



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 01:33 PM EDT

PDB ID : 5VY9  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

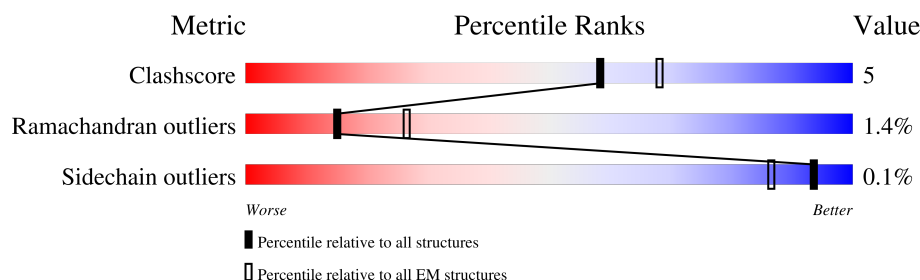
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	<div> <div>44%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	B	908	<div> <div>28%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
1	C	908	<div> <div>21%</div> <div>70%</div> <div>9%</div> <div>21%</div> </div>
1	D	908	<div> <div>29%</div> <div>68%</div> <div>9%</div> <div>21%</div> </div>
1	E	908	<div> <div>37%</div> <div>82%</div> <div>10%</div> <div>6%</div> </div>
1	F	908	<div> <div>44%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
2	P	28	<div> <div>21%</div> <div>89%</div> <div>11%</div> </div>

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.

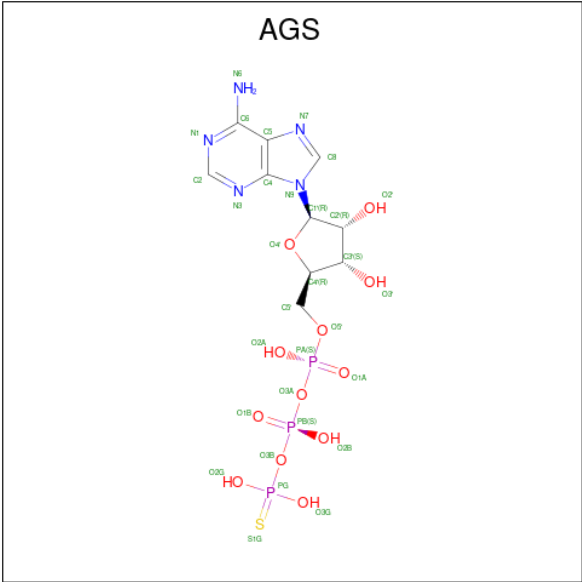
- Molecule 1 is a protein called Heat shock protein 104.

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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).

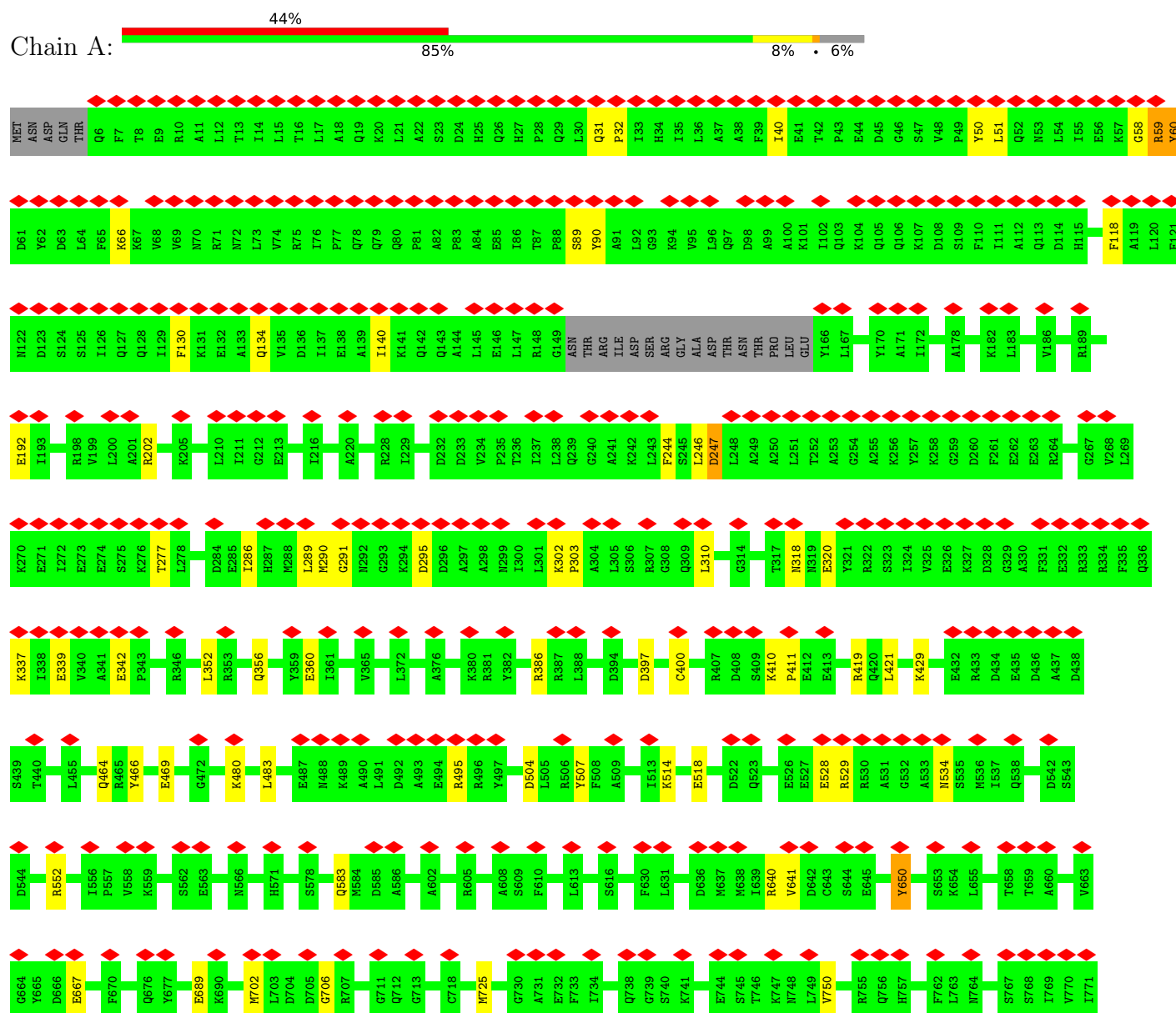


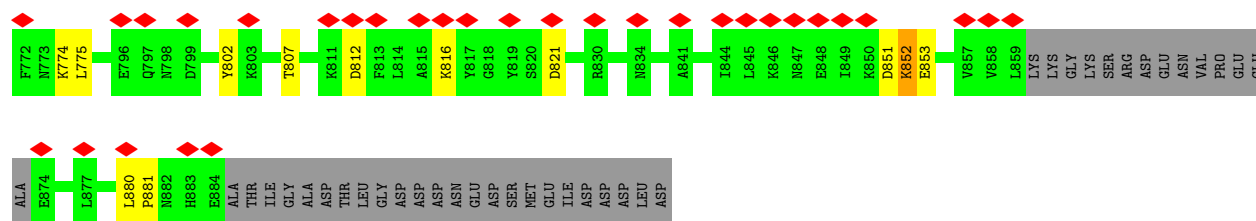
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			61	20	10	23	6	2	
3	D	1	Total	C	N	O	P	S	0
			61	20	10	23	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

### 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.

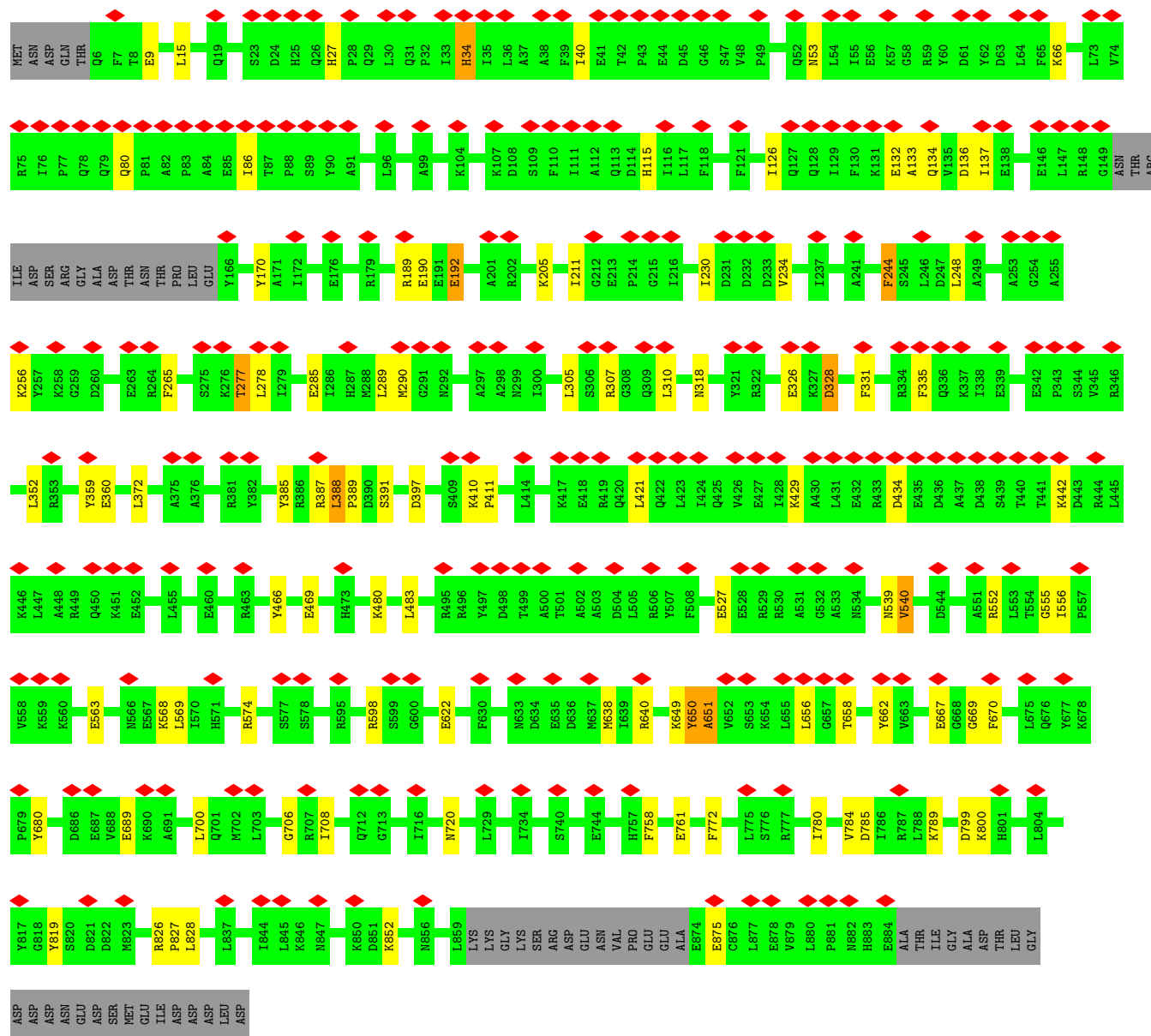
#### • Molecule 1: Heat shock protein 104





• Molecule 1: Heat shock protein 104

Chain B: 28% 82% 11% • 6%

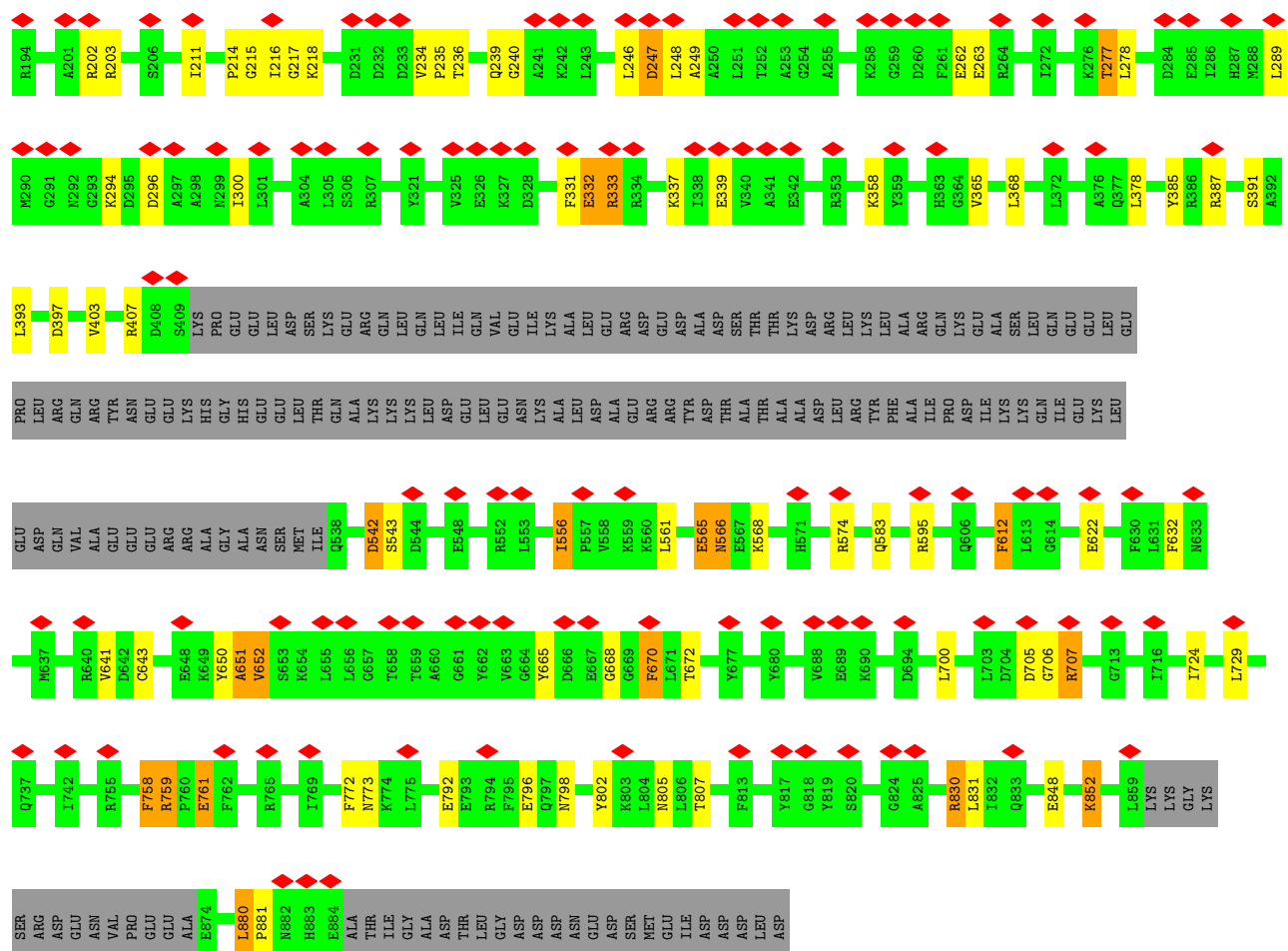


• Molecule 1: Heat shock protein 104

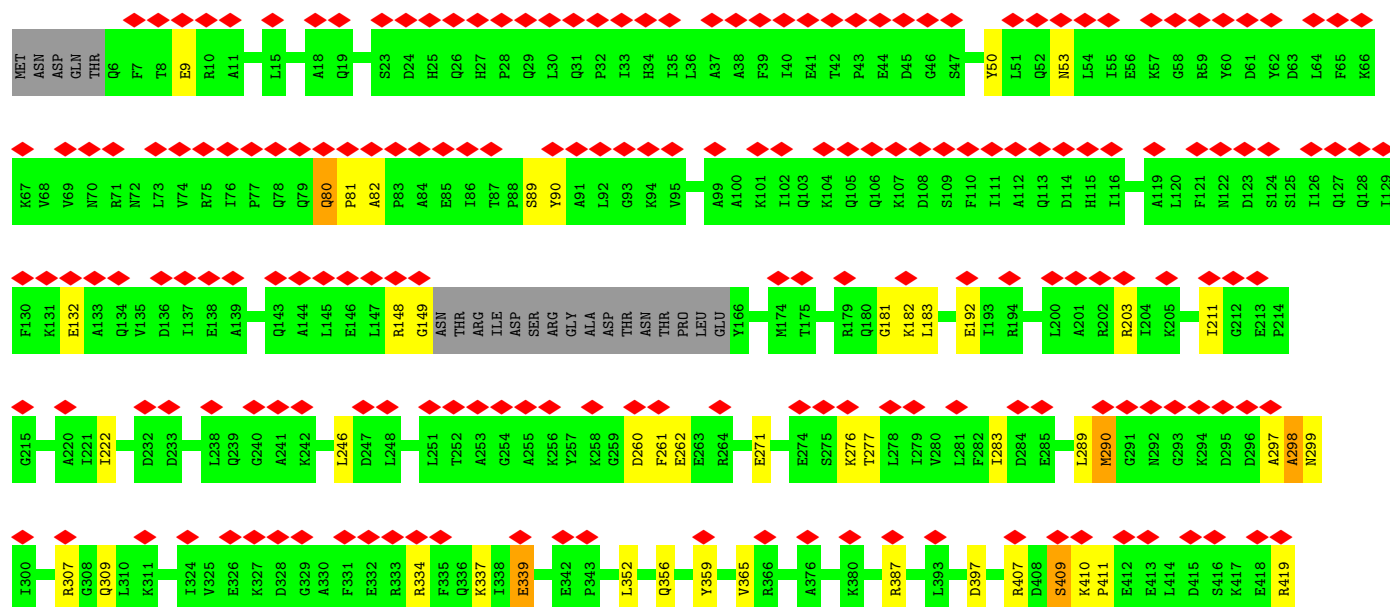
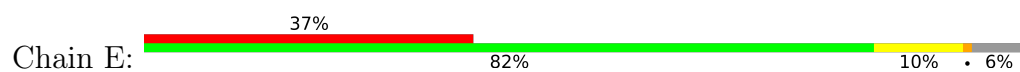
Chain C: 21% 70% 9% • 21%

