O	1:E:82:ALA:N	2.50	0.45
1:F:352:LEU:O	1:F:356:GLN:N	2.50	0.45
1:D:583:GLN:HG2	1:D:773:ASN:H	1.81	0.45
1:E:365:VAL:O	1:E:365:VAL:HG13	2.16	0.45
1:F:610:PHE:CD1	1:F:610:PHE:N	2.83	0.45
1:C:646:LEU:C	1:C:646:LEU:HD23	2.42	0.45
1:A:40:ILE:HG22	1:A:40:ILE:O	2.17	0.45
1:B:137:ILE:HG13	1:B:137:ILE:O	2.17	0.45
1:C:246:LEU:HD22	1:C:246:LEU:N	2.30	0.45
1:E:794:ARG:NE	1:E:794:ARG:C	2.66	0.45
1:F:301:LEU:O	1:F:302:LYS:C	2.59	0.45
1:A:89:SER:OG	1:A:90:TYR:N	2.48	0.45
1:D:880:LEU:HB2	1:D:881:PRO:HD2	1.98	0.45
1:A:583:GLN:OE1	1:A:583:GLN:HA	2.17	0.45
3:B:1001:AGS:O1B	3:B:1001:AGS:O2A	2.34	0.45
1:E:283:ILE:N	1:E:283:ILE:HD12	2.30	0.45
1:A:525:ALA:O	1:A:526:GLU:C	2.57	0.45
1:B:277:THR:OG1	1:B:278:LEU:N	2.50	0.45
1:D:246:LEU:O	1:D:247:ASP:CB	2.65	0.45
1:A:190:GLU:H	1:A:190:GLU:CD	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASP:O	1:A:705:ASP:C	2.60	0.44
1:D:668:GLY:O	1:D:669:GLY:C	2.60	0.44
1:E:289:LEU:O	1:E:290:MET:CB	2.65	0.44
1:D:758:PHE:O	1:D:759:ARG:C	2.58	0.44
1:E:387:ARG:HA	1:E:387:ARG:HE	1.81	0.44
1:E:352:LEU:O	1:E:356:GLN:N	2.50	0.44
1:F:804:LEU:O	1:F:804:LEU:HG	2.17	0.44
1:A:337:LYS:NZ	1:A:339:GLU:OE2	2.50	0.44
1:C:134:GLN:O	1:C:134:GLN:HG2	2.17	0.44
1:E:597:SER:OG	1:E:598:ARG:N	2.51	0.44
1:F:758:PHE:O	1:F:759:ARG:C	2.60	0.44
1:E:183:LEU:N	1:E:183:LEU:HD12	2.32	0.44
1:E:704:ASP:O	1:E:705:ASP:C	2.61	0.44
1:F:630:PHE:CD1	1:F:630:PHE:C	2.95	0.44
1:A:514:LYS:NZ	1:A:518:GLU:OE2	2.50	0.44
1:B:211:ILE:N	1:B:211:ILE:HD12	2.32	0.44
1:E:497:TYR:CE1	1:F:421:LEU:HB3	2.53	0.44
3:A:1002:AGS:O3A	3:A:1002:AGS:S1G	2.76	0.44
1:B:555:GLY:O	1:B:556:ILE:C	2.60	0.44
1:C:601:LEU:O	1:C:602:ALA:C	2.60	0.44
1:D:129:ILE:HG13	1:D:129:ILE:O	2.18	0.44
1:E:141:LYS:O	1:E:142:GLN:C	2.61	0.44
1:F:558:VAL:O	1:F:558:VAL:HG22	2.18	0.44
1:C:542:ASP:OD1	1:C:543:SER:N	2.51	0.43
1:C:655:LEU:H	1:C:655:LEU:CD2	2.31	0.43
1:F:543:SER:O	1:F:544:ASP:C	2.61	0.43
1:F:650:TYR:O	1:F:650:TYR:HD1	2.00	0.43
1:F:835:GLU:OE1	1:F:839:LYS:NZ	2.51	0.43
1:A:649:LYS:O	1:A:650:TYR:C	2.61	0.43
1:B:665:TYR:O	1:B:666:ASP:C	2.59	0.43
1:C:276:LYS:O	1:C:278:LEU:N	2.51	0.43
1:C:835:GLU:OE1	1:C:839:LYS:NZ	2.51	0.43
2:P:15:UNK:O	2:P:16:UNK:CB	2.66	0.43
1:A:360:GLU:OE1	1:A:480:LYS:NZ	2.50	0.43
1:A:699:MET:O	1:A:700:LEU:C	2.60	0.43
1:B:434:ASP:OD2	1:B:442:LYS:NZ	2.49	0.43
1:F:481:LYS:NZ	1:F:485:GLU:OE2	2.49	0.43
1:A:352:LEU:O	1:A:356:GLN:N	2.51	0.43
1:B:658:THR:H	1:B:667:GLU:HB2	1.83	0.43
1:D:798:ASN:OD1	1:D:798:ASN:N	2.50	0.43
1:A:286:ILE:O	1:A:286:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:ARG:N	1:B:827:PRO:CD	2.82	0.43
1:C:246:LEU:N	1:C:246:LEU:CD2	2.82	0.43
1:C:684:LEU:C	1:C:684:LEU:HD23	2.44	0.43
1:B:352:LEU:HB3	1:B:372:LEU:HD22	2.00	0.43
1:E:387:ARG:NE	1:E:387:ARG:CA	2.82	0.43
1:F:828:LEU:O	1:F:829:ASN:C	2.59	0.43
1:C:335:PHE:CD1	1:C:335:PHE:C	2.97	0.43
1:D:174:MET:HE3	1:D:174:MET:O	2.19	0.43
1:D:612:PHE:CD1	1:D:612:PHE:N	2.87	0.43
1:E:558:VAL:HG13	1:E:680:TYR:HH	1.83	0.43
1:F:285:GLU:O	1:F:287:HIS:N	2.52	0.43
1:B:244:PHE:CD1	1:B:244:PHE:N	2.87	0.43
1:D:612:PHE:CD1	1:D:724:ILE:HG23	2.54	0.43
1:E:190:GLU:H	1:E:190:GLU:CD	2.27	0.43
1:F:359:TYR:N	1:F:359:TYR:CD1	2.83	0.43
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.78	0.42
1:A:880:LEU:HB3	1:A:881:PRO:HD3	2.00	0.42
1:B:780:ILE:O	1:B:780:ILE:HG22	2.17	0.42
1:D:368:LEU:HD12	1:D:368:LEU:N	2.34	0.42
1:E:222:ILE:HD13	1:E:222:ILE:HA	1.73	0.42
1:F:583:GLN:OE1	1:F:583:GLN:HA	2.19	0.42
1:A:410:LYS:HB3	1:A:411:PRO:CD	2.49	0.42
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.82	0.42
1:D:50:TYR:CD2	1:D:51:LEU:HG	2.55	0.42
1:F:826:ARG:N	1:F:827:PRO:CD	2.82	0.42
1:A:464:GLN:OE1	1:A:464:GLN:HA	2.19	0.42
1:A:852:LYS:HD2	1:A:852:LYS:N	2.35	0.42
1:B:638:MET:O	1:B:638:MET:HG3	2.16	0.42
1:C:351:ILE:HD12	1:C:351:ILE:HA	1.88	0.42
1:C:644:SER:HB3	1:C:687:GLU:HB2	2.00	0.42
1:D:735:ASN:OD1	1:D:735:ASN:C	2.61	0.42
1:F:80:GLN:O	1:F:82:ALA:N	2.52	0.42
1:A:851:ASP:OD2	1:A:852:LYS:NZ	2.45	0.42
1:B:720:ASN:OD1	1:B:720:ASN:N	2.45	0.42
1:D:186:VAL:CA	3:D:1001:AGS:C2	2.98	0.42
1:E:794:ARG:NE	1:E:794:ARG:CA	2.83	0.42
1:C:333:ARG:HD2	1:C:333:ARG:N	2.35	0.42
1:C:671:LEU:HA	1:C:671:LEU:HD23	1.68	0.42
1:E:795:PHE:O	1:E:796:GLU:C	2.63	0.42
1:F:50:TYR:CD2	1:F:51:LEU:HG	2.55	0.42
1:B:310:LEU:O	1:B:310:LEU:CG	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.84	0.42
1:C:247:ASP:O	1:C:249:ALA:N	2.52	0.42
1:D:236:THR:HA	1:D:239:GLN:HB2	2.00	0.42
1:D:642:ASP:C	1:D:642:ASP:OD1	2.63	0.42
1:E:687:GLU:O	1:E:687:GLU:HG3	2.19	0.42
1:A:774:LYS:NZ	1:A:821:ASP:OD2	2.50	0.42
1:D:186:VAL:HA	3:D:1001:AGS:N1	2.35	0.42
1:D:247:ASP:OD1	1:D:248:LEU:N	2.49	0.42
1:D:565:GLU:O	1:D:568:LYS:N	2.52	0.42
1:E:795:PHE:CD1	1:E:795:PHE:C	2.96	0.42
1:F:568:LYS:O	1:F:569:LEU:HB2	2.19	0.42
1:C:309:GLN:O	1:C:310:LEU:C	2.61	0.42
1:E:428:ILE:O	1:E:432:GLU:N	2.52	0.42
1:D:331:PHE:CG	1:D:332:GLU:N	2.85	0.42
1:D:641:VAL:O	1:D:641:VAL:HG13	2.19	0.42
1:B:49:PRO:C	1:B:53:ASN:HB3	2.45	0.42
1:B:66:LYS:HE2	1:B:66:LYS:HB3	1.87	0.42
1:C:748:ASN:O	1:C:752:GLY:N	2.53	0.42
1:D:190:GLU:H	1:D:190:GLU:CD	2.27	0.42
1:A:66:LYS:HB3	1:A:66:LYS:HE2	1.86	0.41
1:A:659:THR:O	1:A:660:ALA:C	2.63	0.41
1:A:818:GLY:O	1:A:819:TYR:C	2.63	0.41
1:C:780:ILE:O	1:C:781:HIS:C	2.63	0.41
1:E:89:SER:OG	1:E:90:TYR:N	2.53	0.41
1:A:825:ALA:O	1:A:826:ARG:C	2.62	0.41
1:B:360:GLU:OE1	1:B:480:LYS:NZ	2.51	0.41
1:B:708:ILE:O	1:B:708:ILE:HG23	2.14	0.41
1:E:260:ASP:OD1	1:E:261:PHE:N	2.51	0.41
1:B:296:ASP:CG	1:B:296:ASP:O	2.60	0.41
1:B:355:LEU:O	1:B:356:GLN:C	2.63	0.41
1:D:333:ARG:HA	1:D:333:ARG:NE	2.36	0.41
1:D:566:ASN:CG	1:D:567:GLU:H	2.28	0.41
1:E:729:LEU:C	1:E:729:LEU:HD23	2.45	0.41
1:B:305:LEU:HB3	1:B:310:LEU:HB2	2.02	0.41
1:D:186:VAL:CG1	3:D:1001:AGS:N1	2.72	0.41
1:D:216:ILE:HA	1:D:216:ILE:HD12	1.77	0.41
1:D:278:LEU:N	1:D:278:LEU:HD22	2.36	0.41
1:E:276:LYS:HE2	1:E:276:LYS:HB2	1.87	0.41
1:D:186:VAL:HB	3:D:1001:AGS:C6	2.47	0.41
1:D:705:ASP:OD2	1:E:640:ARG:NH1	2.54	0.41
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ILE:HD12	1:D:126:ILE:N	2.35	0.41
1:E:761:GLU:O	1:E:765:ARG:HD3	2.20	0.41
1:F:744:GLU:O	1:F:745:SER:CB	2.68	0.41
1:B:445:LEU:HD12	1:B:445:LEU:C	2.46	0.41
1:C:133:ALA:O	1:C:134:GLN:C	2.62	0.41
1:E:297:ALA:O	1:E:298:ALA:HB3	2.21	0.41
1:A:140:ILE:HD13	1:A:140:ILE:HG21	1.90	0.41
1:B:794:ARG:O	1:B:795:PHE:C	2.63	0.41
1:D:337:LYS:NZ	1:D:339:GLU:OE1	2.54	0.41
1:D:812:ASP:O	1:D:813:PHE:C	2.62	0.41
1:A:53:ASN:CG	1:A:54:LEU:H	2.28	0.41
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.65	0.41
1:B:568:LYS:O	1:B:569:LEU:HB2	2.21	0.41
1:C:355:LEU:O	1:C:356:GLN:C	2.64	0.41
1:C:680:TYR:CD1	1:C:680:TYR:N	2.89	0.41
1:C:802:TYR:HB3	1:C:804:LEU:H	1.86	0.41
1:E:92:LEU:O	1:E:93:GLY:C	2.59	0.41
1:E:410:LYS:HB2	1:E:411:PRO:CD	2.51	0.41
1:E:498:ASP:OD2	1:E:501:THR:N	2.54	0.41
1:B:784:VAL:O	1:B:785:ASP:HB3	2.21	0.41
1:C:33:ILE:HD12	1:C:33:ILE:HA	1.93	0.41
1:D:277:THR:OG1	1:D:278:LEU:N	2.53	0.41
1:F:62:TYR:HA	1:F:65:PHE:HB3	2.03	0.41
1:B:428:ILE:O	1:B:429:LYS:C	2.63	0.40
1:C:299:ASN:CG	1:C:300:ILE:N	2.79	0.40
1:C:717:ASP:N	1:C:717:ASP:OD1	2.53	0.40
1:D:235:PRO:O	1:D:239:GLN:N	2.54	0.40
1:E:307:ARG:HD3	1:E:307:ARG:HA	1.86	0.40
1:C:583:GLN:O	1:C:583:GLN:HG3	2.21	0.40
1:D:90:TYR:CD1	1:D:90:TYR:C	2.99	0.40
1:E:298:ALA:O	1:E:299:ASN:C	2.64	0.40
1:E:629:GLY:O	1:E:633:ASN:N	2.54	0.40
1:E:851:ASP:OD2	1:E:852:LYS:NZ	2.48	0.40
1:B:680:TYR:CD1	1:B:680:TYR:C	2.99	0.40
1:F:815:ALA:HA	1:F:819:TYR:CD1	2.56	0.40
1:F:825:ALA:C	1:F:827:PRO:HD2	2.47	0.40
1:C:302:LYS:HB2	1:C:303:PRO:HD3	2.03	0.40
1:D:300:ILE:HD13	1:D:300:ILE:HA	1.90	0.40
1:E:181:GLY:O	1:E:182:LYS:HB2	2.22	0.40
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.80	0.40
1:C:725:MET:HE2	1:C:725:MET:HB2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:729:LEU:HD23	1:D:729:LEU:O	2.22	0.40
1:E:823:MET:HG3	1:E:824:GLY:N	2.37	0.40
1:F:247:ASP:O	1:F:249:ALA:N	2.54	0.40
1:F:826:ARG:N	1:F:827:PRO:HD2	2.37	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	843/908 (93%)	796 (94%)	38 (4%)	9 (1%)	11	46
1	B	845/908 (93%)	784 (93%)	49 (6%)	12 (1%)	9	40
1	C	713/908 (78%)	671 (94%)	38 (5%)	4 (1%)	21	59
1	D	713/908 (78%)	661 (93%)	36 (5%)	16 (2%)	5	29
1	E	843/908 (93%)	786 (93%)	44 (5%)	13 (2%)	8	40
1	F	843/908 (93%)	789 (94%)	41 (5%)	13 (2%)	8	40
All	All	4800/5448 (88%)	4487 (94%)	246 (5%)	67 (1%)	11	40

