



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:07 PM UTC

PDB ID : 6ZA9 / pdb_00006za9
EMDB ID : EMD-11127
Title : Fo domain of Ovine ATP synthase
Authors : Pinke, G.; Zhou, L.; Sazanov, L.A.
Deposited on : 2020-06-05
Resolution : 3.76 Å(reported)
Based on initial model : 5ARA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

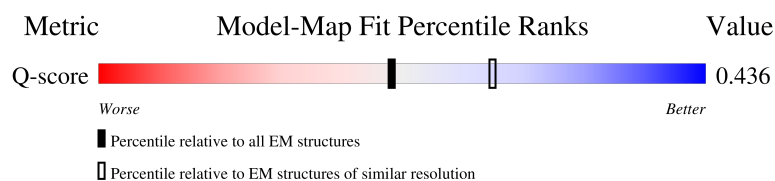
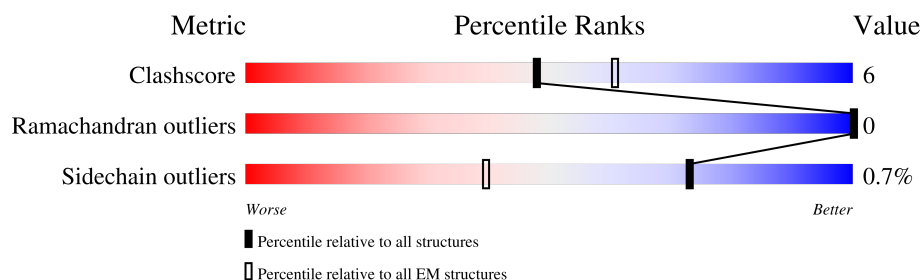
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.76 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	10214 (3.26 - 4.26)

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	1	136	
1	2	136	
1	3	136	
1	4	136	

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Mol	Chain	Length	Quality of chain
1	5	136	
1	6	136	
1	7	136	
1	8	136	
2	K	256	
3	M	161	
4	N	226	
5	O	58	
6	P	60	
7	Q	66	
8	R	88	
9	S	103	
10	T	71	

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
12	CDL	N	401	X	-	-	-
12	CDL	R	301	X	-	-	-
12	CDL	R	302	X	-	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 11067 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 ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	2	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	3	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	4	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	5	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	6	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	7	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
1	8	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

- Molecule 2 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	119	Total	C	N	O	S	0	0
			933	615	144	173	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	58	PHE	ALA	conflict	UNP W5QEA9

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	60	Total	C	N	O	S	0	0
			519	335	84	97	3		

- Molecule 4 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	225	Total	C	N	O	S	0	0
			1734	1150	277	295	12		

- Molecule 5 is a protein called ATP synthase membrane subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	40	Total	C	N	O	S	0	0
			327	219	53	53	2		

- Molecule 6 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	52	Total	C	N	O	S	0	0
			425	281	70	71	3		

- Molecule 7 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	47	Total	C	N	O	S	0	0
			371	248	58	62	3		

- Molecule 8 is a protein called ATP synthase membrane subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	84	Total	C	N	O	S	0	0
			701	461	121	116	3		

- Molecule 9 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	85	Total	C	N	O	S	0	0
			673	448	106	118	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	96	ARG	HIS	conflict	UNP W5Q5U7
S	99	ILE	THR	conflict	UNP W5Q5U7

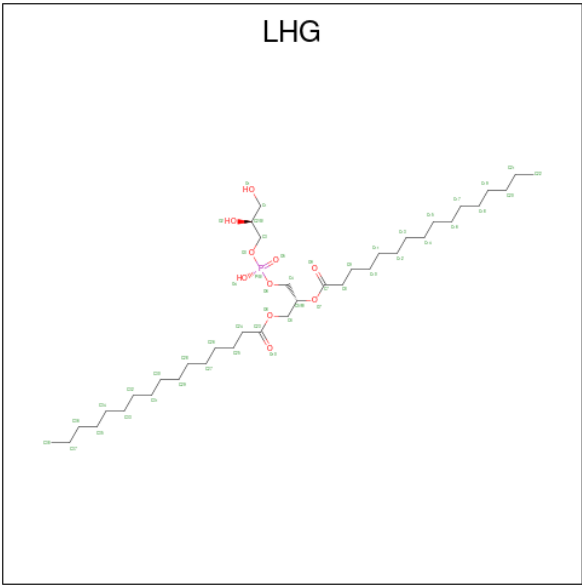
- Molecule 10 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	70	Total	C	N	O	S	0	0
			577	364	106	106	1		