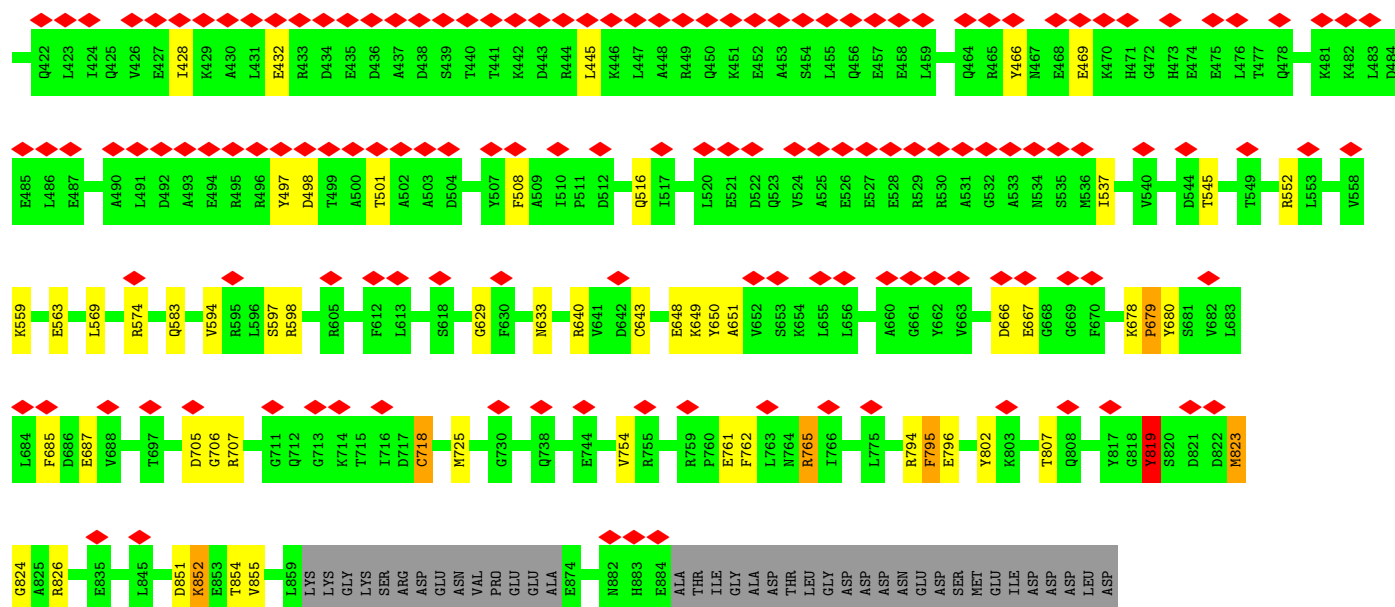




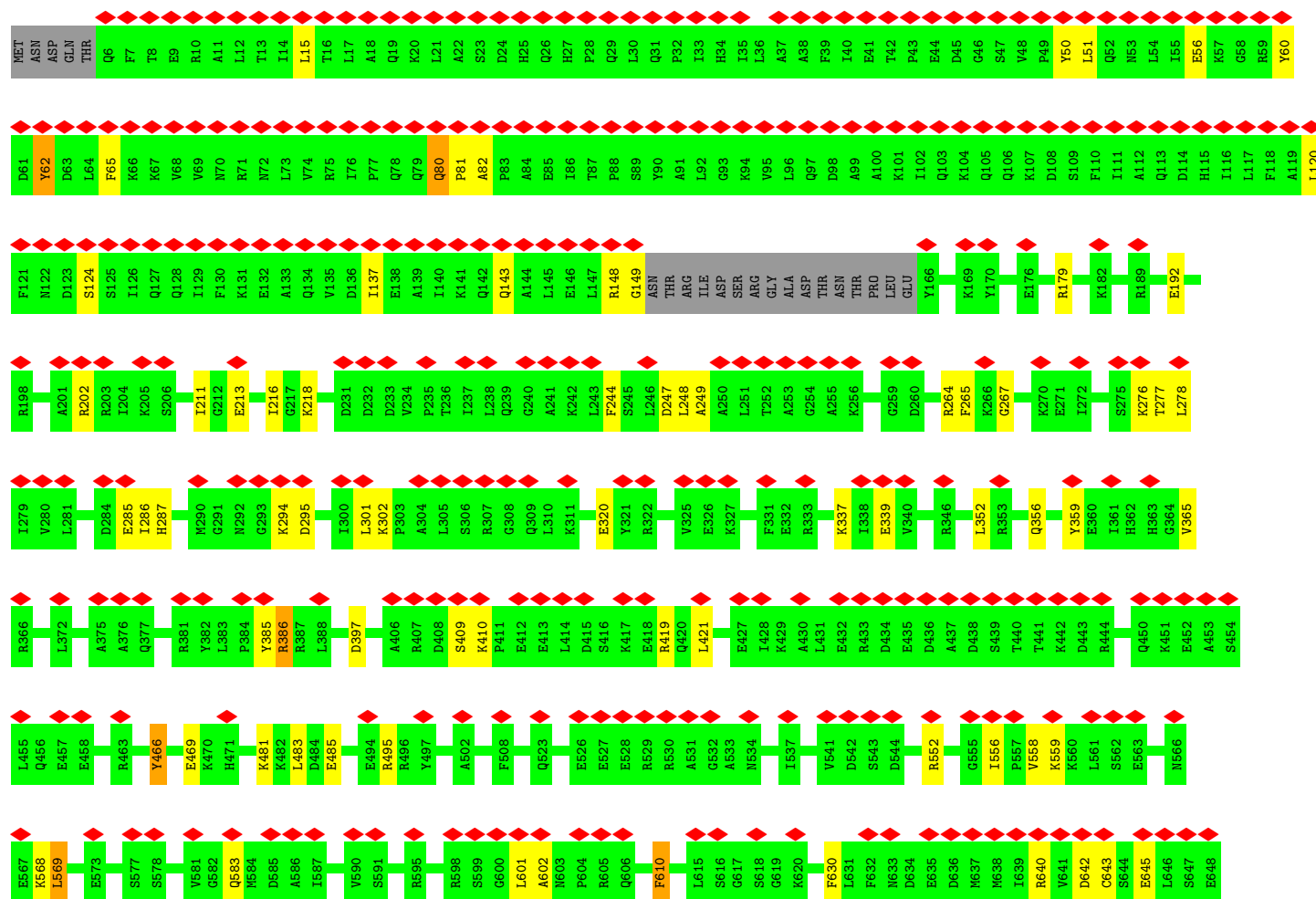
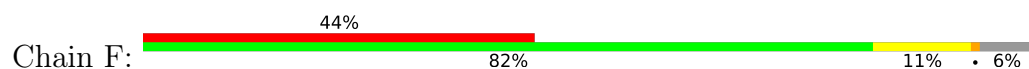


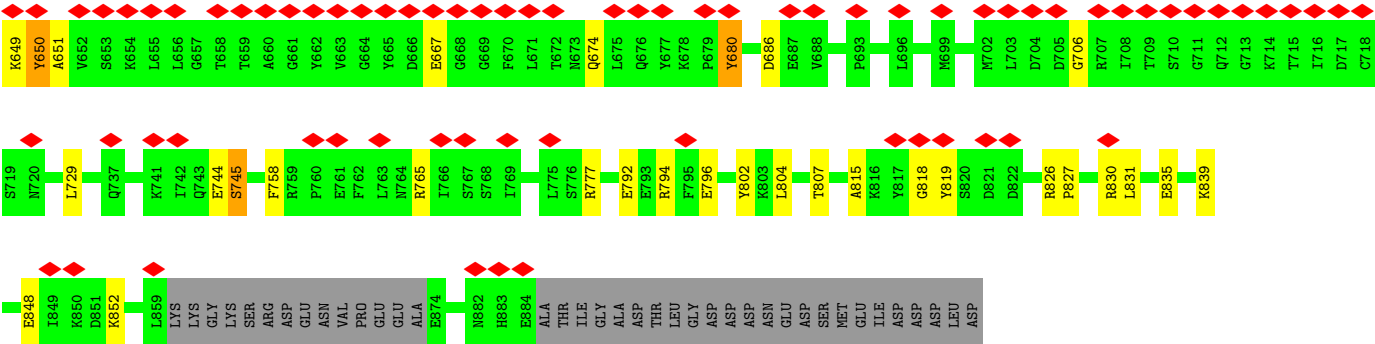
• Molecule 1: Heat shock protein 104



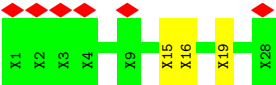
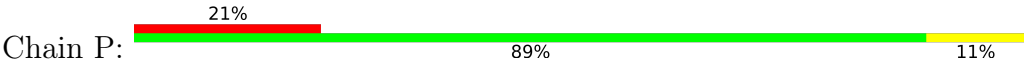


• Molecule 1: Heat shock protein 104





● 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 ( $\text{\AA}$ )	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	15/6810 (0.2%)	0.91	11/9169 (0.1%)
1	B	1.08	19/6811 (0.3%)	0.95	13/9172 (0.1%)
1	C	1.08	19/5747 (0.3%)	0.94	8/7745 (0.1%)
1	D	1.07	19/5747 (0.3%)	0.94	11/7745 (0.1%)
1	E	1.07	16/6810 (0.2%)	0.96	19/9169 (0.2%)
1	F	1.06	18/6810 (0.3%)	0.95	20/9169 (0.2%)
All	All	1.07	106/38735 (0.3%)	0.94	82/52169 (0.2%)

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	652	VAL	CB-CG1	-9.29	1.33	1.52
1	C	652	VAL	CB-CG1	-9.03	1.33	1.52
1	A	400	CYS	CB-SG	-8.15	1.68	1.82
1	F	397	ASP	CB-CG	7.94	1.68	1.51
1	D	802	TYR	CB-CG	-7.86	1.39	1.51
1	E	643	CYS	CB-SG	-7.86	1.68	1.82
1	D	758	PHE	CB-CG	-7.73	1.38	1.51
1	A	667	GLU	CG-CD	-7.72	1.40	1.51
1	D	670	PHE	CB-CG	-7.70	1.38	1.51
1	E	397	ASP	CB-CG	7.39	1.67	1.51
1	F	610	PHE	CB-CG	-7.37	1.38	1.51
1	A	641	VAL	CB-CG2	-7.24	1.37	1.52
1	F	630	PHE	CB-CG	-7.23	1.39	1.51
1	A	397	ASP	CB-CG	7.16	1.66	1.51
1	D	761	GLU	CD-OE1	-7.15	1.17	1.25
1	B	265	PHE	CB-CG	-6.95	1.39	1.51
1	B	670	PHE	CB-CG	-6.92	1.39	1.51
1	C	853	GLU	CD-OE1	-6.86	1.18	1.25
1	A	469	GLU	CD-OE1	-6.72	1.18	1.25
1	D	632	PHE	CB-CG	-6.64	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	802	TYR	CB-CG	-6.50	1.41	1.51
1	C	689	GLU	CD-OE1	-6.49	1.18	1.25
1	B	335	PHE	CG-CD1	-6.36	1.29	1.38
1	C	594	VAL	CB-CG1	-6.33	1.39	1.52
1	A	689	GLU	CD-OE1	-6.29	1.18	1.25
1	C	643	CYS	CB-SG	-6.27	1.71	1.82
1	D	792	GLU	CD-OE2	-6.24	1.18	1.25
1	C	192	GLU	CD-OE1	-6.17	1.18	1.25
1	E	823	MET	CG-SD	-6.08	1.65	1.81
1	B	391	SER	CB-OG	-6.03	1.34	1.42
1	E	594	VAL	CB-CG2	-6.01	1.40	1.52
1	C	190	GLU	CD-OE2	-5.99	1.19	1.25
1	D	332	GLU	CD-OE1	-5.94	1.19	1.25
1	D	397	ASP	CB-CG	5.91	1.64	1.51
1	B	234	VAL	CB-CG1	-5.88	1.40	1.52
1	C	332	GLU	CD-OE1	-5.87	1.19	1.25
1	B	469	GLU	CD-OE1	-5.87	1.19	1.25
1	F	265	PHE	CB-CG	-5.84	1.41	1.51
1	E	132	GLU	CD-OE1	-5.84	1.19	1.25
1	F	667	GLU	CD-OE1	-5.83	1.19	1.25
1	D	848	GLU	CD-OE1	-5.83	1.19	1.25
1	E	718	CYS	CB-SG	-5.83	1.72	1.81
1	C	382	TYR	CB-CG	-5.83	1.43	1.51
1	E	469	GLU	CD-OE1	-5.81	1.19	1.25
1	F	758	PHE	CB-CG	-5.79	1.41	1.51
1	D	263	GLU	CD-OE1	-5.73	1.19	1.25
1	B	622	GLU	CD-OE1	-5.73	1.19	1.25
1	B	244	PHE	CB-CG	-5.70	1.41	1.51
1	D	234	VAL	CB-CG1	-5.66	1.41	1.52
1	C	202	ARG	CG-CD	-5.64	1.37	1.51
1	C	234	VAL	CB-CG1	-5.63	1.41	1.52
1	C	645	GLU	CD-OE2	-5.62	1.19	1.25
1	F	244	PHE	CB-CG	-5.62	1.41	1.51
1	F	192	GLU	CD-OE1	-5.60	1.19	1.25
1	D	622	GLU	CD-OE1	-5.59	1.19	1.25
1	C	792	GLU	CD-OE1	-5.58	1.19	1.25
1	C	792	GLU	CD-OE2	-5.56	1.19	1.25
1	B	328	ASP	CB-CG	-5.55	1.40	1.51
1	B	527	GLU	CD-OE1	-5.53	1.19	1.25
1	E	680	TYR	CB-CG	-5.53	1.43	1.51
1	E	754	VAL	CB-CG1	-5.52	1.41	1.52
1	E	802	TYR	CB-CG	-5.52	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	689	GLU	CD-OE1	-5.49	1.19	1.25
1	C	761	GLU	CD-OE1	-5.49	1.19	1.25
1	B	761	GLU	CD-OE1	-5.49	1.19	1.25
1	C	285	GLU	CD-OE1	-5.46	1.19	1.25
1	D	385	TYR	CB-CG	-5.46	1.43	1.51
1	D	643	CYS	CB-SG	-5.40	1.73	1.81
1	A	244	PHE	CB-CG	-5.37	1.42	1.51
1	E	667	GLU	CD-OE1	-5.37	1.19	1.25
1	F	848	GLU	CD-OE1	-5.37	1.19	1.25
1	F	643	CYS	CB-SG	-5.36	1.73	1.81
1	B	397	ASP	CB-CG	5.33	1.62	1.51
1	B	359	TYR	CB-CG	-5.30	1.43	1.51
1	A	689	GLU	CG-CD	-5.30	1.44	1.51
1	F	792	GLU	CG-CD	-5.30	1.44	1.51
1	D	565	GLU	CD-OE1	-5.30	1.19	1.25
1	F	469	GLU	CD-OE1	-5.29	1.19	1.25
1	A	750	VAL	CB-CG1	-5.25	1.41	1.52
1	B	34	HIS	CB-CG	-5.25	1.40	1.50
1	F	56	GLU	CD-OE1	-5.25	1.19	1.25
1	B	192	GLU	CD-OE1	-5.24	1.19	1.25
1	F	320	GLU	CG-CD	-5.22	1.44	1.51
1	B	758	PHE	CB-CG	-5.22	1.42	1.51
1	A	60	TYR	CB-CG	-5.19	1.43	1.51
1	F	216	ILE	CB-CG1	-5.18	1.39	1.54
1	B	680	TYR	CB-CG	-5.17	1.44	1.51
1	D	391	SER	CB-OG	-5.16	1.35	1.42
1	E	262	GLU	CD-OE1	-5.15	1.20	1.25
1	B	689	GLU	CG-CD	-5.14	1.44	1.51
1	D	792	GLU	CG-CD	-5.14	1.44	1.51
1	F	62	TYR	CE2-CZ	-5.12	1.31	1.38
1	E	339	GLU	CD-OE1	-5.11	1.20	1.25
1	E	765	ARG	CG-CD	-5.10	1.39	1.51
1	C	244	PHE	CB-CG	-5.09	1.42	1.51
1	C	326	GLU	CD-OE1	-5.09	1.20	1.25
1	F	645	GLU	CD-OE1	-5.07	1.20	1.25
1	A	802	TYR	CB-CG	-5.07	1.44	1.51
1	A	853	GLU	CD-OE2	-5.07	1.20	1.25
1	E	271	GLU	CD-OE1	-5.06	1.20	1.25
1	A	320	GLU	CD-OE1	-5.06	1.20	1.25
1	D	190	GLU	CD-OE1	-5.05	1.20	1.25
1	C	682	VAL	CB-CG2	-5.03	1.42	1.52
1	E	762	PHE	CB-CG	-5.03	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	GLU	CD-OE1	-5.02	1.20	1.25
1	A	853	GLU	CD-OE1	-5.00	1.20	1.25