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	THR
1	A	290	MET
1	A	807	THR
1	B	318	ASN
1	B	540	VAL
1	B	650	TYR
1	B	706	GLY
1	C	650	TYR

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Mol	Chain	Res	Type
1	D	28	PRO
1	D	85	GLU
1	D	247	ASP
1	D	277	THR
1	D	542	ASP
1	D	566	ASN
1	D	807	THR
1	E	81	PRO
1	E	277	THR
1	E	290	MET
1	E	569	LEU
1	E	650	TYR
1	E	651	ALA
1	E	706	GLY
1	E	795	PHE
1	E	807	THR
1	F	81	PRO
1	F	286	ILE
1	F	569	LEU
1	F	650	TYR
1	F	745	SER
1	F	807	THR
1	A	59	ARG
1	A	247	ASP
1	A	852	LYS
1	B	277	THR
1	B	388	LEU
1	B	669	GLY
1	B	852	LYS
1	C	248	LEU
1	C	277	THR
1	C	569	LEU
1	D	706	GLY
1	D	852	LYS
1	F	137	ILE
1	F	248	LEU
1	F	706	GLY
1	D	651	ALA
1	E	852	LYS
1	F	686	ASP
1	A	295	ASP
1	A	650	TYR

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Mol	Chain	Res	Type
1	B	248	LEU
1	D	249	ALA
1	D	294	LYS
1	D	880	LEU
1	E	298	ALA
1	E	299	ASN
1	E	679	PRO
1	F	267	GLY
1	F	818	GLY
1	F	852	LYS
1	B	385	TYR
1	B	651	ALA
1	D	89	SER
1	D	561	LEU
1	B	86	ILE
1	D	556	ILE
1	A	706	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	732/783 (94%)	731 (100%)	1 (0%)	88	89
1	B	732/783 (94%)	732 (100%)	0	100	100
1	C	620/783 (79%)	620 (100%)	0	100	100
1	D	620/783 (79%)	619 (100%)	1 (0%)	87	87
1	E	732/783 (94%)	731 (100%)	1 (0%)	88	89
1	F	732/783 (94%)	732 (100%)	0	100	100
All	All	4168/4698 (89%)	4165 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	LEU

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Mol	Chain	Res	Type
1	D	374	THR
1	E	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	79	GLN
1	A	287	HIS
1	A	467	ASN
1	A	523	GLN
1	B	106	GLN
1	B	180	GLN
1	B	808	GLN
1	C	19	GLN
1	C	25	HIS
1	C	29	GLN
1	C	31	GLN
1	C	606	GLN
1	C	829	ASN
1	D	128	GLN
1	D	142	GLN
1	D	287	HIS
1	D	362	HIS
1	D	781	HIS
1	D	829	ASN
1	E	128	GLN
1	E	362	HIS
1	E	422	GLN
1	E	571	HIS
1	E	676	GLN
1	E	712	GLN
1	F	19	GLN
1	F	127	GLN
1	F	292	ASN
1	F	420	GLN
1	F	523	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	A	1001	-	32,33,33	2.08	6 (18%)	45,52,52	2.27	16 (35%)
3	AGS	B	1001	-	32,33,33	2.13	8 (25%)	45,52,52	2.23	15 (33%)
3	AGS	A	1002	-	32,33,33	1.98	6 (18%)	45,52,52	2.22	16 (35%)
3	AGS	D	1002	-	27,32,33	2.44	6 (22%)	39,49,52	5.78	15 (38%)
3	AGS	F	1002	-	32,33,33	2.05	7 (21%)	45,52,52	2.18	13 (28%)
3	AGS	E	1001	-	32,33,33	2.05	8 (25%)	45,52,52	2.23	14 (31%)
3	AGS	E	1002	-	32,33,33	2.38	9 (28%)	45,52,52	2.36	17 (37%)
3	AGS	F	1001	-	32,33,33	1.96	6 (18%)	45,52,52	2.25	15 (33%)
3	AGS	C	1002	-	32,33,33	2.04	7 (21%)	45,52,52	2.33	14 (31%)
3	AGS	D	1001	-	32,33,33	2.38	9 (28%)	45,52,52	2.36	17 (37%)
3	AGS	B	1002	-	32,33,33	2.13	7 (21%)	45,52,52	2.22	13 (28%)
3	AGS	C	1001	-	32,33,33	2.23	10 (31%)	45,52,52	2.15	12 (26%)

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	A	1001	-	-	3/21/38/38	0/3/3/3
3	AGS	B	1001	-	-	8/21/38/38	0/3/3/3
3	AGS	A	1002	-	-	0/21/38/38	0/3/3/3
3	AGS	D	1002	-	-	6/13/36/38	0/3/3/3
3	AGS	F	1002	-	-	6/21/38/38	0/3/3/3
3	AGS	E	1001	-	-	8/21/38/38	0/3/3/3
3	AGS	E	1002	-	-	4/21/38/38	0/3/3/3
3	AGS	F	1001	-	-	10/21/38/38	0/3/3/3
3	AGS	C	1002	-	-	5/21/38/38	0/3/3/3
3	AGS	D	1001	-	-	4/21/38/38	0/3/3/3
3	AGS	B	1002	-	-	9/21/38/38	0/3/3/3
3	AGS	C	1001	-	-	5/21/38/38	0/3/3/3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	AGS	C5-N7	-7.96	1.24	1.39
3	A	1001	AGS	PG-S1G	7.68	2.07	1.90
3	E	1001	AGS	PG-S1G	7.55	2.07	1.90
3	C	1001	AGS	PG-S1G	7.52	2.07	1.90
3	B	1002	AGS	PG-S1G	7.47	2.06	1.90
3	F	1002	AGS	PG-S1G	7.45	2.06	1.90
3	C	1002	AGS	PG-S1G	7.37	2.06	1.90
3	B	1001	AGS	PG-S1G	7.36	2.06	1.90
3	A	1002	AGS	PG-S1G	7.29	2.06	1.90
3	D	1001	AGS	PG-S1G	7.14	2.06	1.90
3	E	1002	AGS	PG-S1G	7.13	2.06	1.90
3	D	1002	AGS	PG-S1G	7.12	2.06	1.90
3	F	1001	AGS	PG-S1G	7.10	2.06	1.90
3	E	1002	AGS	PB-O3A	-5.71	1.53	1.59
3	D	1001	AGS	PB-O3A	-5.69	1.53	1.59
3	D	1001	AGS	C5-C4	5.17	1.48	1.39
3	E	1002	AGS	C5-C4	5.17	1.48	1.39
3	B	1002	AGS	C5-C4	5.16	1.48	1.39
3	E	1001	AGS	C5-C4	5.02	1.48	1.39
3	F	1002	AGS	C5-C4	4.79	1.47	1.39
3	A	1002	AGS	C5-C4	4.68	1.47	1.39
3	A	1001	AGS	C5-C4	4.65	1.47	1.39
3	C	1001	AGS	C5-C4	4.65	1.47	1.39
3	B	1001	AGS	C5-C4	4.51	1.47	1.39
3	C	1002	AGS	C5-C4	4.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	AGS	C5-C4	4.49	1.47	1.39
3	F	1001	AGS	C5-C4	4.47	1.47	1.39
3	C	1001	AGS	PB-O3A	-4.15	1.55	1.59
3	D	1001	AGS	C5-N7	-3.85	1.32	1.39
3	E	1002	AGS	C5-N7	-3.84	1.32	1.39
3	C	1001	AGS	PA-O3A	-3.83	1.55	1.59
3	E	1002	AGS	PA-O3A	-3.72	1.55	1.59
3	D	1001	AGS	PA-O3A	-3.70	1.55	1.59
3	F	1002	AGS	C5-N7	-3.56	1.32	1.39
3	C	1002	AGS	C5-N7	-3.46	1.32	1.39
3	B	1001	AGS	PB-O3A	-3.44	1.55	1.59
3	B	1002	AGS	C5-N7	-3.41	1.32	1.39
3	B	1001	AGS	C5-N7	-3.30	1.33	1.39
3	F	1001	AGS	C5-N7	-3.09	1.33	1.39
3	C	1001	AGS	C5-N7	-2.99	1.33	1.39
3	A	1002	AGS	C5-N7	-2.98	1.33	1.39
3	B	1001	AGS	PB-O3B	-2.97	1.56	1.59
3	A	1001	AGS	C5-N7	-2.95	1.33	1.39
3	B	1001	AGS	PA-O3A	-2.93	1.56	1.59
3	B	1002	AGS	PB-O3A	-2.92	1.56	1.59
3	A	1001	AGS	PB-O3A	-2.86	1.56	1.59
3	E	1001	AGS	C5-N7	-2.85	1.33	1.39
3	A	1001	AGS	PG-O2G	2.78	1.63	1.54
3	C	1002	AGS	PA-O3A	-2.71	1.56	1.59
3	D	1001	AGS	PB-O3B	-2.71	1.56	1.59
3	E	1002	AGS	PB-O3B	-2.71	1.56	1.59
3	C	1001	AGS	PB-O3B	-2.59	1.56	1.59
3	D	1001	AGS	C8-N9	-2.58	1.33	1.37
3	E	1002	AGS	C8-N9	-2.57	1.33	1.37
3	E	1001	AGS	PB-O3B	-2.52	1.56	1.59
3	B	1002	AGS	PG-O2G	2.52	1.62	1.54
3	A	1002	AGS	PG-O2G	2.46	1.62	1.54
3	E	1001	AGS	C5-C6	2.42	1.47	1.41
3	D	1002	AGS	C5-C6	2.40	1.47	1.41
3	F	1002	AGS	PG-O2G	2.38	1.62	1.54
3	C	1002	AGS	PG-O2G	2.37	1.62	1.54
3	C	1001	AGS	C5-C6	2.36	1.47	1.41
3	F	1001	AGS	PA-O3A	-2.35	1.57	1.59
3	F	1002	AGS	PB-O3A	-2.33	1.57	1.59
3	E	1001	AGS	PG-O2G	2.30	1.62	1.54
3	C	1001	AGS	PG-O2G	2.30	1.62	1.54
3	F	1001	AGS	PB-O3A	-2.28	1.57	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1002	AGS	PG-O2G	2.26	1.62	1.54
3	F	1001	AGS	PG-O2G	2.25	1.62	1.54
3	C	1002	AGS	PB-O3B	-2.24	1.57	1.59
3	B	1001	AGS	PG-O2G	2.24	1.62	1.54
3	B	1002	AGS	C5-C6	2.24	1.47	1.41
3	D	1001	AGS	PG-O2G	2.24	1.62	1.54
3	B	1001	AGS	C4-N9	-2.23	1.33	1.37
3	F	1002	AGS	C5-C6	2.23	1.47	1.41
3	C	1002	AGS	PB-O3A	-2.23	1.57	1.59
3	E	1001	AGS	C8-N7	2.23	1.36	1.31
3	D	1002	AGS	PG-O2G	2.21	1.61	1.54
3	A	1002	AGS	C5-C6	2.19	1.47	1.41
3	B	1002	AGS	PB-O3B	-2.17	1.57	1.59
3	D	1002	AGS	PG-O3G	-2.15	1.47	1.54
3	C	1001	AGS	PG-O3G	-2.12	1.47	1.54
3	E	1002	AGS	C5-C6	2.12	1.46	1.41
3	F	1002	AGS	PA-O3A	-2.11	1.57	1.59
3	D	1001	AGS	C5-C6	2.10	1.46	1.41
3	C	1001	AGS	C4-N9	-2.09	1.33	1.37
3	E	1001	AGS	PG-O3G	-2.09	1.47	1.54
3	A	1002	AGS	PB-O3A	-2.07	1.57	1.59
3	A	1001	AGS	C5-C6	2.03	1.46	1.41