There are 3 discrepancies between the modelled and reference sequences:

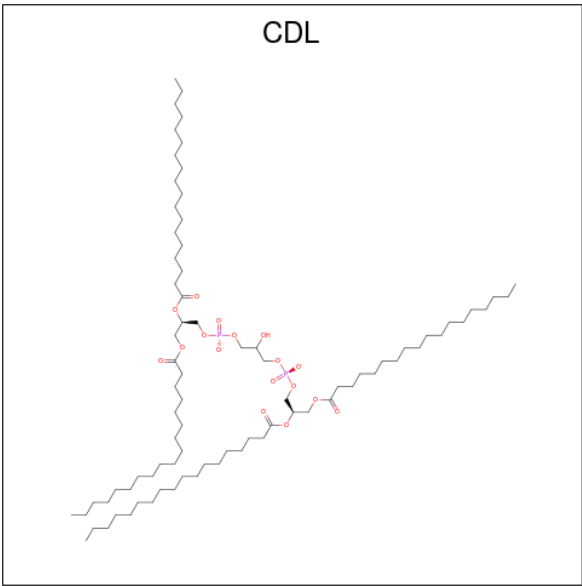
Chain	Residue	Modelled	Actual	Comment	Reference
T	23	MET	VAL	conflict	UNP W5PF18
T	26	GLY	SER	conflict	UNP W5PF18
T	38	GLU	-	insertion	UNP W5PF18

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



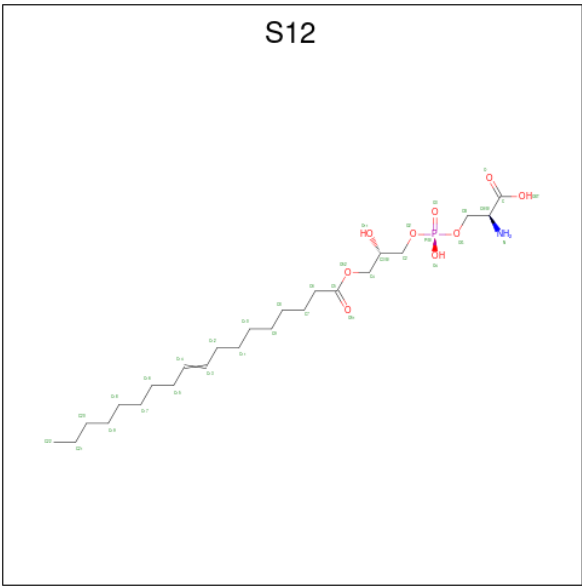
Mol	Chain	Residues	Atoms				AltConf
11	2	1	Total	C	O	P	0
			45	34	10	1	
11	K	1	Total	C	O	P	0
			43	32	10	1	
11	K	1	Total	C	O	P	0
			49	38	10	1	
11	R	1	Total	C	O	P	0
			49	38	10	1	
11	S	1	Total	C	O	P	0
			49	38	10	1	
11	S	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
12	N	1	Total	C	O	P	0
			92	73	17	2	
12	R	1	Total	C	O	P	0
			100	81	17	2	
12	R	1	Total	C	O	P	0
			88	69	17	2	

- Molecule 13 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).