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	202	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	D	707	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	F	419	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	640	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	386	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	E	397	ASP	CB-CG-OD1	8.30	125.77	118.30
1	F	386	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	F	495	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	E	419	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	F	264	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	E	50	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	B	189	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	F	802	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	F	179	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	202	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	D	612	PHE	CB-CG-CD2	7.47	126.03	120.80
1	B	552	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	D	830	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	E	826	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	E	826	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	F	466	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	E	203	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	F	552	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	529	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	F	552	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	F	765	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	60	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	F	777	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	419	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	662	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	A	202	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	E	466	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	D	595	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	466	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	E	680	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	C	382	TYR	CB-CG-CD2	-6.42	117.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	802	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	F	80	GLN	C-N-CD	-6.30	106.74	120.60
1	F	680	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	E	334	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	D	397	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	170	TYR	CB-CG-CD2	-5.98	117.42	121.00
1	F	794	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	118	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	A	495	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	574	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	640	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	359	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	702	MET	CG-SD-CE	5.71	109.34	100.20
1	C	397	ASP	CB-CG-OD1	5.66	123.39	118.30
1	F	385	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	C	385	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	D	75	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	E	80	GLN	C-N-CD	-5.53	108.43	120.60
1	D	574	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	819	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	F	830	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	E	552	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	202	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	359	TYR	CB-CG-CD1	-5.43	117.75	121.00
1	B	387	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	552	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	E	397	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	115	HIS	CA-CB-CG	-5.34	104.52	113.60
1	B	598	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	F	495	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	203	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	359	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	F	60	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	E	407	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	307	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	640	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	759	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	118	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	466	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	C	595	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	E	409	SER	N-CA-CB	5.10	118.14	110.50
1	E	545	THR	CA-CB-CG2	-5.08	105.30	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	D	333	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	B	662	TYR	CB-CG-CD1	5.04	124.03	121.00
1	E	574	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	43	0
1	B	6722	0	6855	60	0
1	C	5669	0	5802	57	0
1	D	5669	0	5802	88	0
1	E	6722	0	6854	66	0
1	F	6722	0	6854	51	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	381	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 (381) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:310:LEU:O	1:A:310:LEU:HG	1.93	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: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:C:53:ASN:C	1:C:53:ASN:OD1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:819:TYR:CD1	1:E:819:TYR:C	2.69	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:E:794:ARG:HE	1:E:794:ARG:C	1.97	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
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:831:LEU:C	1:D:831:LEU:HD13	2.22	0.60
3:B:1002:AGS:O1B	3:B:1002:AGS:O2A	2.18	0.60
1:C:207:ASN:OD1	1:C:207:ASN:C	2.40	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: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: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
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:D:729:LEU:C	1:D:729:LEU:HD23	2.26	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:F:831:LEU:HD23	1:F:831:LEU:C	2.26	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:C:650:TYR:CD1	1:C:650:TYR:C	2.79	0.55
1:E:508:PHE:N	1:E:508:PHE:CD1	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LYS:NZ	1:C:339:GLU:OE2	2.40	0.55
1:A:504:ASP:OD1	1:B:429:LYS:NZ	2.37	0.54
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: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:E:649:LYS:NZ	2:P:19:UNK:O	2.40	0.54
1:D:805:ASN:OD1	1:D:805:ASN:N	2.27	0.53
1:A:483:LEU:C	1:A:483:LEU:HD23	2.29	0.53
1:D:378:LEU:C	1:D:378:LEU:HD23	2.29	0.53
1:F:278:LEU:C	1:F:278:LEU:HD23	2.28	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:E:819:TYR:C	1:E:819:TYR:HD1	2.13	0.53
1:B:136:ASP:OD1	1:B:136:ASP:C	2.46	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
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:650:TYR:CD1	1:D:650:TYR:C	2.82	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:OE1	1:B:9:GLU:N	2.32	0.51
1:B:134:GLN:OE1	1:B:134:GLN:N	2.27	0.51
1:D:700:LEU:HD23	1:D:700:LEU:C	2.30	0.51
1:B:539:ASN:O	1:B:540:VAL:C	2.50	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:H1'	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:A:50:TYR:CD1	1:A:50:TYR:C	2.81	0.50
1:E:794:ARG:O	1:E:796:GLU:N	2.45	0.49
1:F:483:LEU:C	1:F:483:LEU:HD23	2.32	0.49
1:C:187:ILE:C	1:C:187:ILE:HD12	2.33	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:F:148:ARG:O	1:F:149:GLY:C	2.51	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: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:D:670:PHE:C	1:D:670:PHE:CD2	2.87	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: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:B:708:ILE:O	1:B:708:ILE:HG23	2.14	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:D:15:LEU:HD13	1:D:15:LEU:C	2.34	0.48
1:A:246:LEU:O	1:A:247:ASP:CB	2.61	0.48
1:F:213:GLU:O	1:F:218:LYS:NZ	2.47	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: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: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: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:B:388:LEU:O	1:B:389:PRO:C	2.53	0.47
1:D:665:TYR:CD2	1:D:665:TYR:O	2.68	0.47
1:B:819:TYR:N	1:B:819:TYR:HD1	2.13	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: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:C:53:ASN:OD1	1:C:53:ASN:O	2.32	0.46
1:D:296:ASP:O	1:D:296:ASP:CG	2.53	0.46
1:B:53:ASN:OD1	1:B:53:ASN:C	2.53	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: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
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: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:B:421:LEU:C	1:B:421:LEU:HD23	2.35	0.46
1:D:650:TYR:O	1:D:651:ALA:C	2.53	0.46
1:E:337:LYS:NZ	1:E:339:GLU:OE2	2.49	0.46
1:A:812:ASP:O	1:A:816:LYS:N	2.49	0.46
1:D:652:VAL:O	1:D:652:VAL:CG2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:MET:O	1:B:638:MET:HG3	2.16	0.45
1:B:799:ASP:OD2	1:B:800:LYS:NZ	2.47	0.45
1:D:211:ILE:N	1:D:211:ILE:HD12	2.31	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:E:148:ARG:O	1:E:149:GLY:C	2.53	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:HG22	1:C:652:VAL:O	2.17	0.45
1:E:516:GLN:OE1	1:E:516:GLN:HA	2.16	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:HG13	1:E:365:VAL:O	2.16	0.45
1:F:610:PHE:CD1	1:F:610:PHE:N	2.83	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: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: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:E:289:LEU:O	1:E:290:MET:CB	2.65	0.44
1:E:387:ARG:HA	1:E:387:ARG:HE	1.81	0.44
1:C:555:GLY:O	1:C:556:ILE:C	2.55	0.44
1:E:352:LEU:O	1:E:356:GLN:N	2.50	0.44
1:E:678:LYS:O	1:E:679:PRO:C	2.55	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:729:LEU:HD23	1:F:729:LEU:C	2.38	0.44
1:E:183:LEU:N	1:E:183:LEU:HD12	2.32	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:D:129:ILE:HG13	1:D:129:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:VAL:O	1:F:558:VAL:HG22	2.18	0.44
1:A:528:GLU:H	1:A:528:GLU:CD	2.21	0.43
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: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: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: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:F:15:LEU:HD23	1:F:15:LEU:C	2.39	0.43
1:A:286:ILE:O	1:A:286:ILE:HG22	2.17	0.43
1:B:483:LEU:HD23	1:B:483:LEU:C	2.38	0.43
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: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:D:612:PHE:CD1	1:D:612:PHE:N	2.87	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:A:421:LEU:HD23	1:A:421:LEU:C	2.39	0.43
1:E:445:LEU:C	1:E:445:LEU:HD12	2.39	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:C:409:SER:O	1:C:409:SER:OG	2.32	0.42
1:D:368:LEU:HD12	1:D:368:LEU:N	2.34	0.42
1:D:565:GLU:O	1:D:566:ASN:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:53:ASN:C	1:E:53:ASN:OD1	2.57	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: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
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: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:542:ASP:CG	1:D:543:SER:H	2.20	0.42
1:D:565:GLU:O	1:D:568:LYS:N	2.52	0.42
1:F:568:LYS:O	1:F:569:LEU:HB2	2.19	0.42
1:D:831:LEU:C	1:D:831:LEU:CD1	2.88	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:E:9:GLU:H	1:E:9:GLU:CD	2.14	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:A:66:LYS:HB3	1:A:66:LYS:HE2	1.86	0.41
1:E:89:SER:OG	1:E:90:TYR:N	2.53	0.41
1:F:601:LEU:O	1:F:602:ALA:C	2.59	0.41
1:B:190:GLU:H	1:B:190:GLU:CD	2.21	0.41
1:B:360:GLU:OE1	1:B:480:LYS:NZ	2.51	0.41
1:E:260:ASP:OD1	1:E:261:PHE:N	2.51	0.41
1:D:333:ARG:HA	1:D:333:ARG:NE	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:409:SER:O	1:E:410:LYS:C	2.59	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:D:758:PHE:O	1:D:759:ARG:C	2.58	0.41
1:A:534:ASN:OD1	1:A:534:ASN:C	2.59	0.41
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.91	0.41
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:642:ASP:OD1	1:F:642:ASP:C	2.59	0.41
1:F:744:GLU:O	1:F:745:SER:CB	2.68	0.41
1:E:297:ALA:O	1:E:298:ALA:HB3	2.21	0.41
1:A:60:TYR:CD1	1:A:60:TYR:C	2.93	0.41
1:A:140:ILE:HD13	1:A:140:ILE:HG21	1.90	0.41
1:B:700:LEU:HD12	1:B:700:LEU:C	2.40	0.41
1:D:337:LYS:NZ	1:D:339:GLU:OE1	2.54	0.41
1:B:132:GLU:O	1:B:133:ALA:C	2.59	0.41
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.65	0.41
1:B:326:GLU:OE2	1:C:714:LYS:NZ	2.51	0.41
1:B:568:LYS:O	1:B:569:LEU:HB2	2.21	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: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:C:183:LEU:HD23	1:C:183:LEU:C	2.42	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:F:409:SER:O	1:F:410:LYS:C	2.57	0.41
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:B:555:GLY:O	1:B:556:ILE:C	2.60	0.40
1:C:583:GLN:O	1:C:583:GLN:HG3	2.21	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:C:646:LEU:HD23	1:C:646:LEU:C	2.42	0.40
1:F:815:ALA:HA	1:F:819:TYR:CD1	2.56	0.40
1:C:302:LYS:HB2	1:C:303:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:794:ARG:NE	1:E:794:ARG:C	2.66	0.40
1:F:301:LEU:O	1:F:302:LYS:C	2.59	0.40
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.80	0.40
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

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	14	52
1	B	845/908 (93%)	784 (93%)	49 (6%)	12 (1%)	11	46
1	C	713/908 (78%)	671 (94%)	38 (5%)	4 (1%)	25	66
1	D	713/908 (78%)	661 (93%)	36 (5%)	16 (2%)	6	35
1	E	843/908 (93%)	786 (93%)	44 (5%)	13 (2%)	10	46
1	F	843/908 (93%)	789 (94%)	41 (5%)	13 (2%)	10	46
All	All	4800/5448 (88%)	4487 (94%)	246 (5%)	67 (1%)	15	46

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	THR
1	A	290	MET
1	A	807	THR

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Mol	Chain	Res	Type
1	B	318	ASN
1	B	540	VAL
1	B	650	TYR
1	B	706	GLY
1	C	650	TYR
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

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Mol	Chain	Res	Type
1	D	651	ALA
1	E	852	LYS
1	F	686	ASP
1	A	295	ASP
1	A	650	TYR
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%)	93	96
1	B	732/783 (94%)	731 (100%)	1 (0%)	93	96
1	C	620/783 (79%)	619 (100%)	1 (0%)	93	96
1	D	620/783 (79%)	620 (100%)	0	100	100
1	E	732/783 (94%)	731 (100%)	1 (0%)	93	96
1	F	732/783 (94%)	732 (100%)	0	100	100
All	All	4168/4698 (89%)	4164 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	LEU
1	B	256	LYS
1	C	702	MET
1	E	819	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	GLN
1	B	606	GLN
1	C	829	ASN
1	D	720	ASN
1	D	829	ASN
1	E	128	GLN
1	E	883	HIS
1	F	523	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides 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	1002	-	26,33,33	1.92	6 (23%)	26,52,52	2.20	8 (30%)
3	AGS	D	1001	-	26,33,33	1.89	7 (26%)	26,52,52	2.38	10 (38%)
3	AGS	B	1002	-	26,33,33	1.97	6 (23%)	26,52,52	1.93	7 (26%)
3	AGS	E	1002	-	26,33,33	1.88	7 (26%)	26,52,52	2.38	10 (38%)
3	AGS	F	1002	-	26,33,33	1.93	6 (23%)	26,52,52	1.87	7 (26%)
3	AGS	C	1002	-	26,33,33	1.88	6 (23%)	26,52,52	2.00	7 (26%)
3	AGS	F	1001	-	26,33,33	1.84	7 (26%)	26,52,52	2.11	7 (26%)
3	AGS	D	1002	-	24,32,33	2.15	7 (29%)	25,49,52	5.76	6 (24%)
3	AGS	E	1001	-	26,33,33	1.92	5 (19%)	26,52,52	2.01	7 (26%)
3	AGS	B	1001	-	26,33,33	1.84	4 (15%)	26,52,52	2.07	6 (23%)
3	AGS	C	1001	-	26,33,33	1.91	5 (19%)	26,52,52	2.07	6 (23%)
3	AGS	A	1001	-	26,33,33	1.97	5 (19%)	26,52,52	2.10	6 (23%)