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	C4-N9-C1'	20.43	174.41	126.63
3	D	1002	AGS	C1'-N9-C8	-20.30	82.04	127.09
3	D	1002	AGS	C4-N9-C8	-12.72	92.39	105.74
3	D	1002	AGS	C5-C4-N3	-8.68	114.77	126.72
3	D	1002	AGS	C5-C4-N9	8.23	114.78	105.81
3	D	1001	AGS	C5-C4-N3	-6.92	117.19	126.72
3	E	1002	AGS	C5-C4-N3	-6.92	117.19	126.72
3	F	1001	AGS	C5-C4-N3	-6.81	117.33	126.72
3	C	1002	AGS	C5-C4-N3	-6.73	117.45	126.72
3	B	1002	AGS	C5-C4-N3	-6.64	117.57	126.72
3	E	1001	AGS	C5-C4-N3	-6.56	117.69	126.72
3	F	1002	AGS	C5-C4-N3	-6.53	117.72	126.72
3	B	1001	AGS	C5-C4-N3	-6.44	117.84	126.72
3	A	1001	AGS	C5-C4-N3	-6.41	117.89	126.72
3	F	1001	AGS	N3-C4-N9	6.33	137.94	127.17
3	A	1002	AGS	C5-C4-N3	-6.31	118.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	AGS	PB-O3B-PG	-6.31	110.08	133.17
3	B	1002	AGS	PB-O3B-PG	-6.29	110.16	133.17
3	C	1002	AGS	PB-O3B-PG	-6.27	110.23	133.17
3	C	1002	AGS	N3-C4-N9	6.21	137.73	127.17
3	C	1001	AGS	PB-O3B-PG	-6.09	110.88	133.17
3	D	1001	AGS	N3-C4-N9	5.98	137.33	127.17
3	E	1002	AGS	N3-C4-N9	5.97	137.33	127.17
3	A	1001	AGS	N3-C4-N9	5.95	137.28	127.17
3	B	1001	AGS	N3-C4-N9	5.88	137.17	127.17
3	C	1001	AGS	C5-C4-N3	-5.86	118.64	126.72
3	E	1001	AGS	PB-O3B-PG	-5.76	112.09	133.17
3	D	1001	AGS	PB-O3B-PG	-5.66	112.47	133.17
3	E	1002	AGS	PB-O3B-PG	-5.66	112.47	133.17
3	F	1002	AGS	N3-C4-N9	5.58	136.66	127.17
3	B	1002	AGS	N3-C4-N9	5.53	136.58	127.17
3	E	1001	AGS	N3-C4-N9	5.52	136.56	127.17
3	A	1002	AGS	N3-C4-N9	5.50	136.53	127.17
3	D	1002	AGS	C4-C5-N7	-5.49	104.30	110.58
3	D	1002	AGS	N9-C8-N7	5.31	121.47	113.94
3	A	1001	AGS	PB-O3B-PG	-5.20	114.13	133.17
3	F	1002	AGS	PB-O3B-PG	-5.09	114.54	133.17
3	C	1001	AGS	N3-C4-N9	4.90	135.51	127.17
3	F	1001	AGS	PB-O3B-PG	-4.79	115.64	133.17
3	D	1002	AGS	C2-N3-C4	4.38	122.54	111.83
3	A	1002	AGS	PB-O3B-PG	-4.34	117.29	133.17
3	A	1002	AGS	O3A-PA-O1A	-3.49	100.21	110.70
3	A	1001	AGS	O2G-PG-O3B	3.46	116.19	104.64
3	A	1002	AGS	C2-N3-C4	3.44	120.24	111.83
3	C	1002	AGS	N6-C6-N1	3.42	126.00	118.38
3	A	1001	AGS	N6-C6-N1	3.40	125.94	118.38
3	C	1001	AGS	C4-C5-N7	-3.39	106.71	110.58
3	F	1001	AGS	C2-N3-C4	3.38	120.09	111.83
3	F	1001	AGS	N6-C6-N1	3.38	125.90	118.38
3	E	1001	AGS	O3A-PA-O1A	-3.37	100.56	110.70
3	F	1002	AGS	C2-N3-C4	3.37	120.06	111.83
3	C	1002	AGS	C2-N3-C4	3.37	120.06	111.83
3	E	1002	AGS	C2-N3-C4	3.37	120.05	111.83
3	B	1001	AGS	C2-N3-C4	3.37	120.05	111.83
3	E	1001	AGS	C2-N3-C4	3.36	120.04	111.83
3	D	1001	AGS	C2-N3-C4	3.36	120.04	111.83
3	A	1002	AGS	O2G-PG-O3B	3.34	115.80	104.64
3	A	1001	AGS	C2-N3-C4	3.30	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	AGS	C2-N3-C4	3.27	119.83	111.83
3	B	1001	AGS	N6-C6-N1	3.27	125.66	118.38
3	C	1001	AGS	C2-N3-C4	3.24	119.75	111.83
3	A	1002	AGS	N6-C6-N1	3.24	125.59	118.38
3	B	1002	AGS	C4-C5-N7	-3.20	106.92	110.58
3	B	1002	AGS	N6-C6-N1	3.16	125.42	118.38
3	D	1001	AGS	O2G-PG-O3B	3.15	115.16	104.64
3	E	1002	AGS	O2G-PG-O3B	3.14	115.13	104.64
3	F	1001	AGS	O2G-PG-O3B	3.14	115.12	104.64
3	E	1002	AGS	N6-C6-N1	3.10	125.28	118.38
3	C	1002	AGS	O2G-PG-O3B	3.09	114.96	104.64
3	D	1001	AGS	N6-C6-N1	3.08	125.24	118.38
3	C	1001	AGS	O3A-PA-O1A	-3.04	101.56	110.70
3	E	1001	AGS	C4-C5-N7	-3.02	107.13	110.58
3	D	1002	AGS	O2G-PG-O3B	3.00	114.65	104.64
3	A	1002	AGS	C4-C5-N7	-2.98	107.17	110.58
3	D	1001	AGS	C4-C5-N7	-2.96	107.19	110.58
3	D	1002	AGS	C6-C5-C4	2.96	121.22	117.18
3	F	1002	AGS	O2G-PG-O3B	2.96	114.51	104.64
3	E	1002	AGS	C4-C5-N7	-2.95	107.21	110.58
3	F	1002	AGS	C4-C5-N7	-2.93	107.23	110.58
3	D	1002	AGS	N6-C6-N1	2.91	124.85	118.38
3	B	1001	AGS	C4-N9-C8	2.88	108.76	105.74
3	A	1001	AGS	C4-N9-C8	2.87	108.75	105.74
3	E	1001	AGS	O2G-PG-O3B	2.83	114.09	104.64
3	F	1001	AGS	C5-C6-N6	-2.83	116.29	123.29
3	C	1001	AGS	C5-N7-C8	2.80	107.85	103.45
3	A	1001	AGS	C5-C6-N6	-2.74	116.49	123.29
3	E	1002	AGS	O2B-PB-O1B	2.74	125.17	112.44
3	D	1001	AGS	O2B-PB-O1B	2.73	125.15	112.44
3	C	1002	AGS	C5'-C4'-C3'	-2.72	105.41	115.21
3	A	1001	AGS	O2B-PB-O1B	2.70	125.01	112.44
3	C	1002	AGS	C5-C6-N6	-2.70	116.61	123.29
3	F	1001	AGS	C4-N9-C8	2.68	108.56	105.74
3	F	1002	AGS	C5-N7-C8	2.68	107.67	103.45
3	E	1002	AGS	O3A-PB-O1B	-2.68	102.64	110.70
3	C	1001	AGS	C4-N9-C8	2.68	108.55	105.74
3	D	1001	AGS	O3A-PB-O1B	-2.67	102.68	110.70
3	F	1002	AGS	O2A-PA-O3A	2.65	114.45	107.27
3	F	1002	AGS	N6-C6-N1	2.64	124.26	118.38
3	D	1002	AGS	N3-C2-N1	-2.63	124.61	128.58
3	C	1001	AGS	O2G-PG-O3B	2.63	113.41	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	AGS	N3-C2-N1	-2.61	124.63	128.58
3	F	1002	AGS	N3-C2-N1	-2.58	124.68	128.58
3	B	1002	AGS	O2G-PG-O3B	2.57	113.22	104.64
3	B	1001	AGS	N3-C2-N1	-2.57	124.70	128.58
3	A	1002	AGS	C4-N9-C8	2.56	108.43	105.74
3	C	1002	AGS	O3A-PA-O1A	-2.55	103.02	110.70
3	E	1001	AGS	C5-N7-C8	2.55	107.46	103.45
3	D	1001	AGS	C1'-N9-C8	-2.53	121.49	127.09
3	E	1002	AGS	C1'-N9-C8	-2.52	121.50	127.09
3	F	1001	AGS	C1'-N9-C8	-2.52	121.50	127.09
3	C	1002	AGS	C4-N9-C8	2.52	108.39	105.74
3	B	1001	AGS	O2G-PG-O3B	2.52	113.04	104.64
3	B	1002	AGS	C5'-C4'-C3'	-2.50	106.20	115.21
3	E	1001	AGS	N6-C6-N1	2.50	123.94	118.38
3	C	1001	AGS	N3-C2-N1	-2.50	124.81	128.58
3	A	1002	AGS	C5-N7-C8	2.49	107.37	103.45
3	B	1001	AGS	O3A-PA-O1A	-2.49	103.21	110.70
3	A	1002	AGS	C5-C6-N6	-2.47	117.17	123.29
3	C	1002	AGS	N3-C2-N1	-2.47	124.85	128.58
3	D	1002	AGS	C5'-C4'-C3'	-2.46	106.35	115.21
3	E	1001	AGS	C4-N9-C8	2.45	108.31	105.74
3	F	1001	AGS	O3A-PA-O1A	-2.45	103.34	110.70
3	D	1001	AGS	O5'-C5'-C4'	-2.44	100.69	108.99
3	E	1001	AGS	C2'-C3'-C4'	2.43	107.30	102.61
3	E	1002	AGS	O5'-C5'-C4'	-2.42	100.75	108.99
3	A	1001	AGS	N3-C2-N1	-2.42	124.92	128.58
3	B	1002	AGS	C5-N7-C8	2.42	107.25	103.45
3	A	1002	AGS	O2B-PB-O1B	2.41	123.66	112.44
3	A	1001	AGS	C1'-N9-C8	-2.40	121.78	127.09
3	B	1001	AGS	C5-C6-N6	-2.39	117.36	123.29
3	B	1002	AGS	O3A-PA-O1A	-2.38	103.53	110.70
3	A	1001	AGS	C4-C5-N7	-2.38	107.86	110.58
3	F	1002	AGS	O2B-PB-O1B	2.37	123.48	112.44
3	E	1002	AGS	O3A-PA-O1A	-2.35	103.63	110.70
3	B	1001	AGS	O3'-C3'-C4'	-2.35	104.33	111.08
3	D	1001	AGS	O3A-PA-O1A	-2.35	103.64	110.70
3	C	1002	AGS	C5-N7-C8	2.35	107.14	103.45
3	F	1002	AGS	O3A-PA-O1A	-2.32	103.72	110.70
3	D	1002	AGS	C5-N7-C8	2.30	107.06	103.45
3	F	1001	AGS	N3-C2-N1	-2.29	125.11	128.58
3	D	1001	AGS	C5-N7-C8	2.29	107.05	103.45
3	F	1001	AGS	C4-C5-N7	-2.28	107.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	O3A-PA-O1A	-2.28	103.84	110.70
3	E	1002	AGS	N3-C2-N1	-2.28	125.13	128.58
3	D	1001	AGS	C6-C5-C4	2.27	120.28	117.18
3	E	1002	AGS	C6-C5-C4	2.27	120.28	117.18
3	E	1002	AGS	C5-N7-C8	2.27	107.02	103.45
3	D	1001	AGS	N3-C2-N1	-2.27	125.15	128.58
3	F	1001	AGS	C5-N7-C8	2.26	107.00	103.45
3	A	1001	AGS	C5-N7-C8	2.25	106.99	103.45
3	C	1001	AGS	O2B-PB-O1B	2.24	122.85	112.44
3	F	1002	AGS	C5'-C4'-C3'	-2.21	107.27	115.21
3	D	1001	AGS	O5'-PA-O1A	2.20	117.66	108.94
3	A	1001	AGS	O3B-PB-O1B	-2.20	104.09	110.70
3	B	1002	AGS	N3-C2-N1	-2.20	125.26	128.58
3	E	1002	AGS	O5'-PA-O1A	2.19	117.62	108.94
3	F	1001	AGS	O2A-PA-O1A	2.19	122.63	112.44
3	B	1002	AGS	O2B-PB-O1B	2.18	122.58	112.44
3	B	1001	AGS	C4-C5-N7	-2.17	108.10	110.58
3	C	1002	AGS	C4-C5-N7	-2.17	108.10	110.58
3	A	1001	AGS	O3A-PA-O1A	-2.16	104.20	110.70
3	F	1001	AGS	O2B-PB-O1B	2.16	122.50	112.44
3	E	1001	AGS	N3-C2-N1	-2.16	125.32	128.58
3	B	1001	AGS	O2A-PA-O1A	2.15	122.43	112.44
3	A	1002	AGS	C2'-C1'-N9	-2.12	108.03	113.30
3	C	1002	AGS	C2'-C1'-N9	-2.07	108.17	113.30
3	B	1002	AGS	C5-C6-N6	-2.05	118.21	123.29
3	C	1001	AGS	N9-C8-N7	-2.04	111.04	113.94
3	A	1002	AGS	O2A-PA-O1A	2.04	121.92	112.44
3	E	1002	AGS	C2'-C3'-C4'	2.02	106.52	102.61
3	B	1001	AGS	O2B-PB-O1B	2.02	121.84	112.44
3	B	1001	AGS	C5-N7-C8	2.02	106.62	103.45
3	A	1002	AGS	O4'-C1'-N9	2.02	111.96	108.09
3	D	1001	AGS	C2'-C3'-C4'	2.02	106.50	102.61
3	E	1001	AGS	O2A-PA-O1A	2.01	121.81	112.44
3	A	1001	AGS	C2'-C3'-C4'	2.01	106.49	102.61
3	E	1001	AGS	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
3	B	1001	AGS	PB-O3B-PG-O3G
3	B	1001	AGS	C5'-O5'-PA-O2A
3	B	1002	AGS	PB-O3B-PG-O2G
3	B	1002	AGS	PB-O3B-PG-O3G
3	B	1002	AGS	C5'-O5'-PA-O2A
3	B	1002	AGS	C5'-O5'-PA-O3A
3	C	1001	AGS	C5'-O5'-PA-O2A
3	C	1001	AGS	C5'-O5'-PA-O3A
3	C	1001	AGS	O4'-C1'-N9-C8
3	C	1001	AGS	O4'-C1'-N9-C4
3	D	1002	AGS	C5'-O5'-PA-O1A
3	D	1002	AGS	C5'-O5'-PA-O3A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	E	1001	AGS	C5'-O5'-PA-O3A
3	F	1001	AGS	PB-O3B-PG-O2G
3	F	1001	AGS	PB-O3B-PG-O3G
3	F	1001	AGS	C5'-O5'-PA-O3A
3	F	1002	AGS	PB-O3B-PG-O2G
3	F	1002	AGS	PB-O3B-PG-O3G
3	A	1001	AGS	C3'-C4'-C5'-O5'
3	C	1002	AGS	C3'-C4'-C5'-O5'
3	D	1001	AGS	O4'-C4'-C5'-O5'
3	E	1002	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	C3'-C4'-C5'-O5'
3	C	1002	AGS	O4'-C4'-C5'-O5'
3	D	1001	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	O4'-C4'-C5'-O5'
3	E	1002	AGS	C3'-C4'-C5'-O5'
3	B	1002	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	C3'-C4'-C5'-O5'
3	F	1002	AGS	C3'-C4'-C5'-O5'
3	F	1001	AGS	O4'-C4'-C5'-O5'
3	F	1001	AGS	C3'-C4'-C5'-O5'
3	B	1002	AGS	C2'-C1'-N9-C4
3	F	1002	AGS	O4'-C4'-C5'-O5'
3	D	1001	AGS	C2'-C1'-N9-C4
3	E	1002	AGS	C2'-C1'-N9-C4
3	E	1001	AGS	PG-O3B-PB-O1B
3	D	1002	AGS	O4'-C1'-N9-C4
3	D	1001	AGS	C2'-C1'-N9-C8
3	E	1002	AGS	C2'-C1'-N9-C8