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	1002	-	-	1/17/38/38	0/3/3/3
3	AGS	D	1001	-	-	2/17/38/38	0/3/3/3
3	AGS	B	1002	-	-	7/17/38/38	0/3/3/3
3	AGS	E	1002	-	-	2/17/38/38	0/3/3/3
3	AGS	F	1002	-	-	6/17/38/38	0/3/3/3
3	AGS	C	1002	-	-	4/17/38/38	0/3/3/3
3	AGS	F	1001	-	-	9/17/38/38	0/3/3/3
3	AGS	D	1002	-	-	3/9/36/38	0/3/3/3
3	AGS	E	1001	-	-	7/17/38/38	0/3/3/3
3	AGS	B	1001	-	-	7/17/38/38	0/3/3/3
3	AGS	C	1001	-	-	4/17/38/38	0/3/3/3
3	AGS	A	1001	-	-	3/17/38/38	0/3/3/3

All (71) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	AGS	PG-S1G	7.67	2.07	1.90
3	E	1001	AGS	PG-S1G	7.54	2.07	1.90
3	C	1001	AGS	PG-S1G	7.51	2.07	1.90
3	B	1002	AGS	PG-S1G	7.45	2.06	1.90
3	F	1002	AGS	PG-S1G	7.44	2.06	1.90
3	C	1002	AGS	PG-S1G	7.36	2.06	1.90
3	B	1001	AGS	PG-S1G	7.35	2.06	1.90
3	A	1002	AGS	PG-S1G	7.28	2.06	1.90
3	D	1001	AGS	PG-S1G	7.12	2.06	1.90
3	E	1002	AGS	PG-S1G	7.12	2.06	1.90
3	D	1002	AGS	PG-S1G	7.11	2.06	1.90
3	F	1001	AGS	PG-S1G	7.09	2.06	1.90
3	D	1002	AGS	C5-N7	-4.18	1.24	1.39
3	A	1002	AGS	C2'-C1'	-2.80	1.49	1.53
3	D	1001	AGS	C5-C4	2.79	1.48	1.40
3	E	1002	AGS	C5-C4	2.79	1.48	1.40
3	B	1002	AGS	C5-C4	2.78	1.48	1.40
3	D	1002	AGS	C2'-C1'	-2.78	1.49	1.53
3	D	1002	AGS	O4'-C1'	2.75	1.44	1.41
3	B	1002	AGS	O4'-C1'	2.75	1.44	1.41
3	A	1001	AGS	PG-O2G	2.71	1.63	1.54
3	E	1001	AGS	C5-C4	2.69	1.48	1.40
3	F	1002	AGS	O4'-C1'	2.64	1.44	1.41
3	F	1002	AGS	C5-C4	2.53	1.47	1.40
3	A	1002	AGS	C5-C4	2.46	1.47	1.40
3	B	1002	AGS	PG-O2G	2.46	1.62	1.54
3	C	1002	AGS	O4'-C1'	2.45	1.44	1.41
3	A	1001	AGS	C5-C4	2.44	1.47	1.40
3	C	1001	AGS	C5-C4	2.44	1.47	1.40
3	A	1001	AGS	C2-N3	2.40	1.36	1.32
3	A	1002	AGS	PG-O2G	2.39	1.62	1.54
3	B	1001	AGS	C5-C4	2.35	1.47	1.40
3	C	1002	AGS	C5-C4	2.34	1.47	1.40
3	D	1002	AGS	C5-C4	2.33	1.47	1.40
3	F	1002	AGS	PG-O2G	2.32	1.62	1.54
3	F	1001	AGS	C5-C4	2.32	1.47	1.40
3	C	1002	AGS	PG-O2G	2.31	1.62	1.54
3	C	1002	AGS	C2-N3	2.28	1.35	1.32
3	E	1001	AGS	PG-O2G	2.24	1.62	1.54
3	C	1001	AGS	PG-O2G	2.24	1.62	1.54
3	D	1002	AGS	PG-O3G	-2.22	1.47	1.54
3	C	1001	AGS	O4'-C1'	2.22	1.44	1.41
3	E	1002	AGS	PG-O2G	2.20	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	AGS	PG-O3G	-2.19	1.47	1.54
3	F	1001	AGS	PG-O2G	2.19	1.62	1.54
3	A	1002	AGS	O4'-C1'	2.18	1.44	1.41
3	B	1001	AGS	PG-O2G	2.18	1.62	1.54
3	D	1001	AGS	PG-O2G	2.17	1.62	1.54
3	E	1001	AGS	PG-O3G	-2.16	1.47	1.54
3	D	1002	AGS	PG-O2G	2.15	1.61	1.54
3	F	1001	AGS	C2-N3	2.13	1.35	1.32
3	D	1001	AGS	C5-N7	-2.11	1.32	1.39
3	E	1002	AGS	C5-N7	-2.11	1.32	1.39
3	A	1001	AGS	O4'-C1'	2.10	1.44	1.41
3	D	1001	AGS	O4'-C1'	2.10	1.44	1.41
3	E	1002	AGS	O4'-C1'	2.08	1.44	1.41
3	F	1001	AGS	O4'-C1'	2.07	1.44	1.41
3	F	1001	AGS	C2'-C1'	-2.06	1.50	1.53
3	F	1001	AGS	PG-O3G	-2.06	1.48	1.54
3	E	1001	AGS	C2-N3	2.06	1.35	1.32
3	A	1002	AGS	C2-N3	2.05	1.35	1.32
3	B	1001	AGS	PG-O3G	-2.05	1.48	1.54
3	B	1002	AGS	C2-N3	2.03	1.35	1.32
3	E	1002	AGS	C2'-C1'	-2.03	1.50	1.53
3	F	1002	AGS	C2'-C1'	-2.03	1.50	1.53
3	F	1002	AGS	PG-O3G	-2.02	1.48	1.54
3	B	1002	AGS	PG-O3G	-2.02	1.48	1.54
3	C	1002	AGS	PG-O3G	-2.02	1.48	1.54
3	D	1001	AGS	C2'-C1'	-2.02	1.50	1.53
3	D	1001	AGS	PG-O3G	-2.01	1.48	1.54
3	E	1002	AGS	PG-O3G	-2.00	1.48	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	C1'-N9-C4	27.19	174.41	126.64
3	D	1001	AGS	PA-O3A-PB	-7.94	105.60	132.83
3	E	1002	AGS	PA-O3A-PB	-7.92	105.64	132.83
3	A	1002	AGS	PA-O3A-PB	-7.29	107.83	132.83
3	C	1001	AGS	PA-O3A-PB	-7.08	108.52	132.83
3	B	1001	AGS	PA-O3A-PB	-6.99	108.84	132.83
3	F	1001	AGS	PA-O3A-PB	-6.79	109.54	132.83
3	E	1001	AGS	PA-O3A-PB	-6.53	110.40	132.83
3	A	1001	AGS	PA-O3A-PB	-6.41	110.82	132.83
3	B	1002	AGS	PA-O3A-PB	-5.96	112.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	AGS	PA-O3A-PB	-5.69	113.28	132.83
3	F	1002	AGS	PA-O3A-PB	-5.16	115.14	132.83
3	D	1002	AGS	C4-C5-N7	-4.89	104.30	109.40
3	C	1002	AGS	N6-C6-N1	3.58	126.00	118.57
3	A	1001	AGS	N6-C6-N1	3.55	125.94	118.57
3	F	1001	AGS	N6-C6-N1	3.53	125.90	118.57
3	A	1001	AGS	O2G-PG-O3B	3.46	116.19	104.64
3	B	1001	AGS	N6-C6-N1	3.41	125.66	118.57
3	A	1002	AGS	N6-C6-N1	3.38	125.59	118.57
3	A	1002	AGS	O2G-PG-O3B	3.34	115.80	104.64
3	B	1002	AGS	N6-C6-N1	3.30	125.42	118.57
3	E	1002	AGS	N6-C6-N1	3.23	125.28	118.57
3	D	1001	AGS	N6-C6-N1	3.21	125.24	118.57
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	C	1002	AGS	O2G-PG-O3B	3.09	114.96	104.64
3	D	1002	AGS	N6-C6-N1	3.02	124.85	118.57
3	D	1002	AGS	O2G-PG-O3B	3.00	114.65	104.64
3	F	1002	AGS	O2G-PG-O3B	2.96	114.51	104.64
3	E	1001	AGS	C3'-C2'-C1'	2.84	105.25	100.98
3	E	1001	AGS	O2G-PG-O3B	2.83	114.09	104.64
3	F	1002	AGS	N6-C6-N1	2.74	124.26	118.57
3	F	1001	AGS	C5-C6-N6	-2.68	116.29	120.35
3	C	1001	AGS	O2G-PG-O3B	2.63	113.41	104.64
3	E	1002	AGS	O2B-PB-O1B	2.62	125.17	112.24
3	D	1001	AGS	O2B-PB-O1B	2.61	125.15	112.24
3	C	1002	AGS	C5'-C4'-C3'	-2.61	105.41	115.18
3	D	1002	AGS	N3-C2-N1	-2.61	124.61	128.68
3	A	1002	AGS	N3-C2-N1	-2.59	124.63	128.68
3	E	1001	AGS	N6-C6-N1	2.59	123.94	118.57
3	C	1001	AGS	C4-C5-N7	-2.58	106.71	109.40
3	A	1002	AGS	C3'-C2'-C1'	2.58	104.87	100.98
3	A	1001	AGS	O2B-PB-O1B	2.58	125.01	112.24
3	B	1002	AGS	O2G-PG-O3B	2.57	113.22	104.64
3	F	1002	AGS	N3-C2-N1	-2.56	124.68	128.68
3	B	1001	AGS	N3-C2-N1	-2.55	124.70	128.68
3	A	1001	AGS	C5-C6-N6	-2.54	116.49	120.35
3	B	1001	AGS	O2G-PG-O3B	2.52	113.04	104.64
3	C	1001	AGS	N3-C2-N1	-2.48	124.81	128.68
3	C	1002	AGS	C5-C6-N6	-2.46	116.61	120.35
3	C	1002	AGS	N3-C2-N1	-2.45	124.85	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	AGS	C3'-C2'-C1'	2.43	104.64	100.98
3	E	1002	AGS	C1'-N9-C4	2.42	130.90	126.64
3	D	1001	AGS	O5'-C5'-C4'	-2.41	100.69	108.99
3	D	1001	AGS	C1'-N9-C4	2.41	130.87	126.64
3	A	1001	AGS	N3-C2-N1	-2.40	124.92	128.68
3	E	1001	AGS	C2'-C3'-C4'	2.40	107.30	102.64
3	B	1002	AGS	C5'-C4'-C3'	-2.40	106.20	115.18
3	E	1002	AGS	O5'-C5'-C4'	-2.40	100.75	108.99
3	B	1002	AGS	C4-C5-N7	-2.38	106.92	109.40
3	D	1002	AGS	C5'-C4'-C3'	-2.36	106.35	115.18
3	B	1001	AGS	O3'-C3'-C4'	-2.32	104.33	111.05
3	A	1002	AGS	O2B-PB-O1B	2.31	123.66	112.24
3	F	1001	AGS	N3-C2-N1	-2.28	125.11	128.68
3	F	1002	AGS	O2B-PB-O1B	2.27	123.48	112.24
3	E	1002	AGS	N3-C2-N1	-2.27	125.13	128.68
3	D	1001	AGS	N3-C2-N1	-2.26	125.15	128.68
3	D	1001	AGS	O5'-PA-O1A	2.20	117.66	109.07
3	E	1002	AGS	O5'-PA-O1A	2.19	117.62	109.07
3	B	1002	AGS	N3-C2-N1	-2.19	125.26	128.68
3	E	1001	AGS	C4-C5-N7	-2.18	107.13	109.40
3	E	1001	AGS	N3-C2-N1	-2.15	125.32	128.68
3	C	1001	AGS	O2B-PB-O1B	2.15	122.85	112.24
3	A	1002	AGS	C4-C5-N7	-2.14	107.17	109.40
3	D	1001	AGS	C4-C5-N7	-2.12	107.19	109.40
3	F	1002	AGS	C5'-C4'-C3'	-2.11	107.27	115.18
3	E	1002	AGS	C4-C5-N7	-2.10	107.21	109.40
3	F	1001	AGS	O2A-PA-O1A	2.10	122.63	112.24
3	A	1002	AGS	C5-C6-N6	-2.09	117.17	120.35
3	B	1002	AGS	O2B-PB-O1B	2.09	122.58	112.24
3	E	1002	AGS	C3'-C2'-C1'	2.08	104.11	100.98
3	F	1002	AGS	C4-C5-N7	-2.08	107.23	109.40
3	D	1001	AGS	C3'-C2'-C1'	2.08	104.10	100.98
3	F	1001	AGS	O2B-PB-O1B	2.07	122.50	112.24
3	B	1001	AGS	O2A-PA-O1A	2.06	122.43	112.24
3	C	1001	AGS	C3'-C2'-C1'	2.00	103.99	100.98

There are no chirality outliers.

All (55) 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	1001	AGS	C5'-O5'-PA-O3A
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	1002	AGS	C3'-C4'-C5'-O5'
3	D	1002	AGS	C5'-O5'-PA-O1A
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	D	1001	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	O4'-C4'-C5'-O5'
3	E	1002	AGS	C3'-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	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	E	1001	AGS	PG-O3B-PB-O1B
3	F	1002	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	C5'-O5'-PA-O3A
3	D	1002	AGS	C5'-O5'-PA-O3A
3	C	1002	AGS	PB-O3A-PA-O2A
3	B	1001	AGS	C5'-O5'-PA-O1A
3	C	1001	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-O2A
3	B	1002	AGS	O4'-C4'-C5'-O5'

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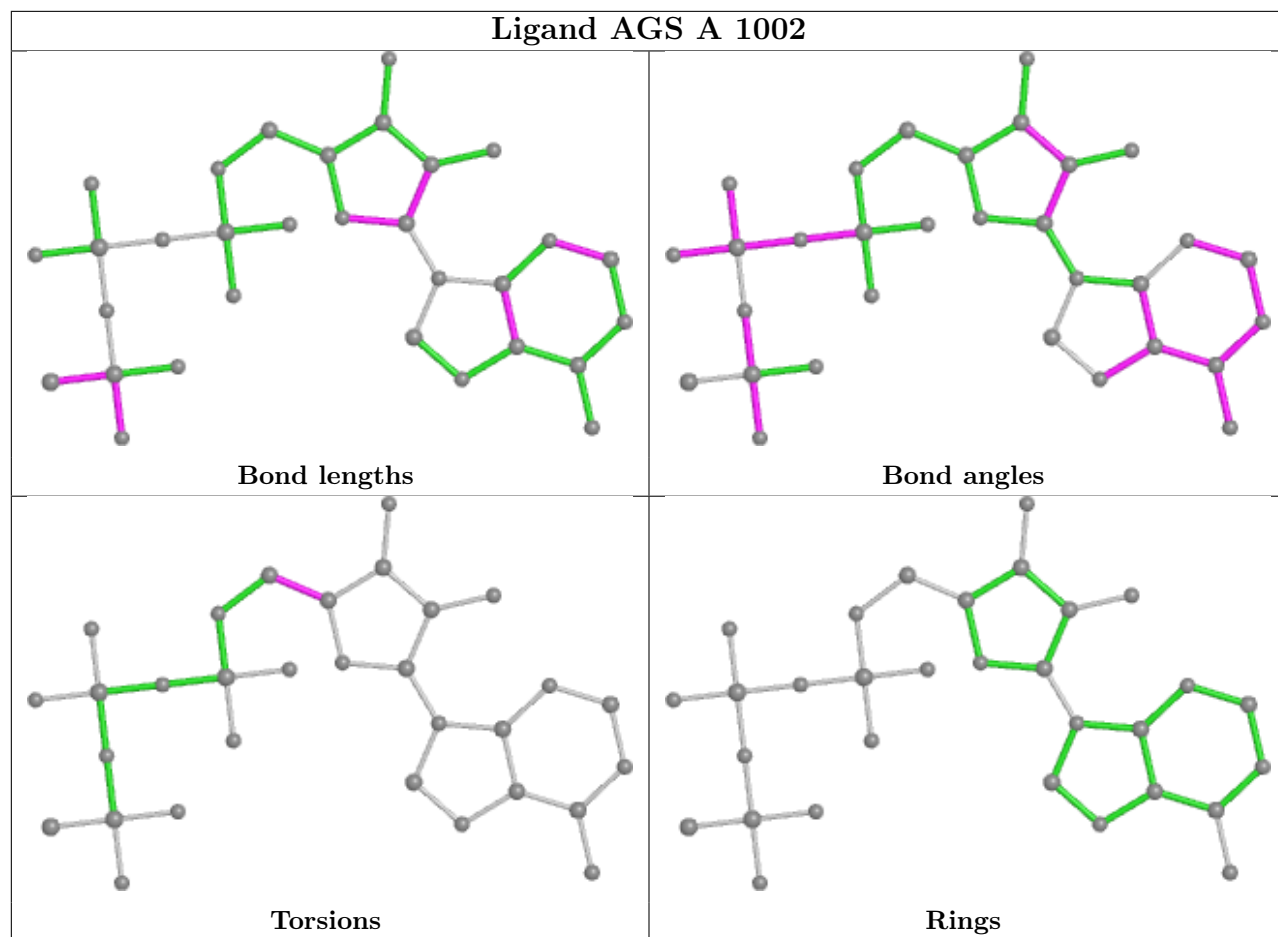
Mol	Chain	Res	Type	Atoms
3	F	1002	AGS	PB-O3A-PA-O2A
3	A	1001	AGS	PG-O3B-PB-O2B
3	B	1002	AGS	PG-O3B-PB-O1B
3	E	1001	AGS	PG-O3B-PB-O2B
3	F	1001	AGS	PG-O3B-PB-O1B
3	F	1002	AGS	PG-O3B-PB-O2B
3	A	1002	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	O4'-C4'-C5'-O5'
3	F	1001	AGS	PA-O3A-PB-O1B
3	C	1002	AGS	C5'-O5'-PA-O1A
3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