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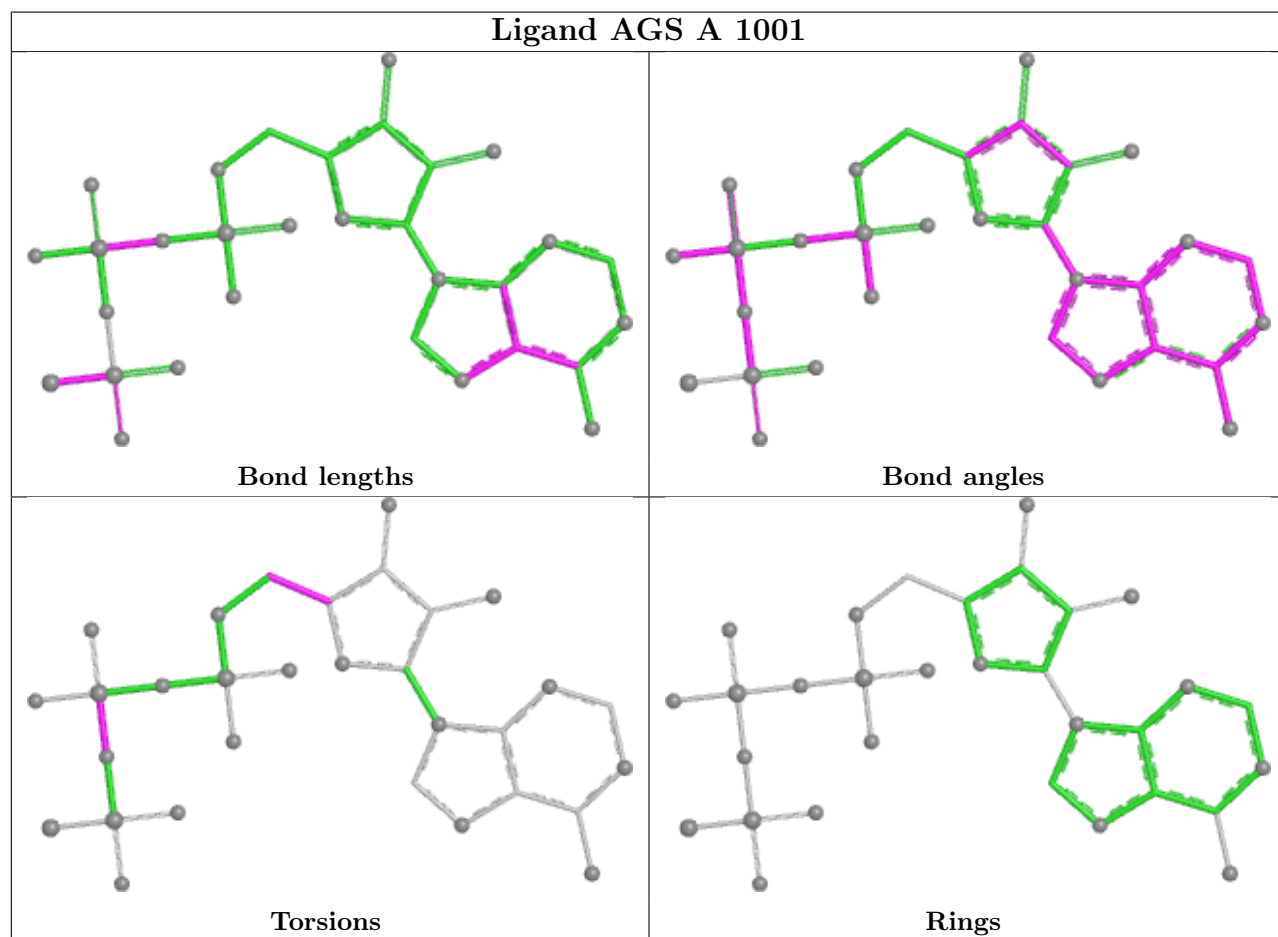
Mol	Chain	Res	Type	Atoms
3	C	1002	AGS	PB-O3A-PA-O2A
3	B	1002	AGS	C2'-C1'-N9-C8
3	D	1002	AGS	C2'-C1'-N9-C8
3	B	1002	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	C5'-O5'-PA-O1A
3	B	1001	AGS	C5'-O5'-PA-O3A
3	C	1001	AGS	C5'-O5'-PA-O1A
3	C	1002	AGS	C5'-O5'-PA-O1A
3	D	1002	AGS	C5'-O5'-PA-O2A
3	E	1001	AGS	C5'-O5'-PA-O1A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

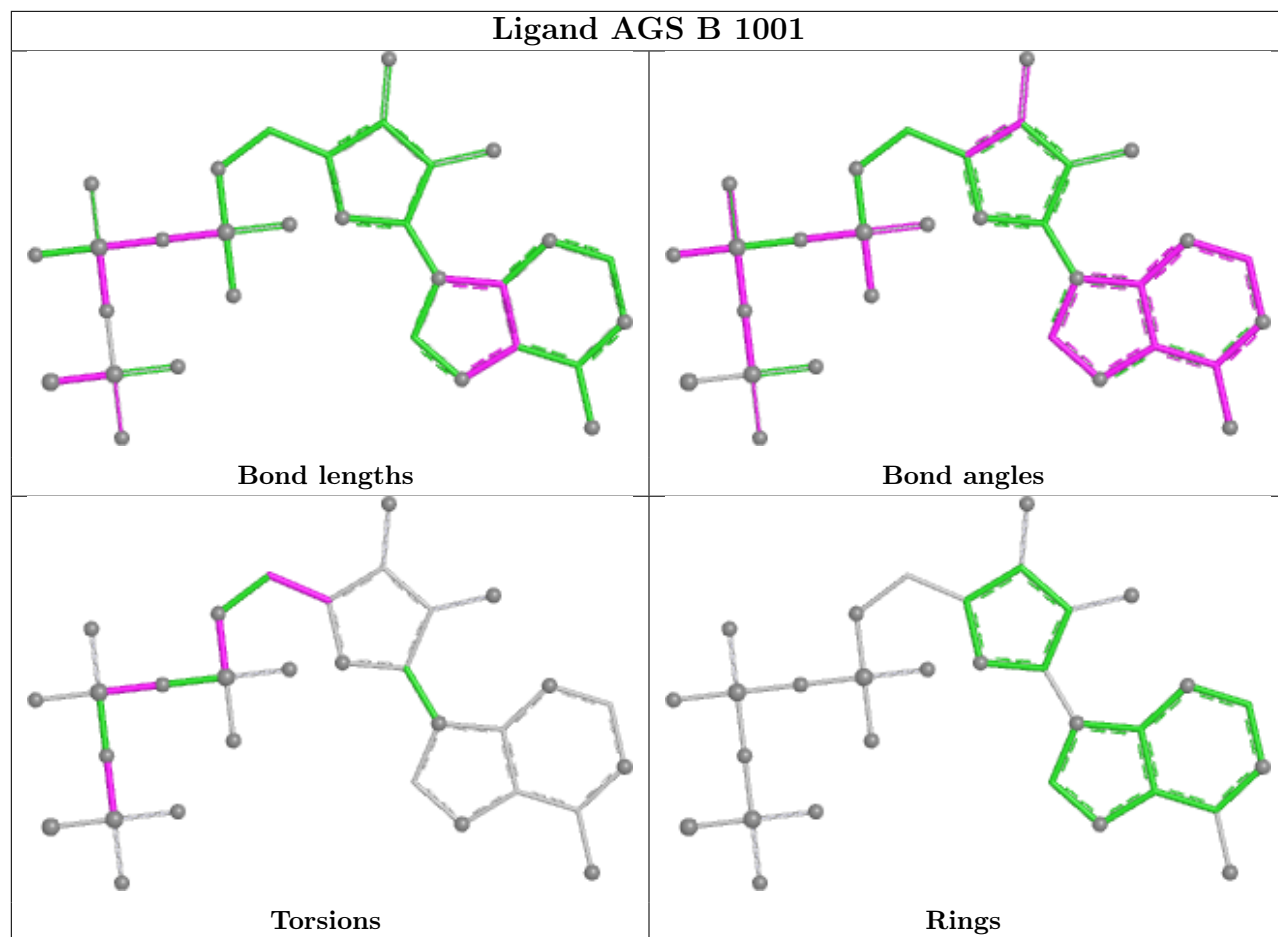
There are no ring outliers.

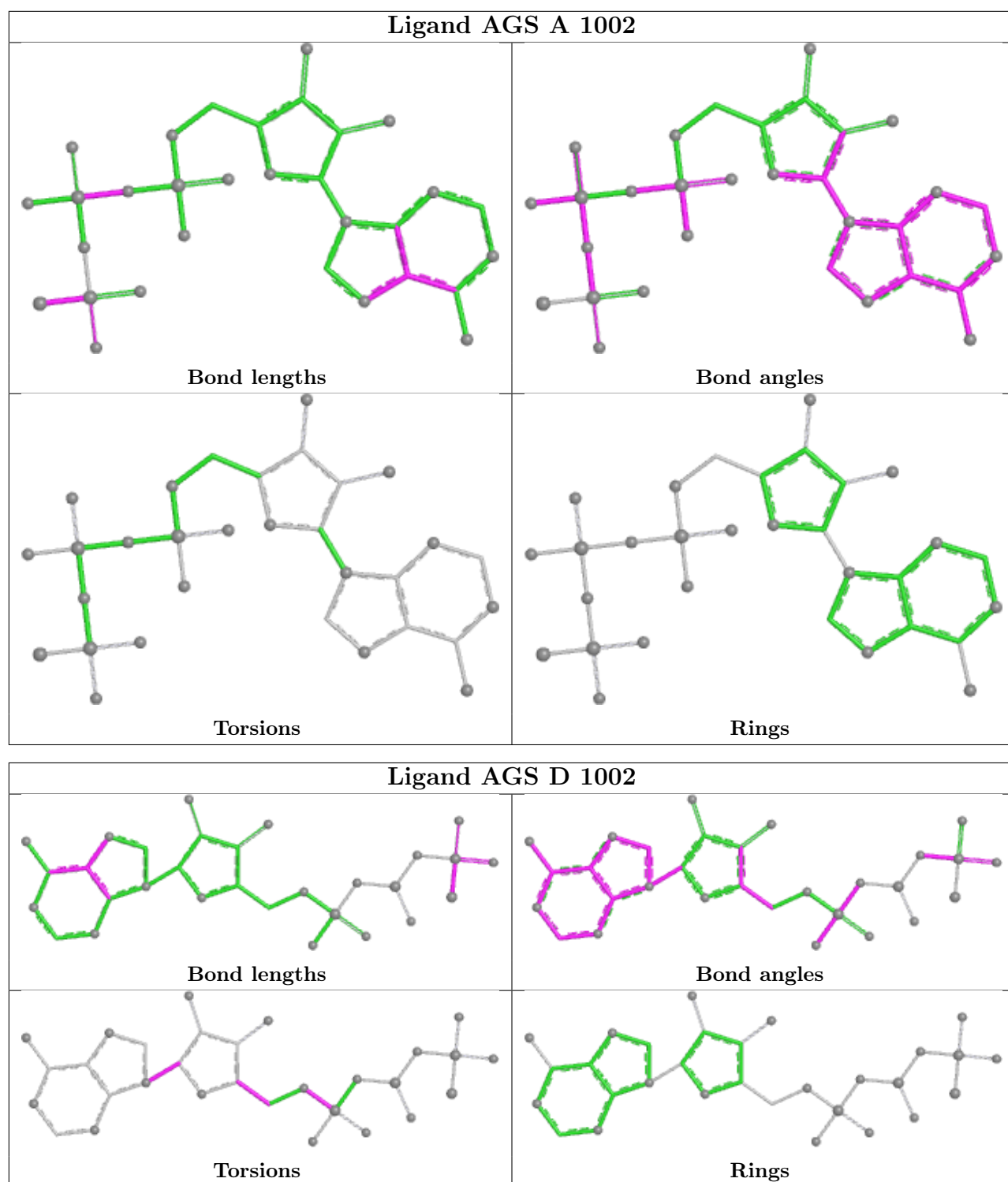
12 monomers are involved in 45 short contacts:

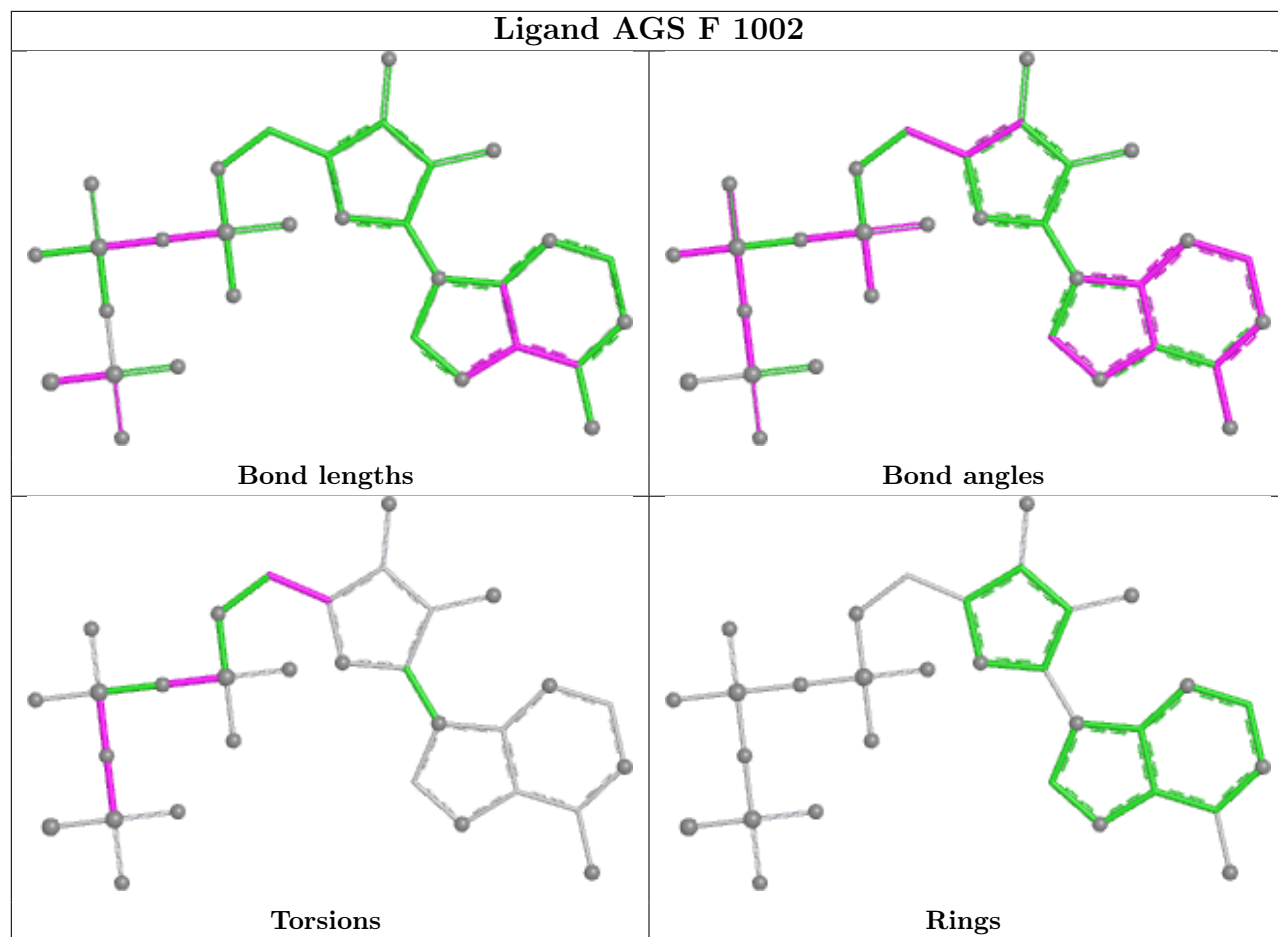
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AGS	1	0
3	B	1001	AGS	5	0
3	A	1002	AGS	2	0
3	D	1002	AGS	1	0
3	F	1002	AGS	1	0
3	E	1001	AGS	4	0
3	E	1002	AGS	1	0
3	F	1001	AGS	2	0
3	C	1002	AGS	1	0
3	D	1001	AGS	22	0
3	B	1002	AGS	3	0
3	C	1001	AGS	2	0

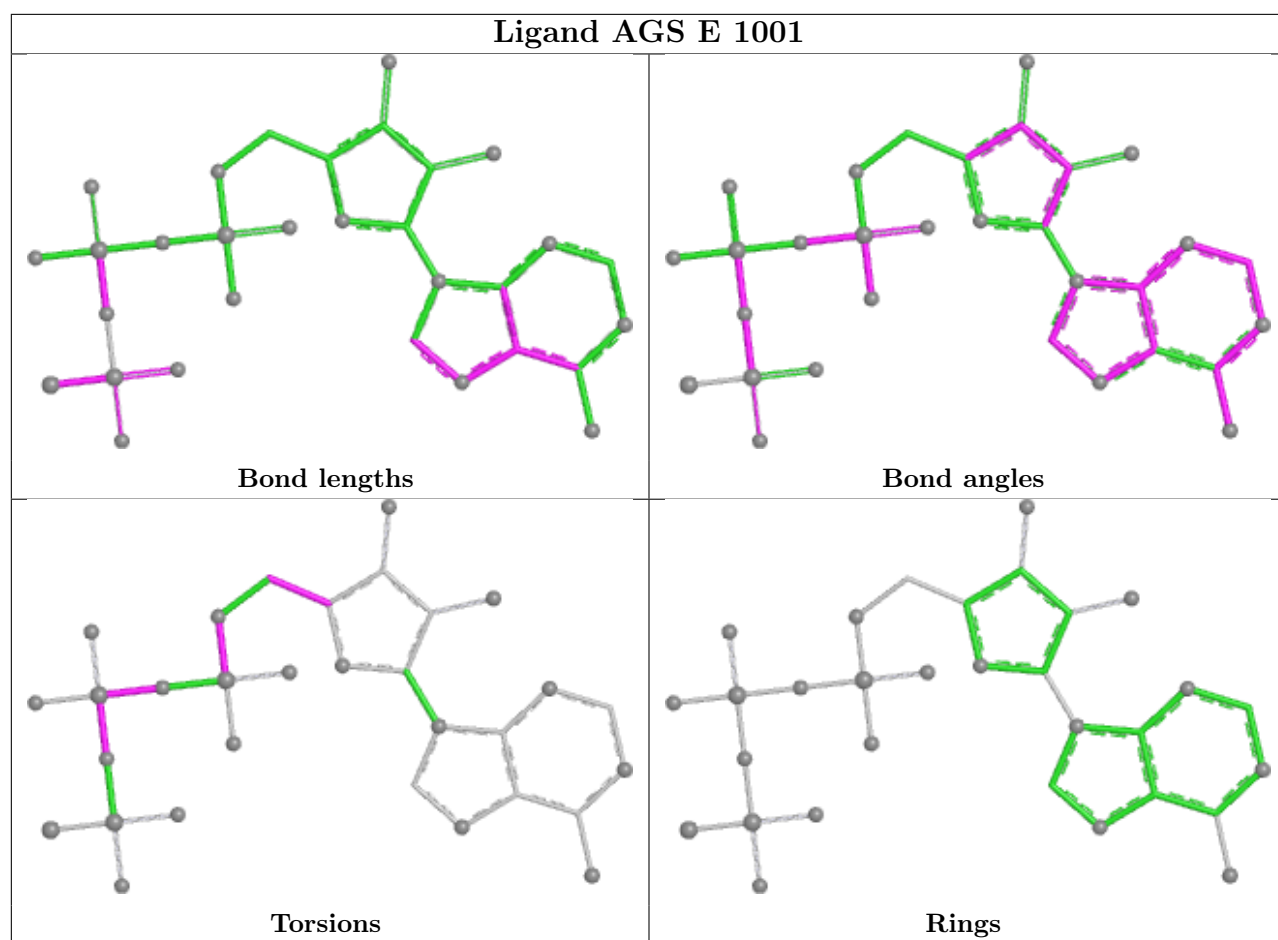
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