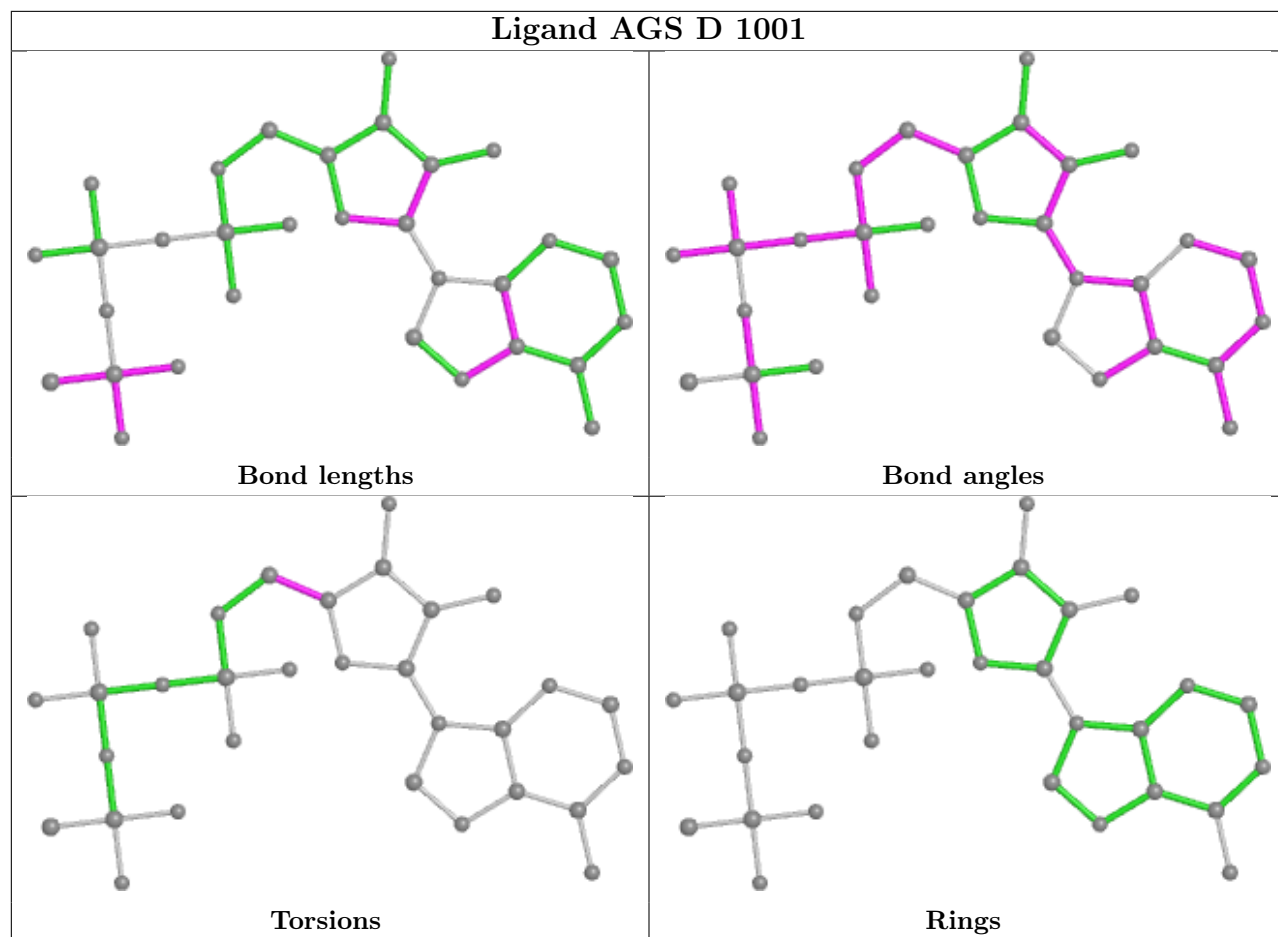
There are no ring outliers.

12 monomers are involved in 45 short contacts:

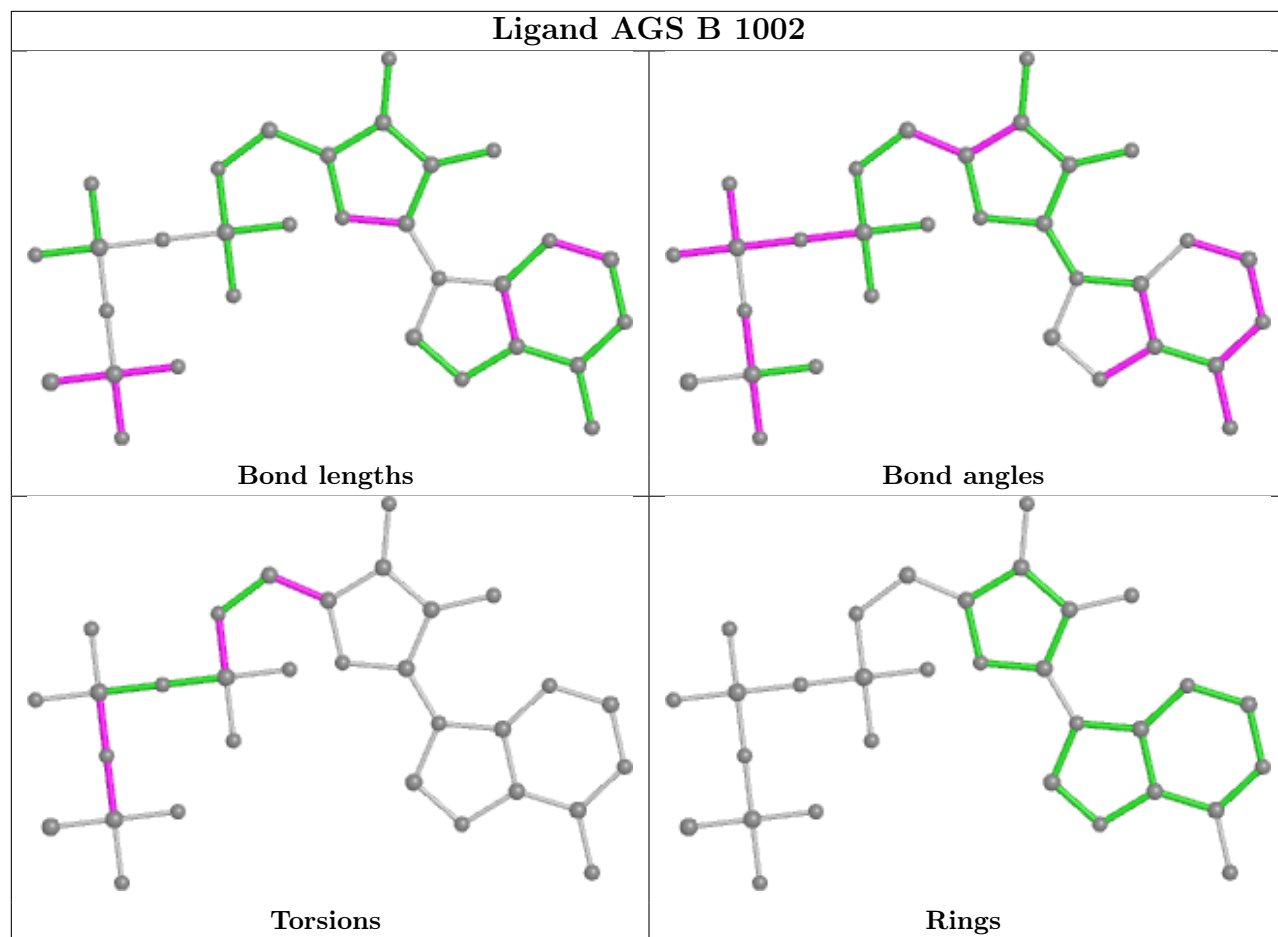
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	AGS	2	0
3	D	1001	AGS	22	0
3	B	1002	AGS	3	0
3	E	1002	AGS	1	0
3	F	1002	AGS	1	0
3	C	1002	AGS	1	0
3	F	1001	AGS	2	0
3	D	1002	AGS	1	0
3	E	1001	AGS	4	0
3	B	1001	AGS	5	0
3	C	1001	AGS	2	0
3	A	1001	AGS	1	0

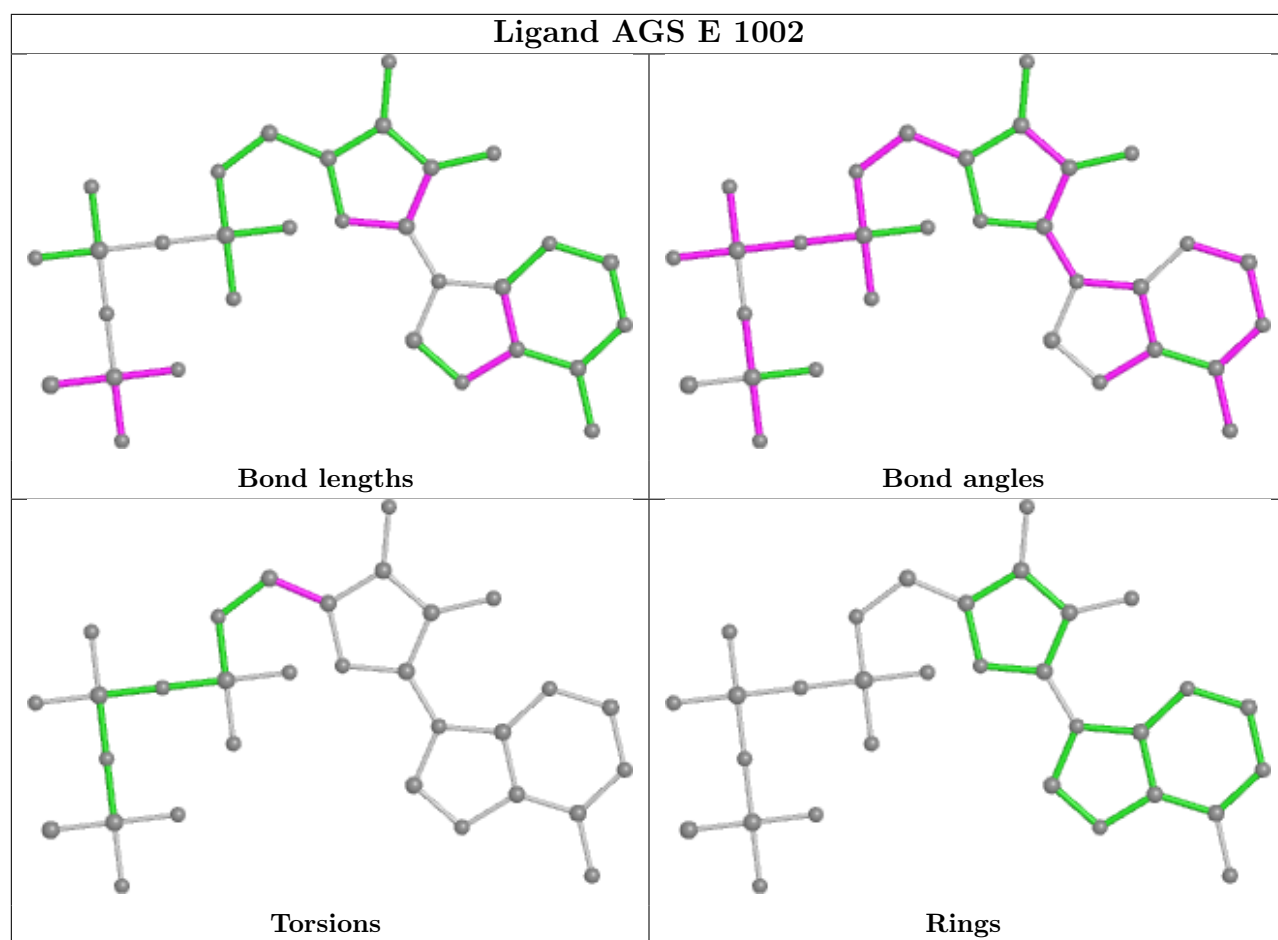
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