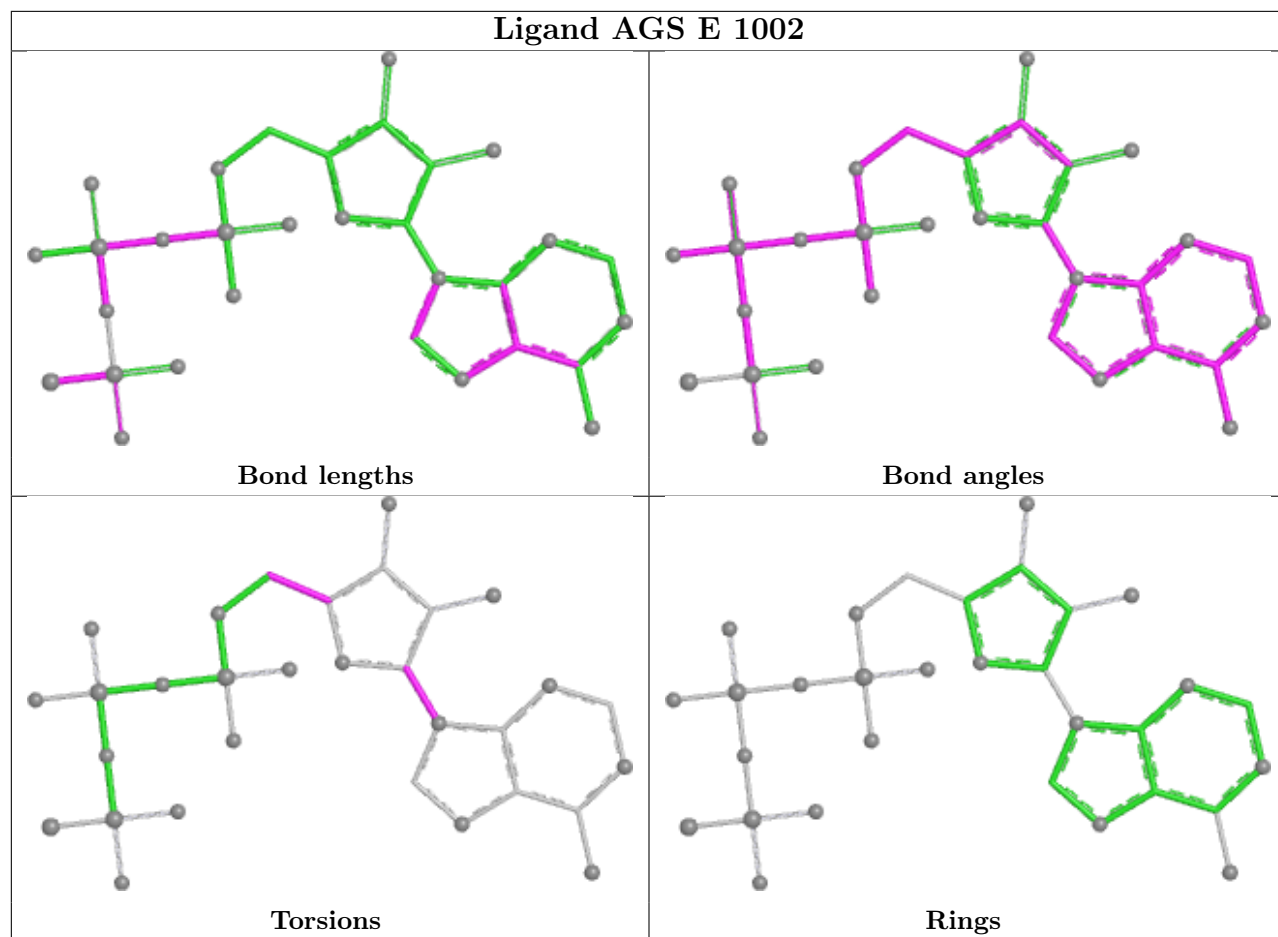


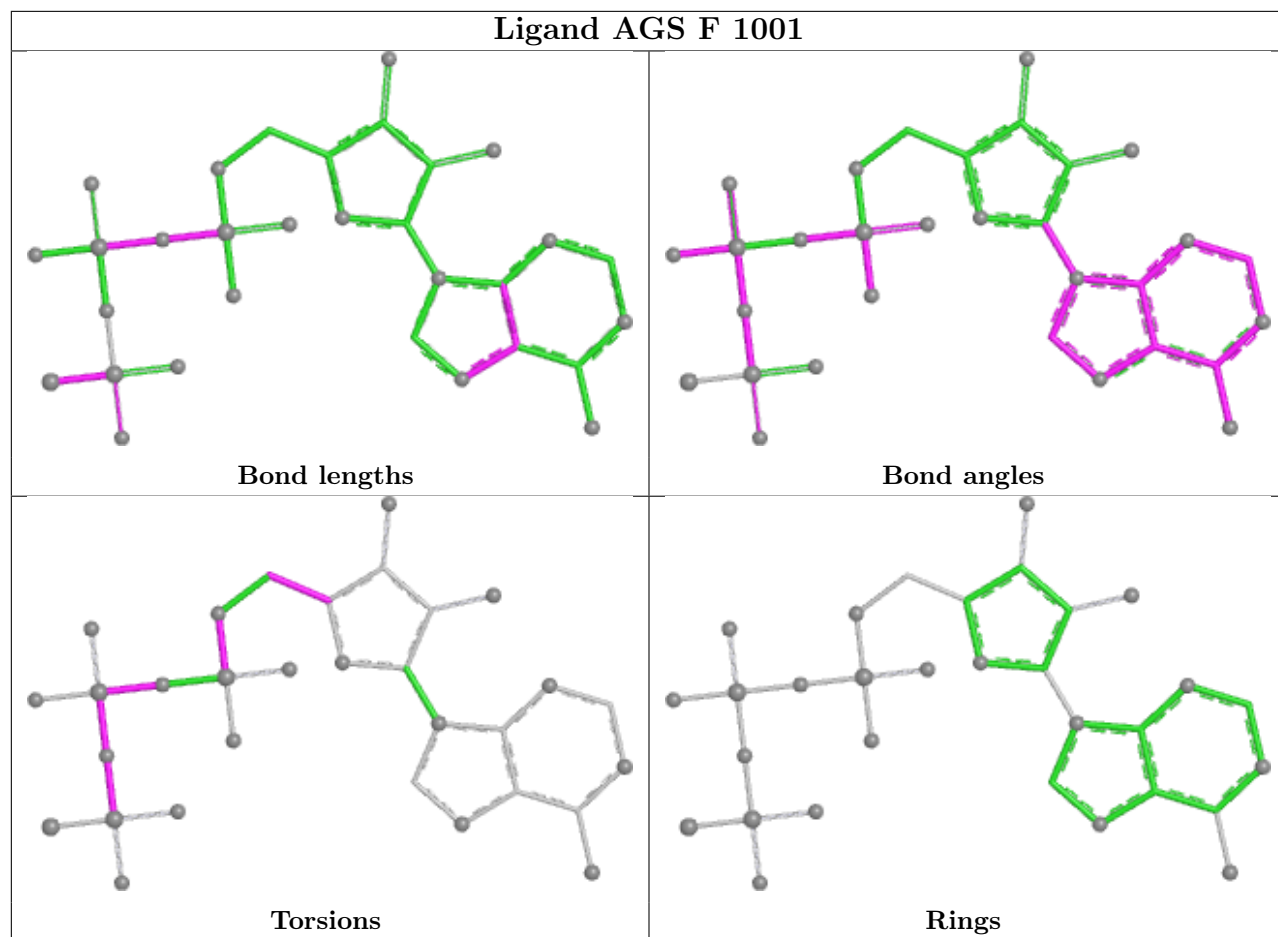


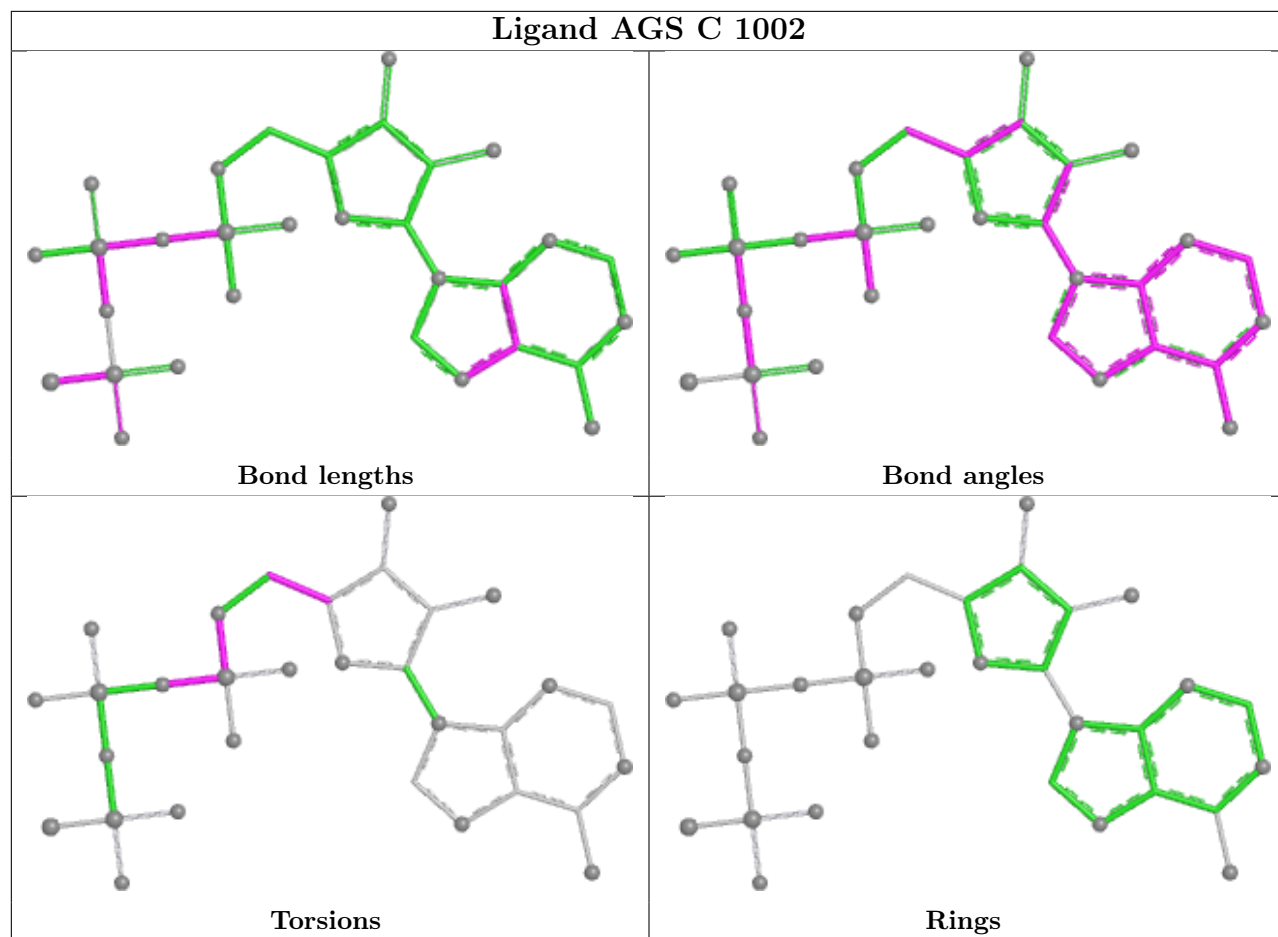


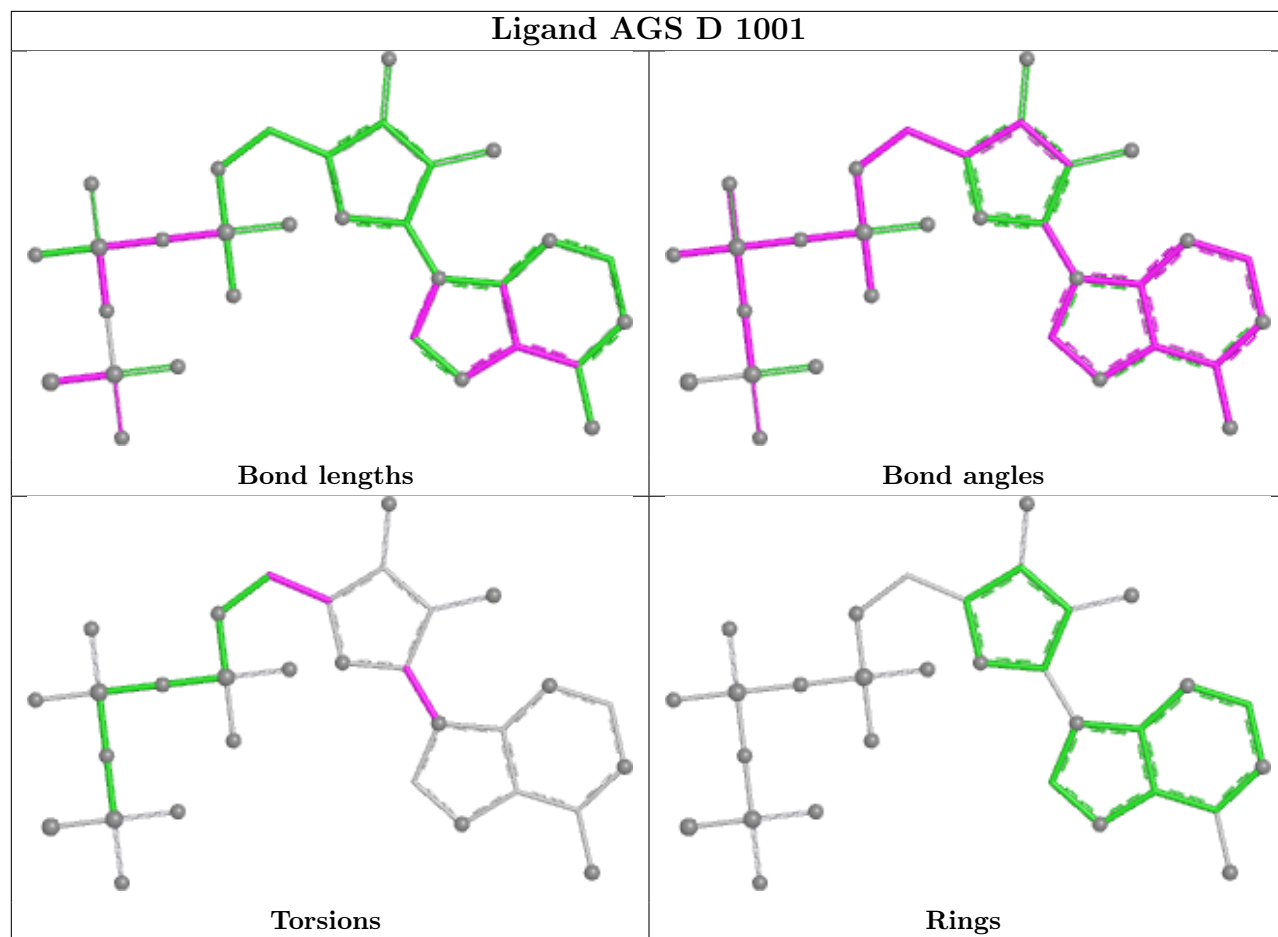


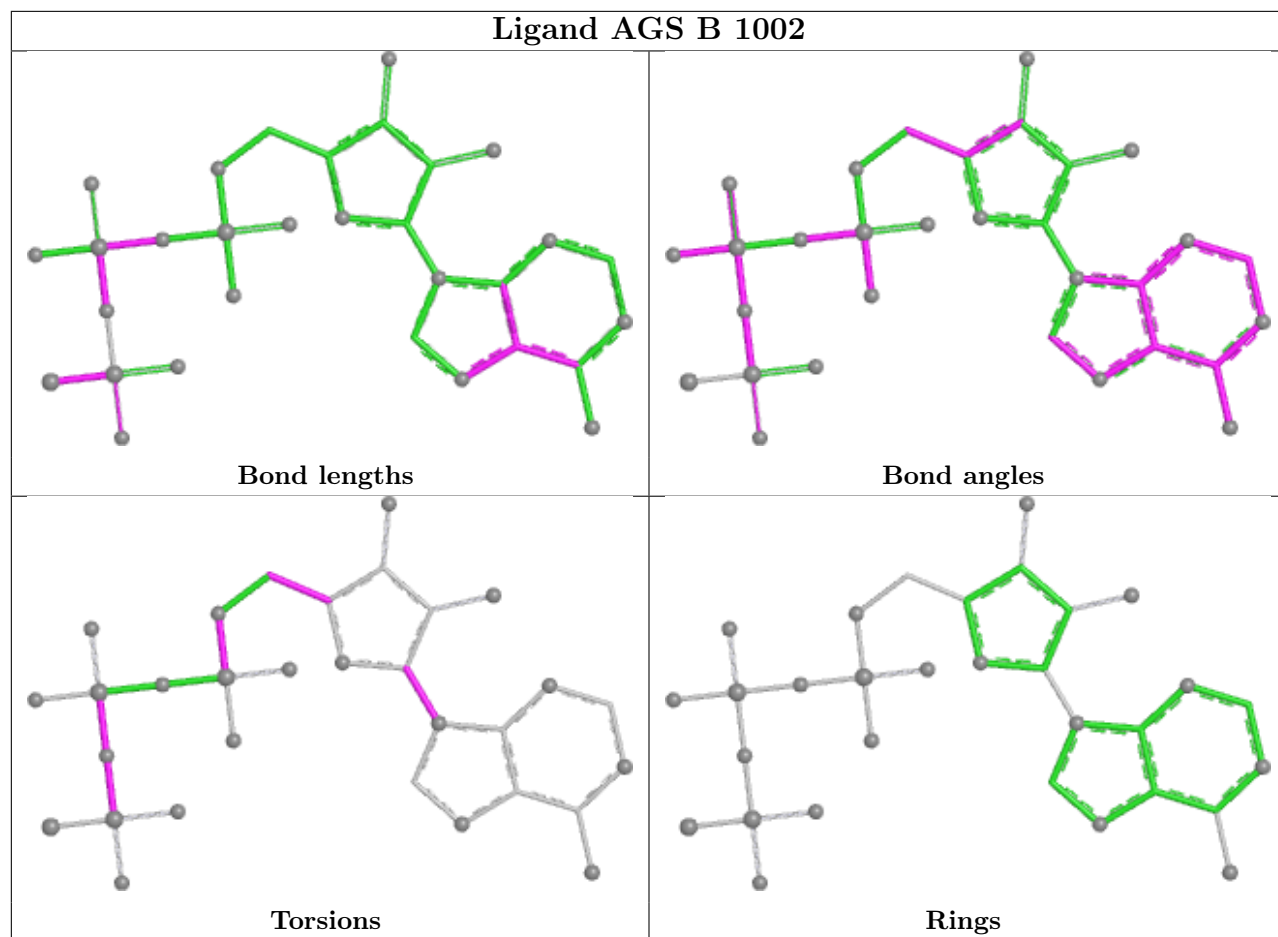


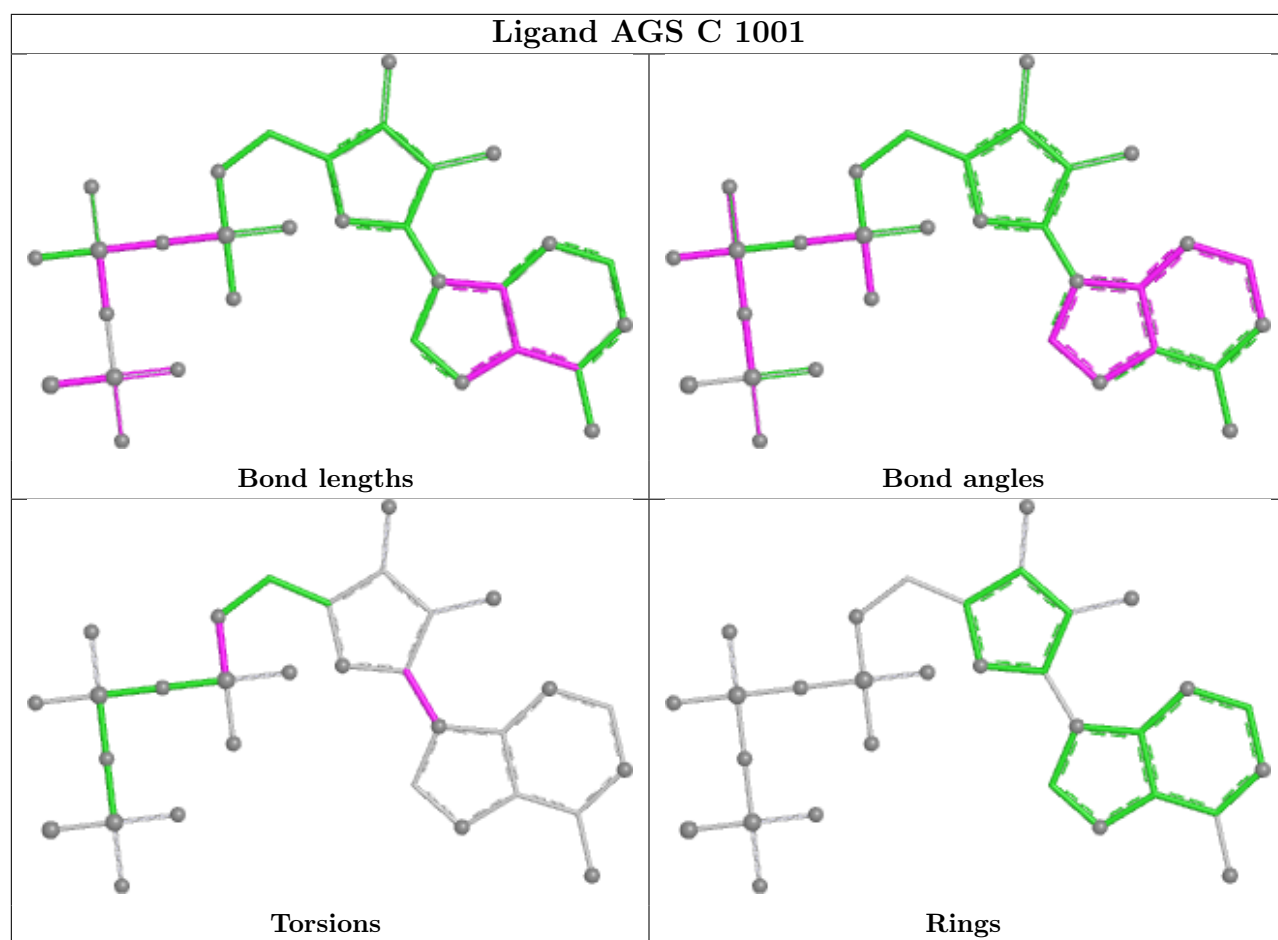












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

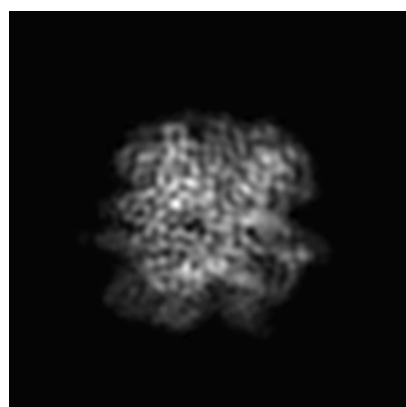
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8745. These allow visual inspection of the internal detail of the map and identification of artifacts.

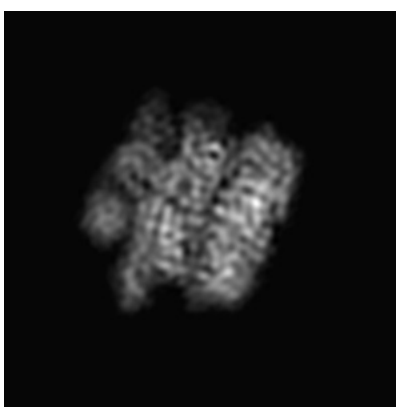
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

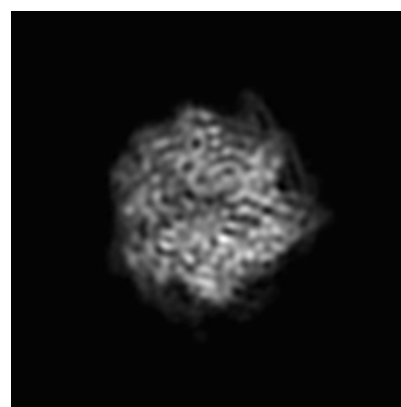
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

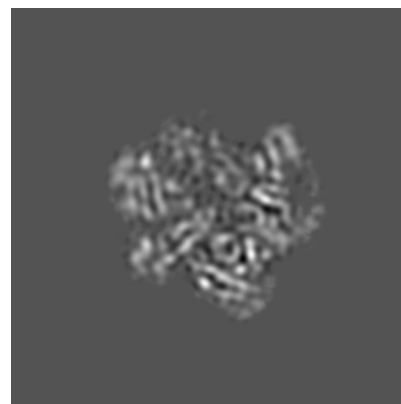
6.2.1 Primary map



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: 123



Y Index: 105

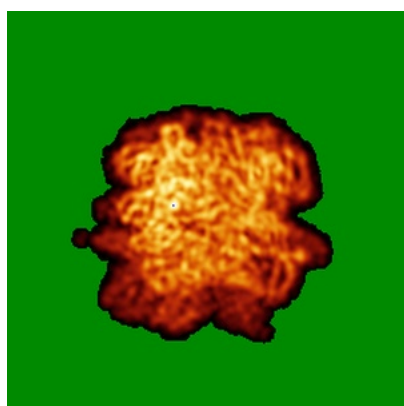


Z Index: 161

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

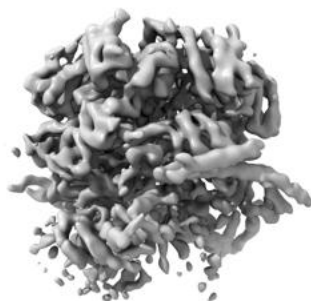


Z

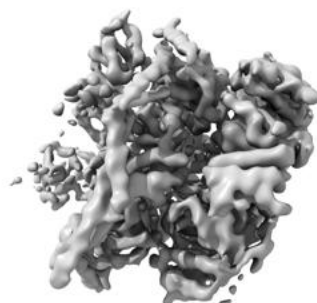
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

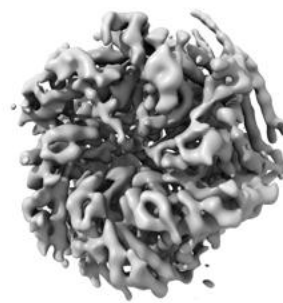
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

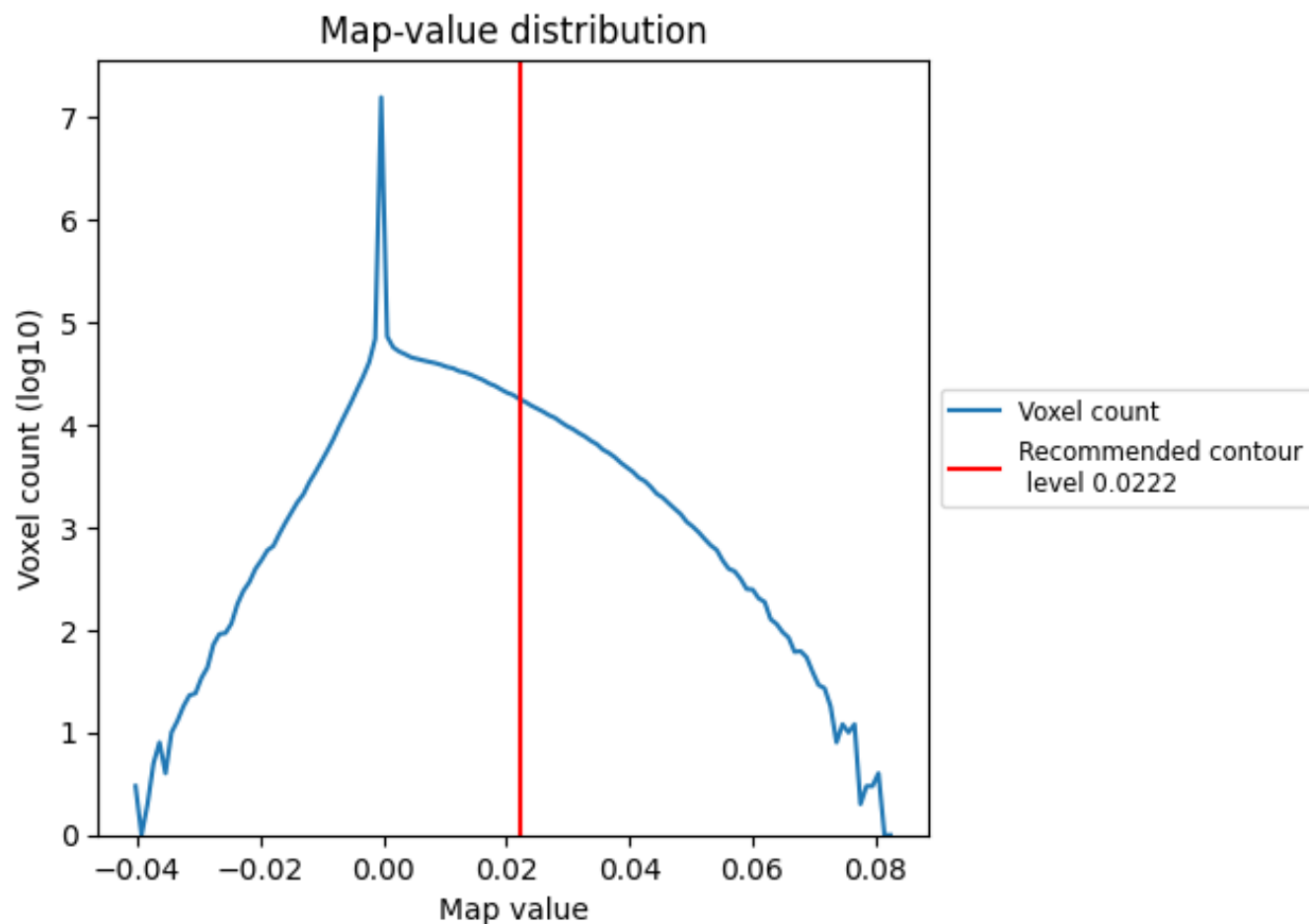
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

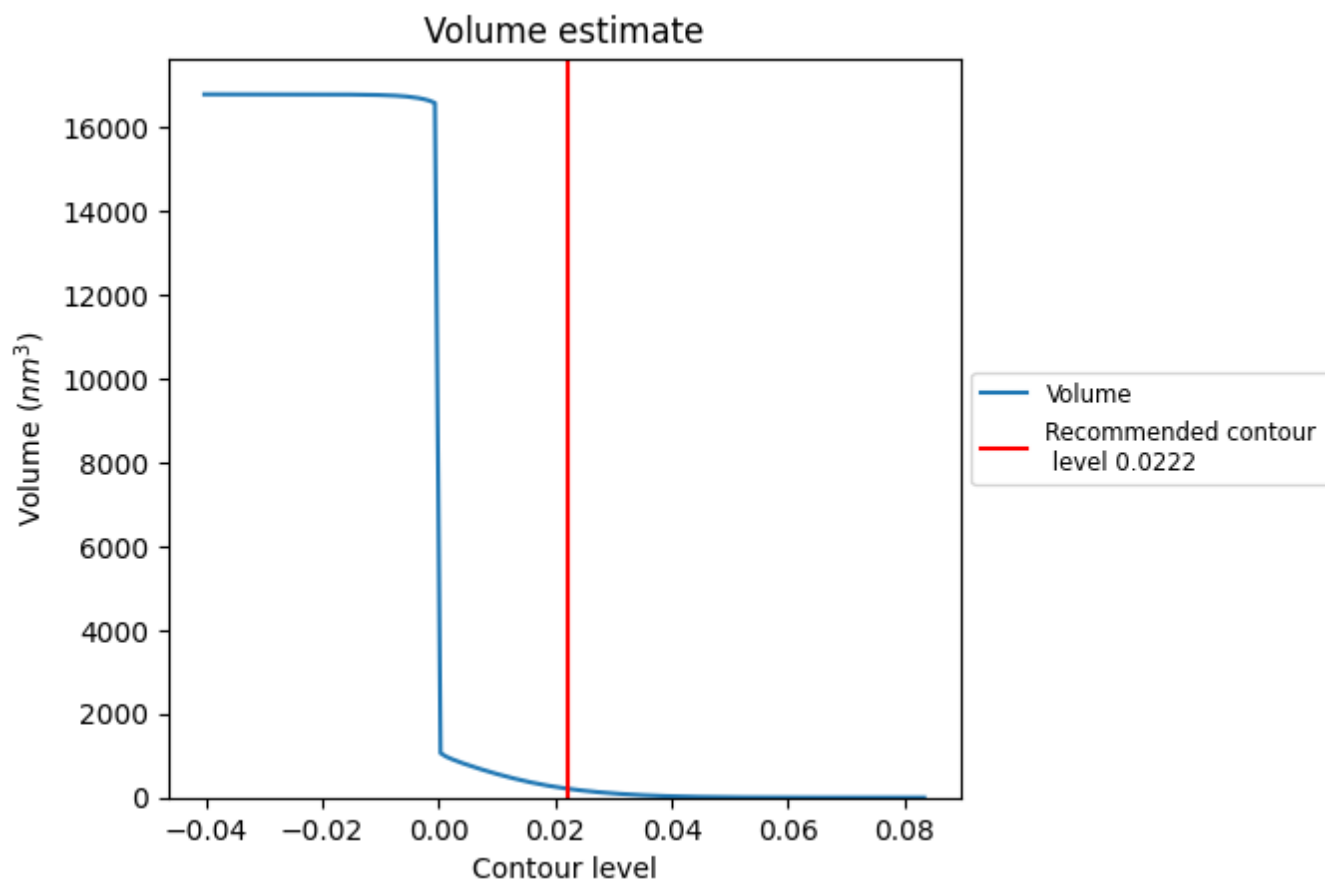
This section contains the results of statistical analysis of the map.