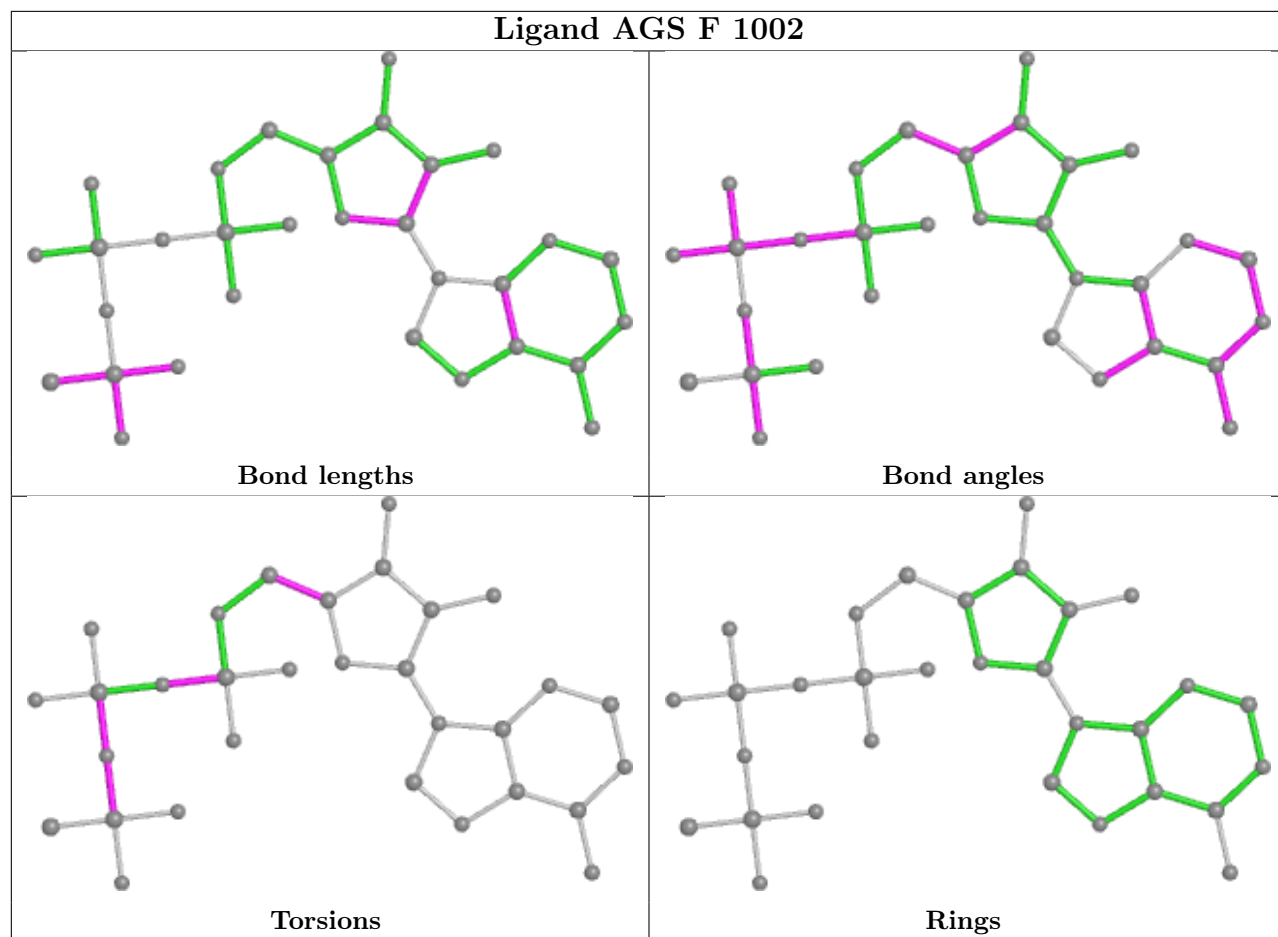


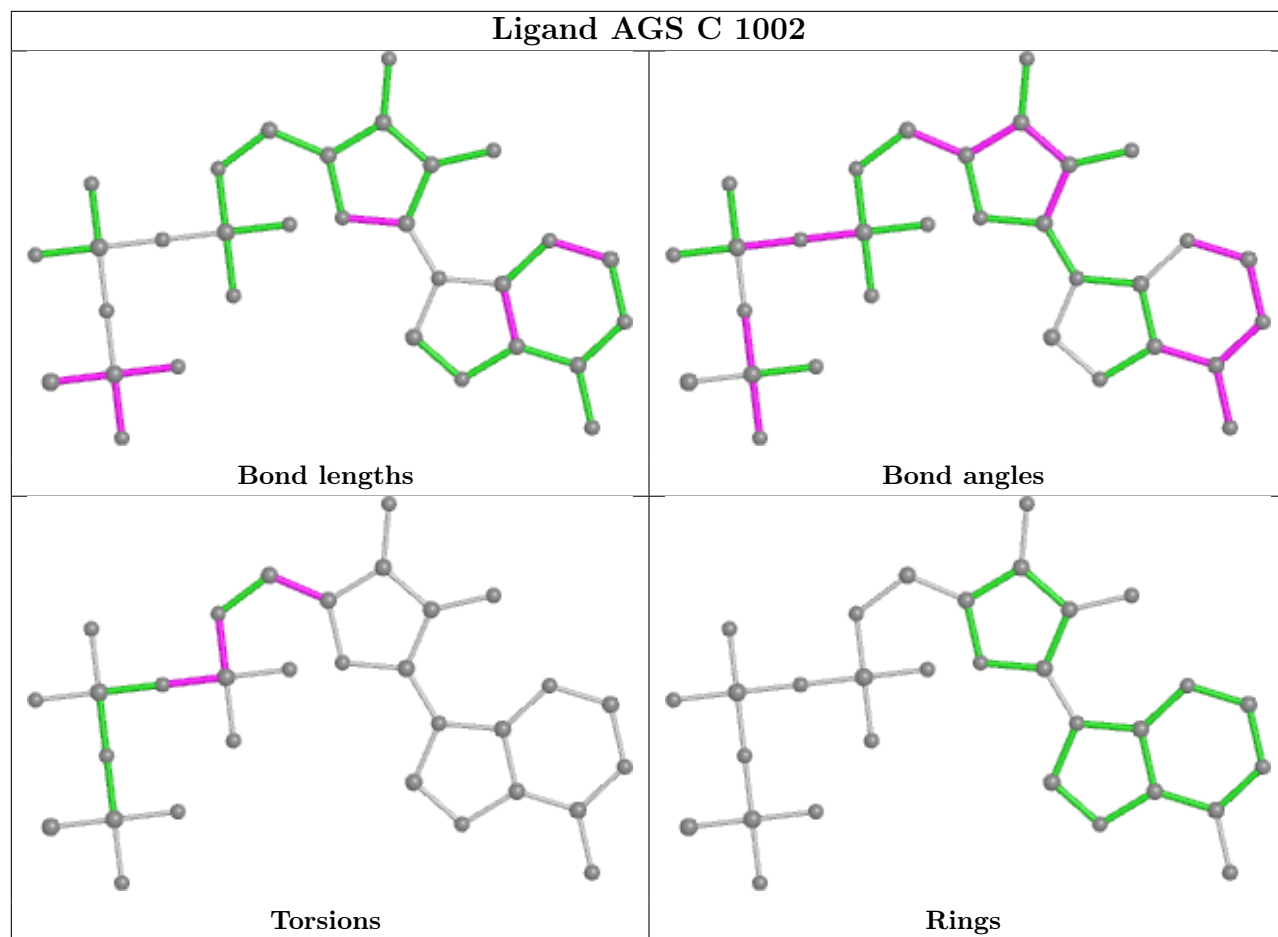


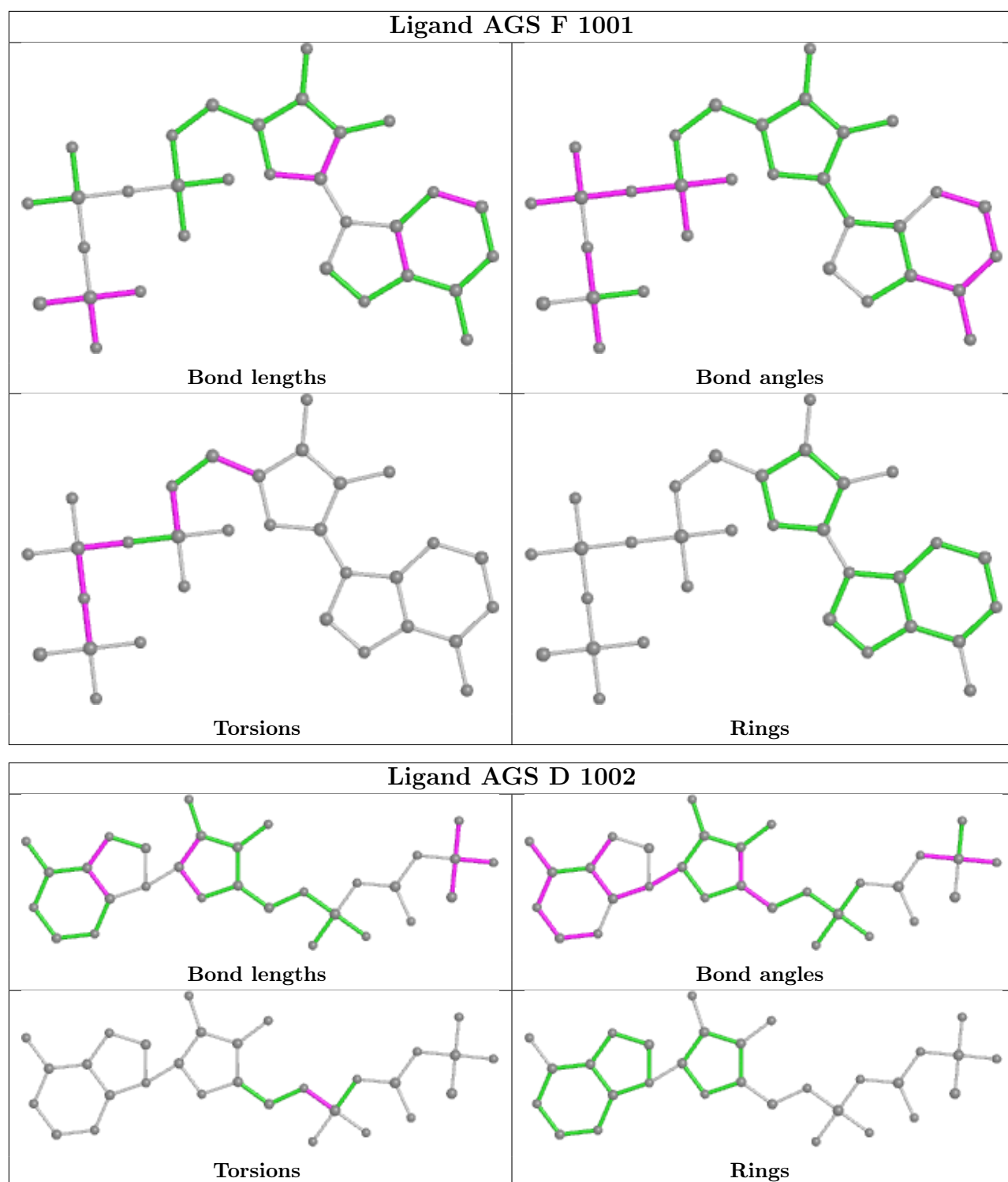


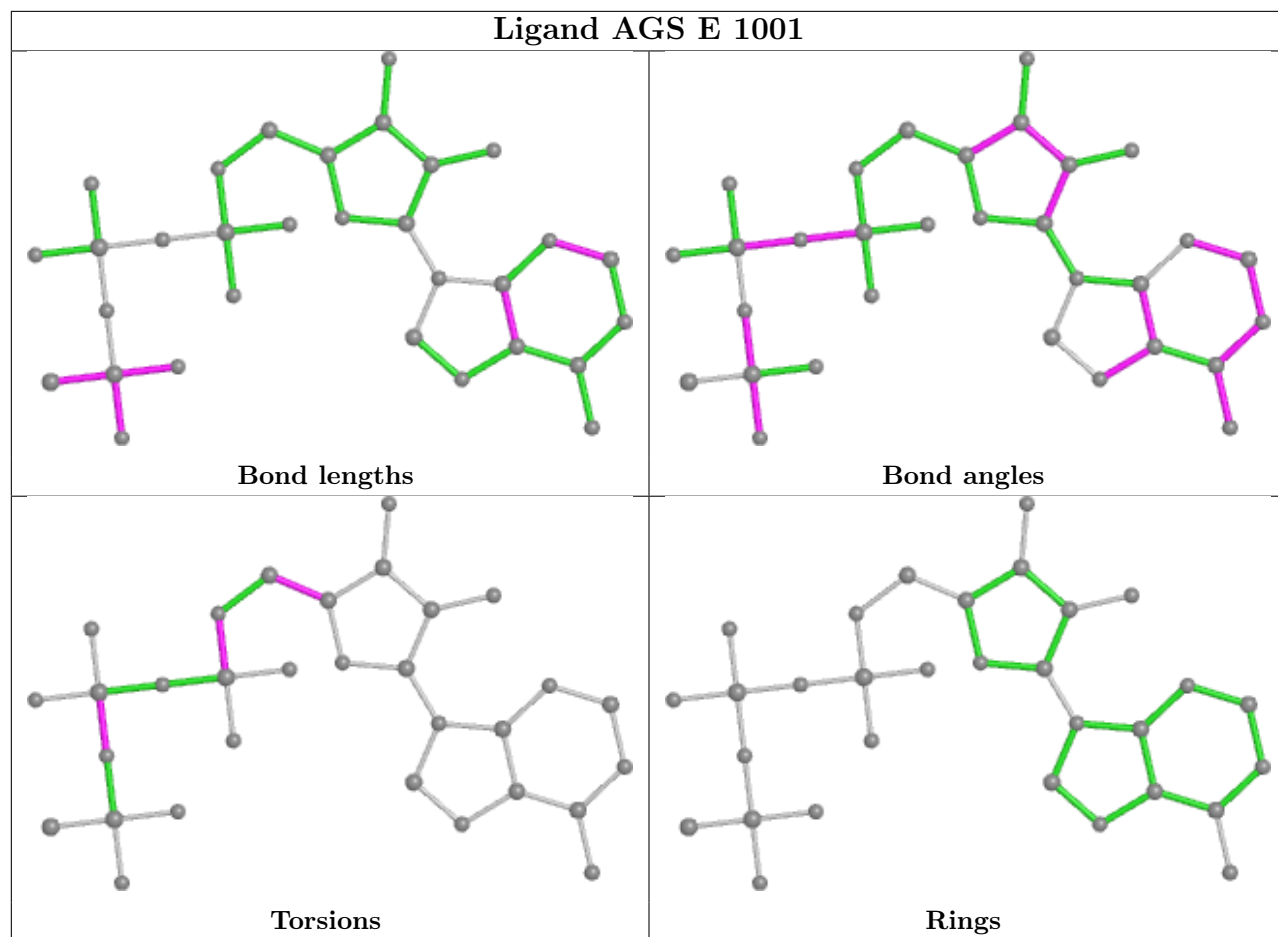


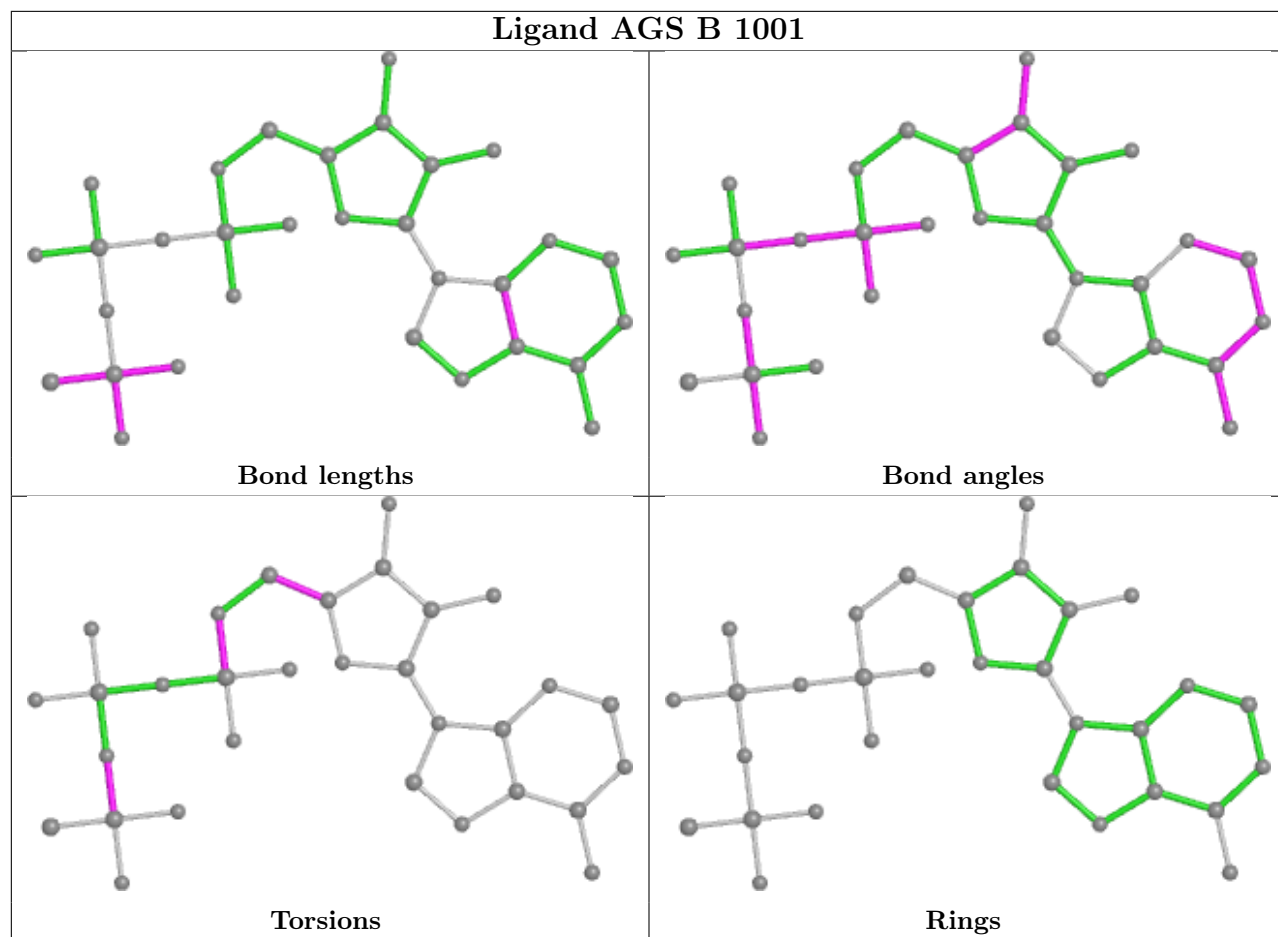


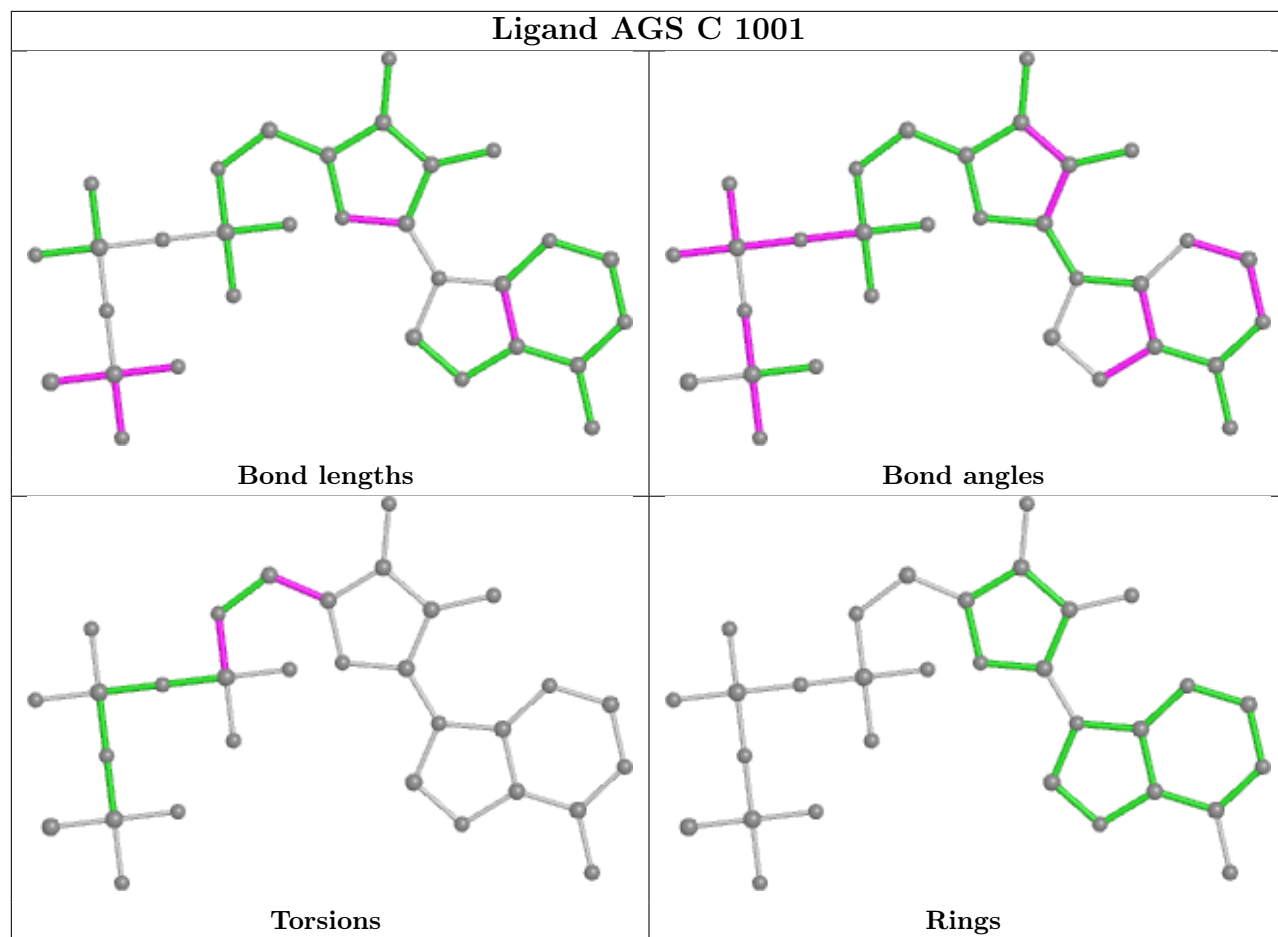




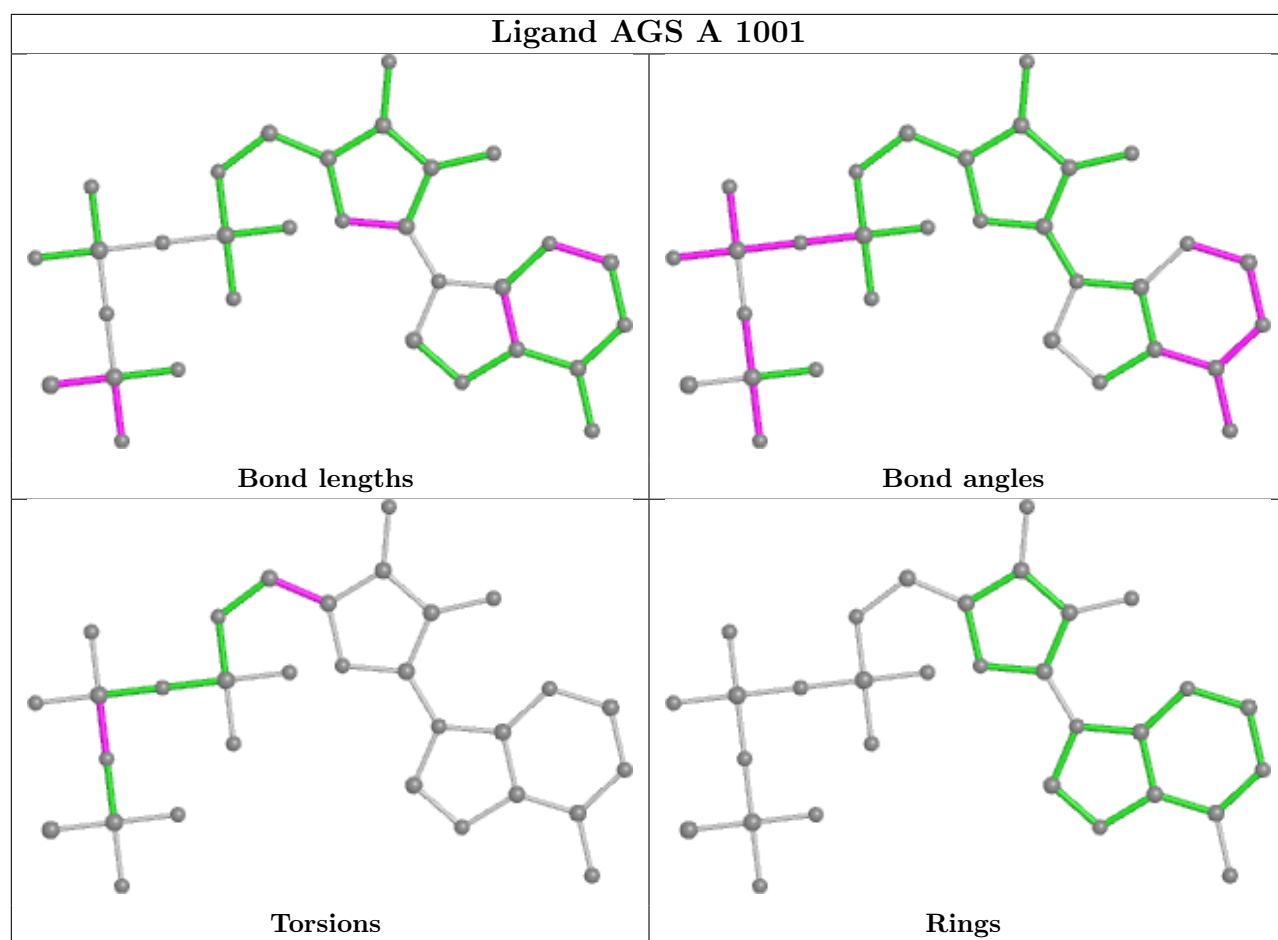












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

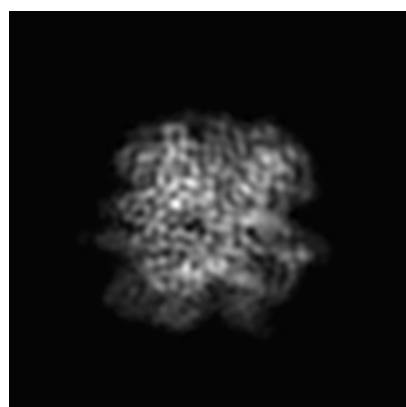
## 6 Map visualisation [i](#)

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.

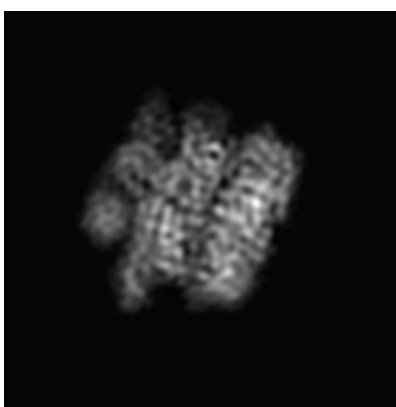
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

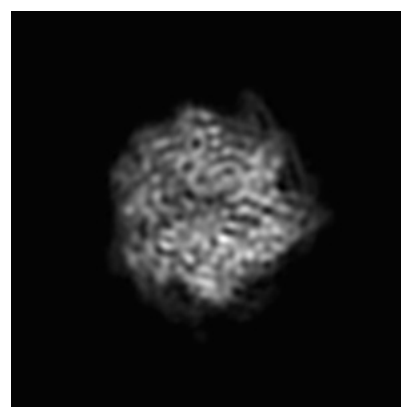
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

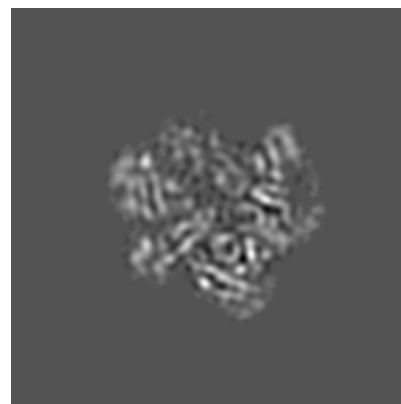
#### 6.2.1 Primary map



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](#)

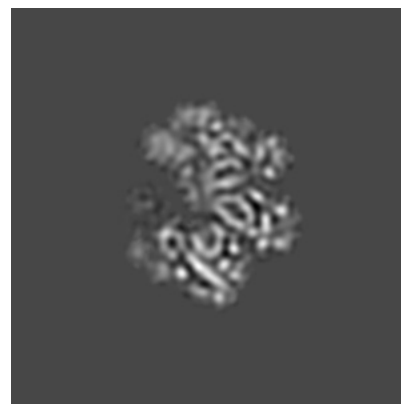
### 6.3.1 Primary map



X Index: 123



Y Index: 105

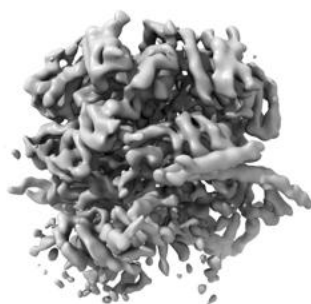


Z Index: 161

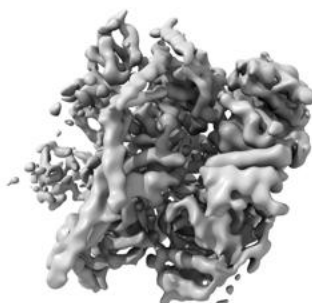
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

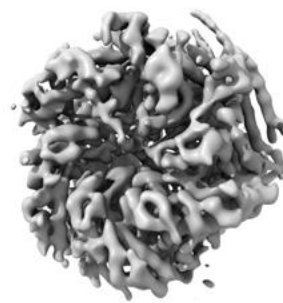
### 6.4.1 Primary map



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.

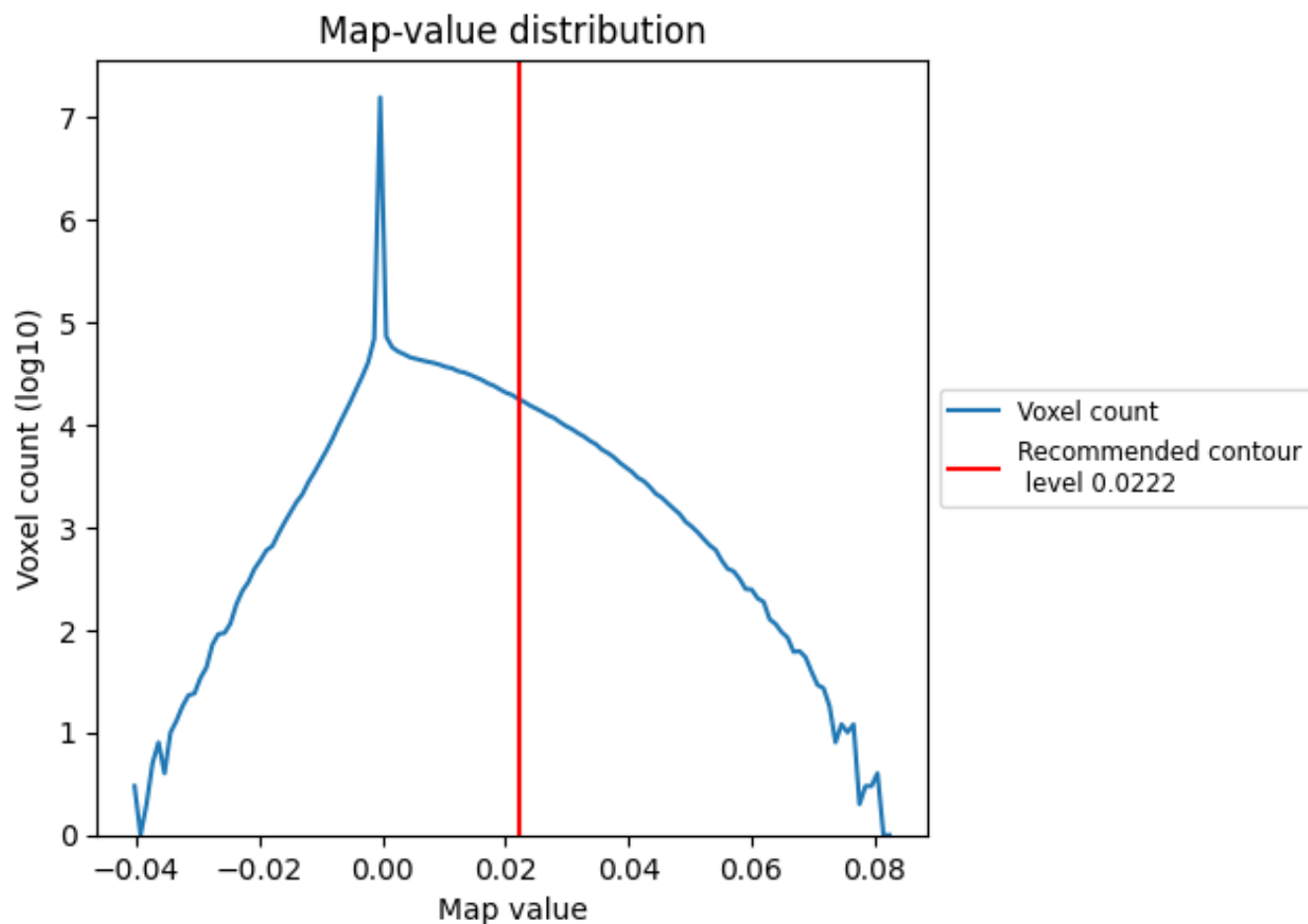
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