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.

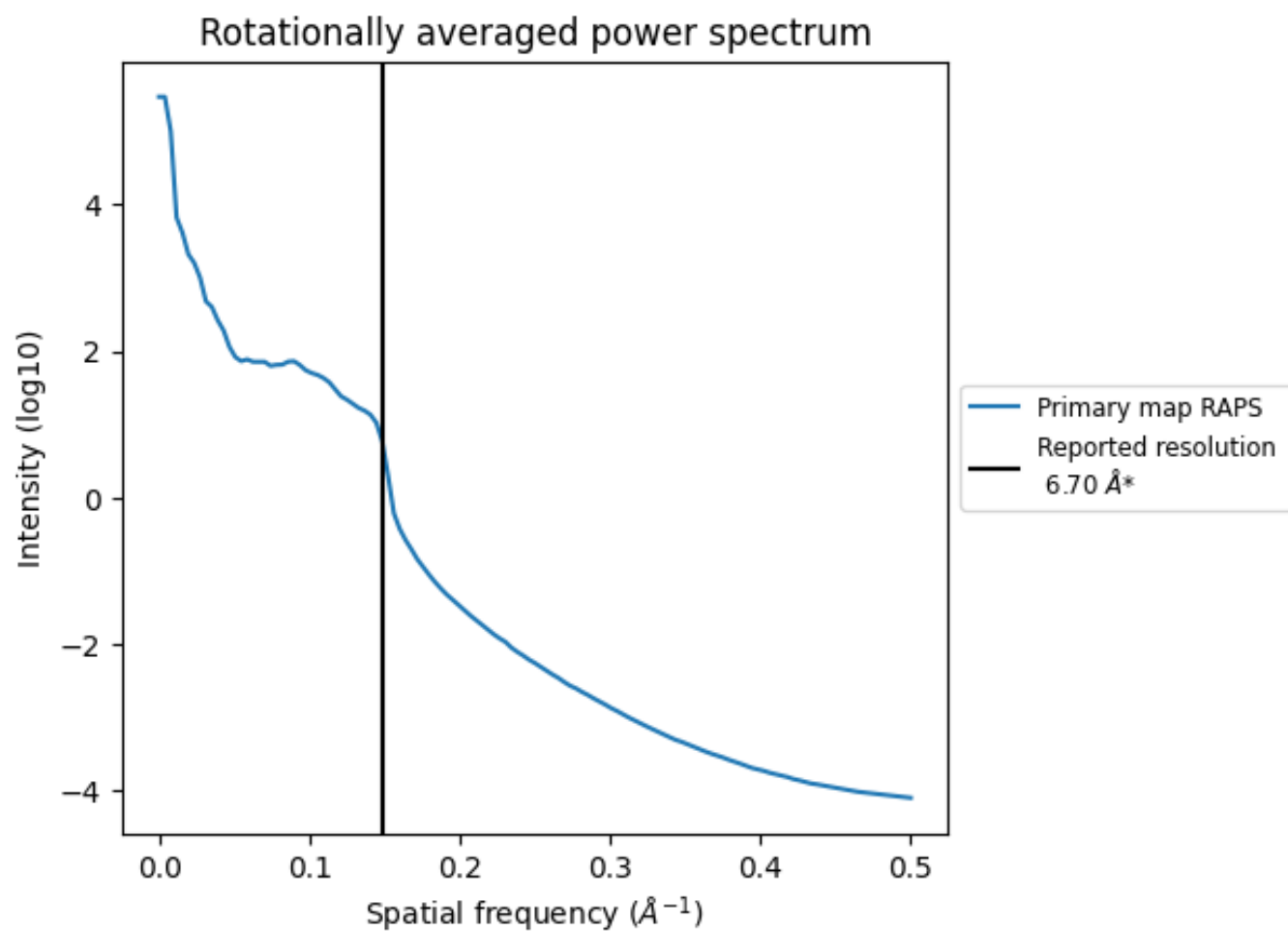
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 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 0.149 Å⁻¹

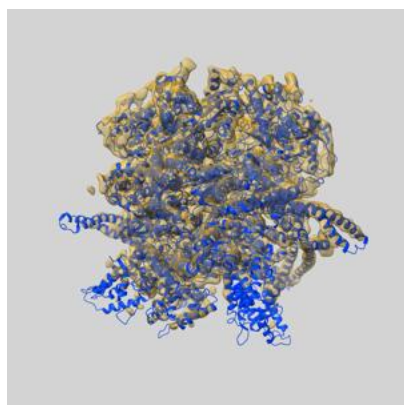
8 Fourier-Shell correlation

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

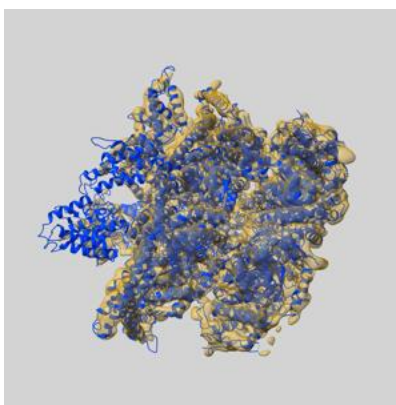
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8745 and PDB model 5VY9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

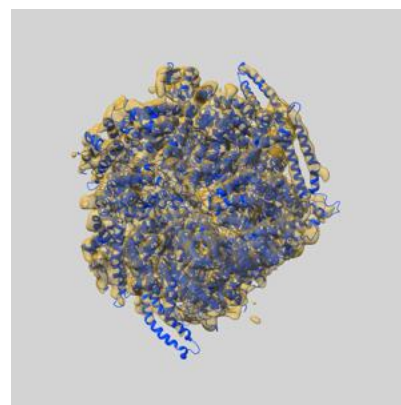
9.1 Map-model overlay [i](#)



X



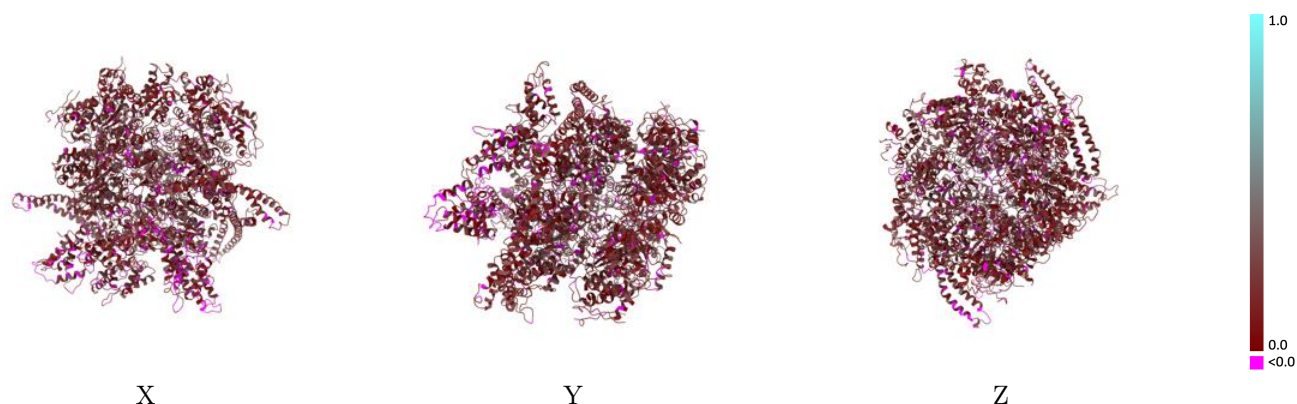
Y



Z

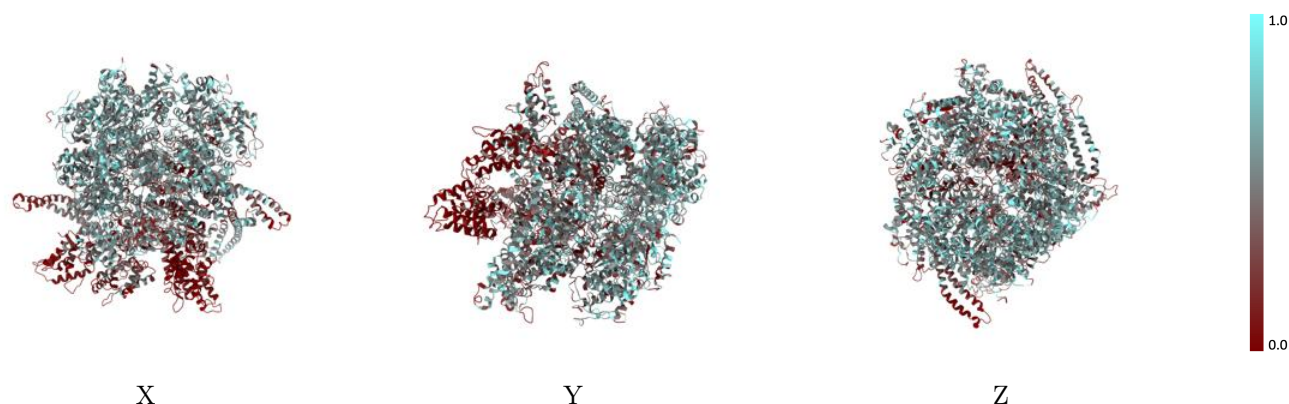
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



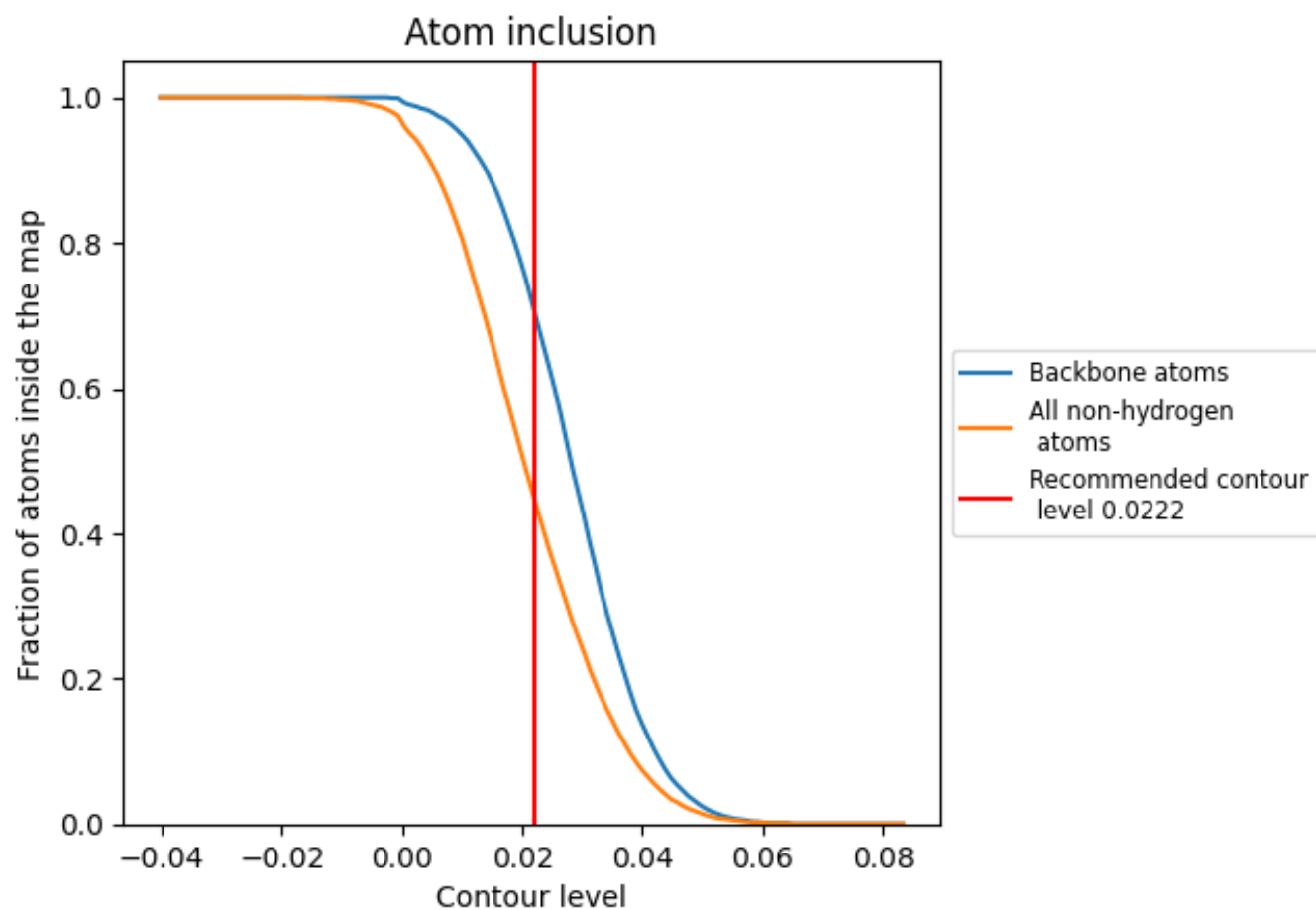
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0222).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 44% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4420	0.1610
A	0.3930	0.1580
B	0.4910	0.1680
C	0.5220	0.1720
D	0.4440	0.1600
E	0.4330	0.1620
F	0.3740	0.1440
P	0.6710	0.3040

1.0

0.0

<0.0