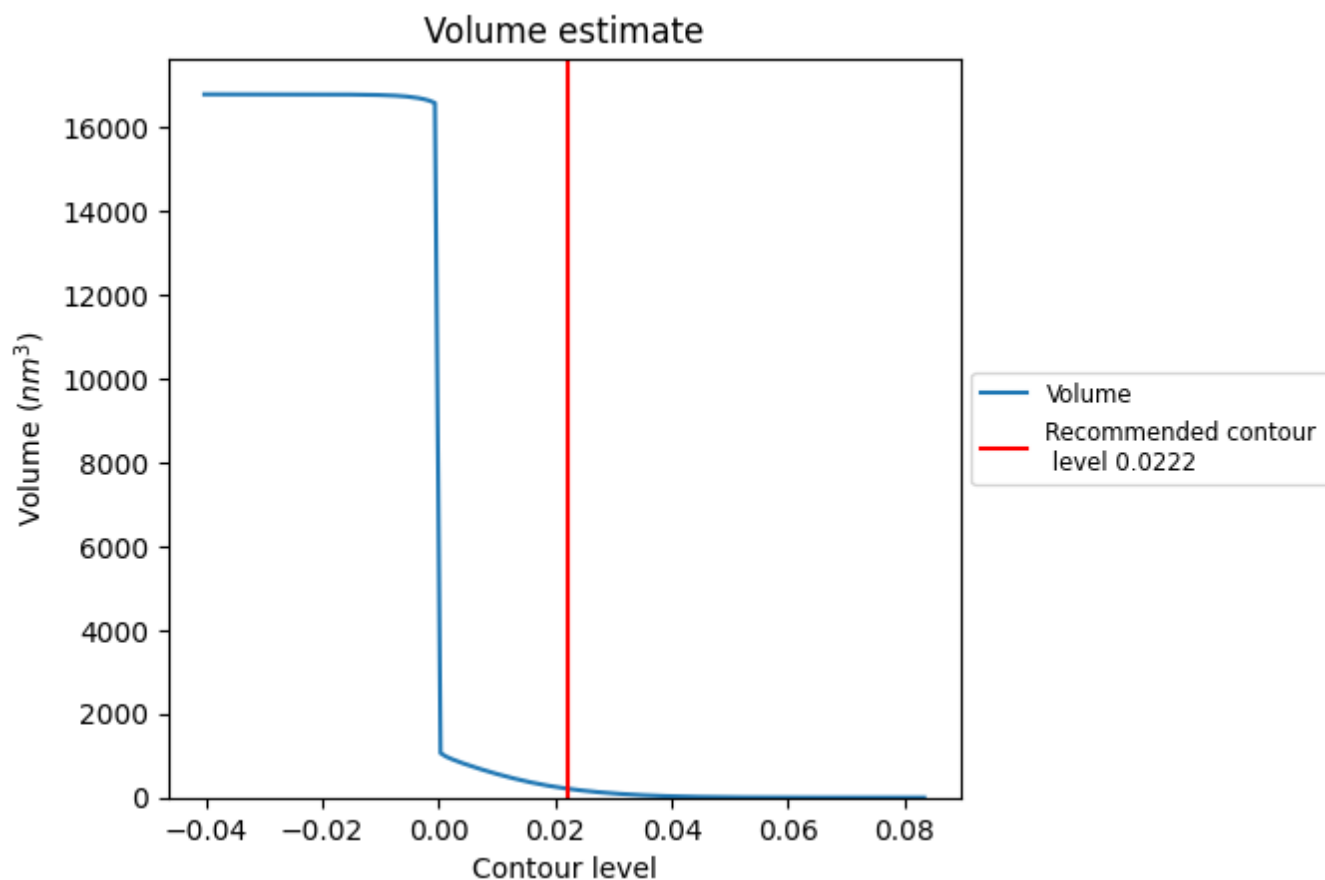
This section contains the results of statistical analysis of the map.

### 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.

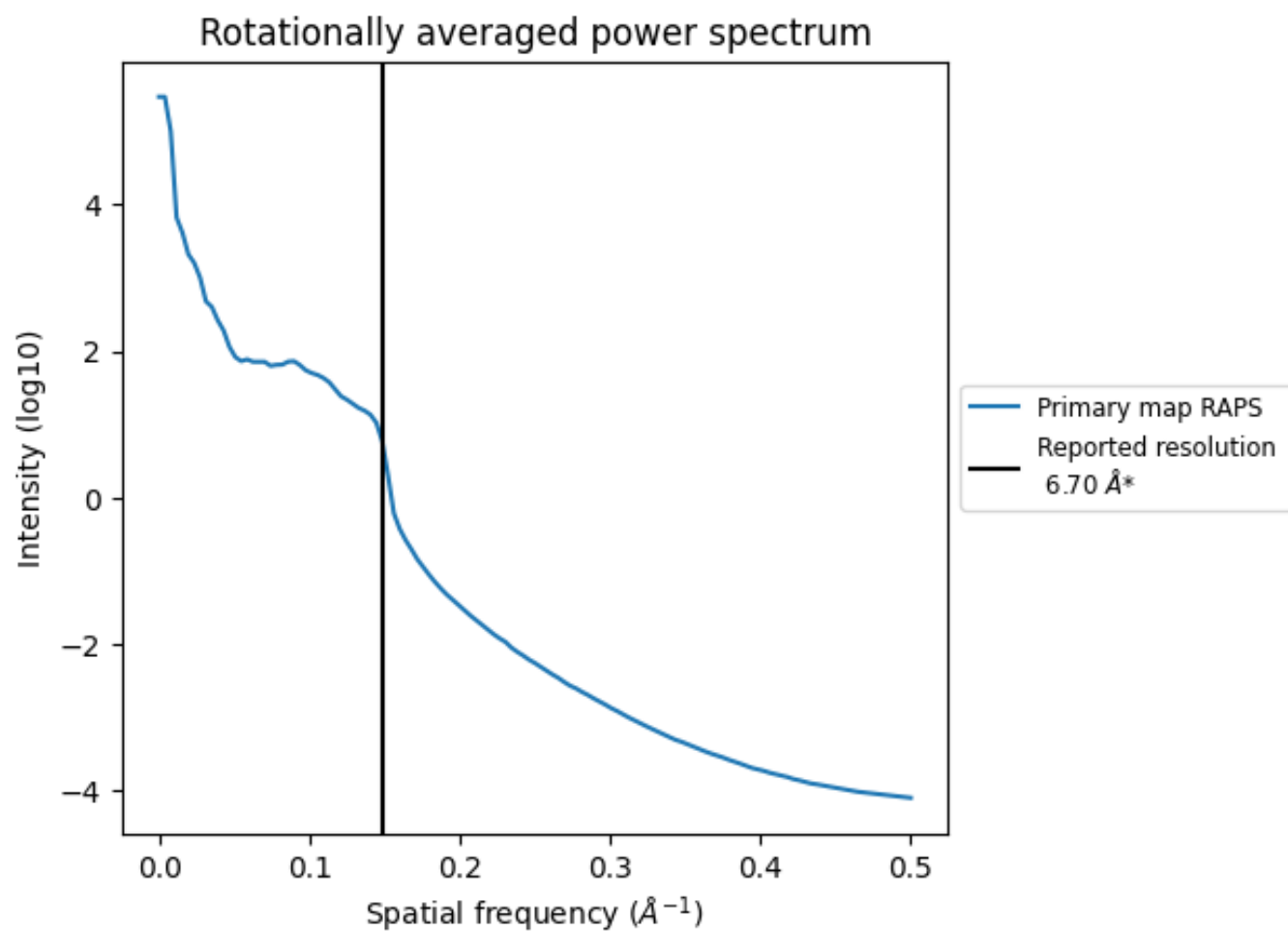
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm<sup>3</sup>; 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<sup>-1</sup>

## 8 Fourier-Shell correlation

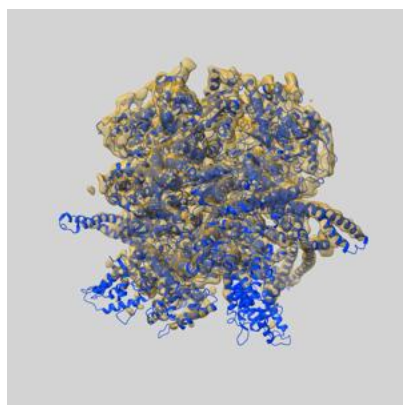
This section was not generated. No FSC curve or half-maps provided.



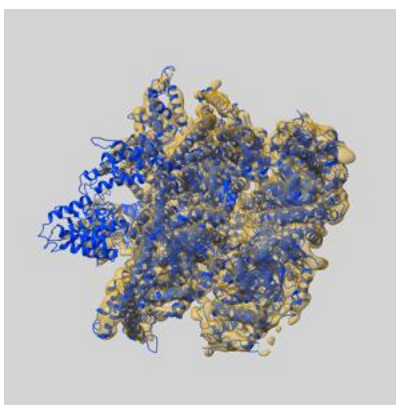
## 9 Map-model fit [i](#)

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](#).

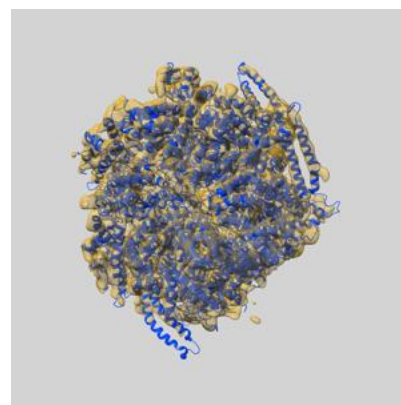
### 9.1 Map-model overlay [i](#)



X



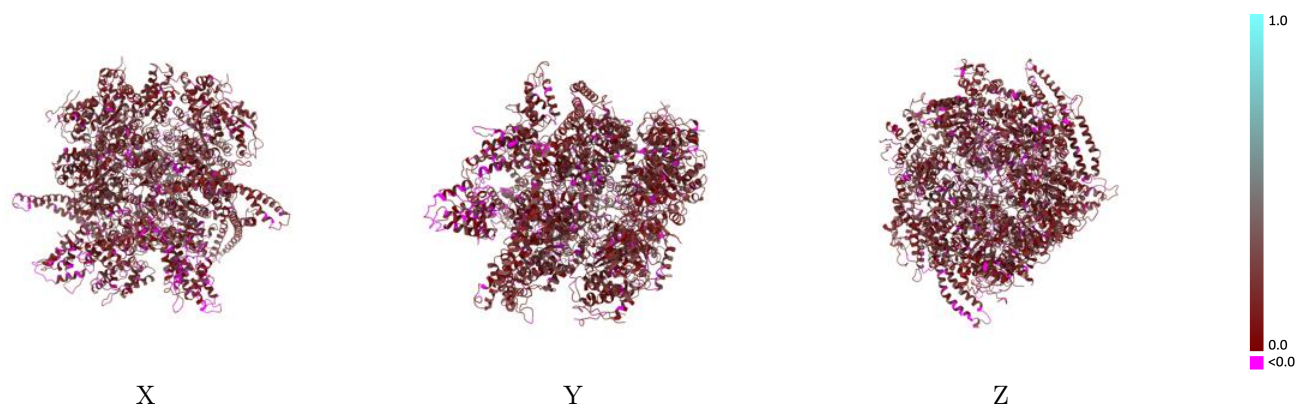
Y



Z

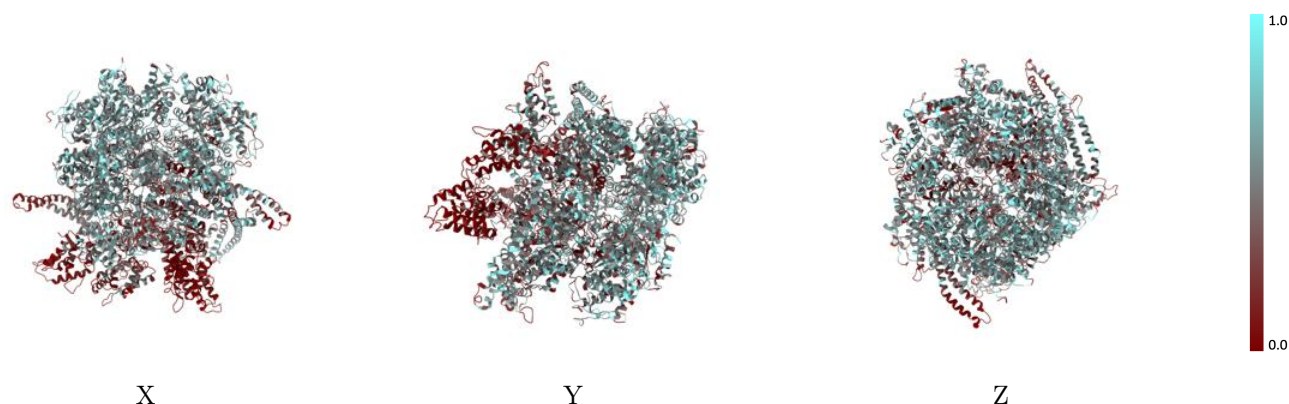
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



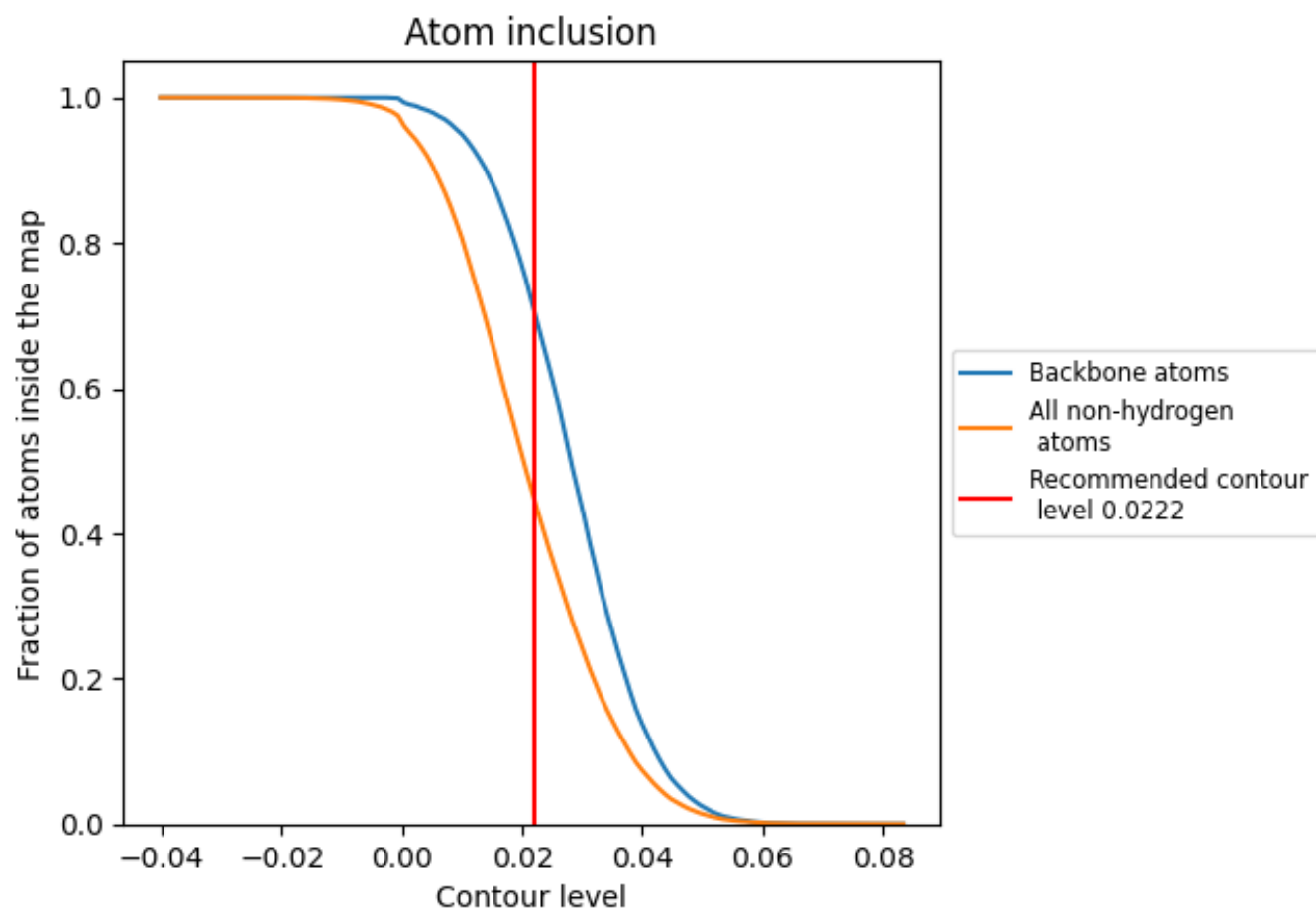
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.4415	<div></div> 0.1610
A	<div></div> 0.3929	<div></div> 0.1580
B	<div></div> 0.4907	<div></div> 0.1680
C	<div></div> 0.5222	<div></div> 0.1720
D	<div></div> 0.4443	<div></div> 0.1600
E	<div></div> 0.4330	<div></div> 0.1620
F	<div></div> 0.3740	<div></div> 0.1440
P	<div></div> 0.6714	<div></div> 0.3040

1.0

0.0

<0.0