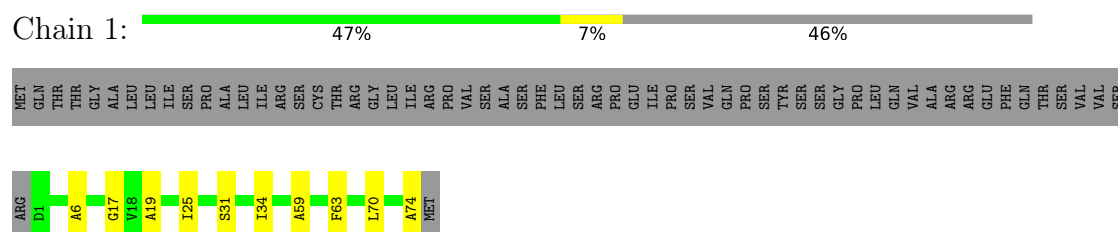


Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			35	24	1	9	1	

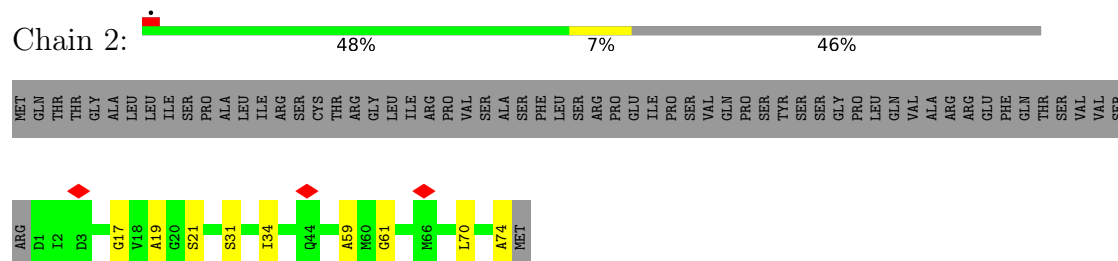
3 Residue-property plots [i](#)

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

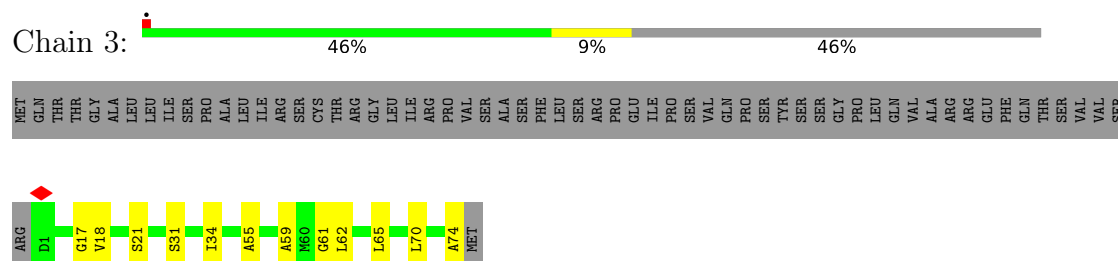
- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial



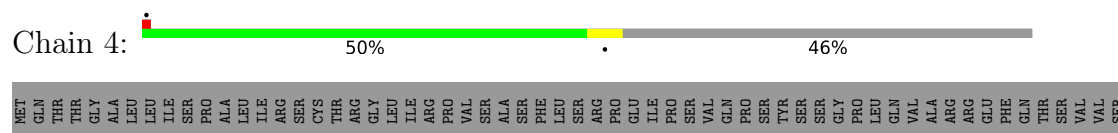
- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial

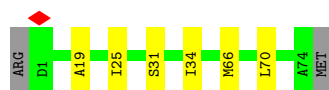


- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial

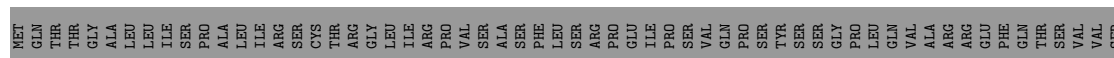


- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial

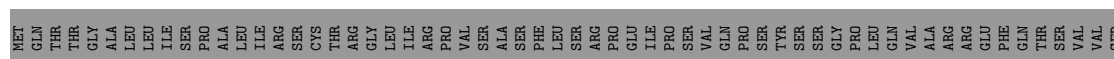




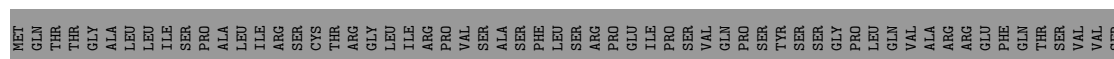
- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial



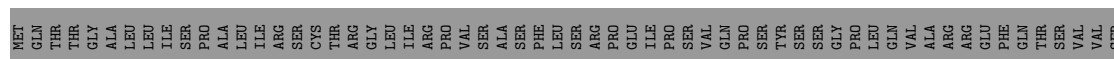
- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial



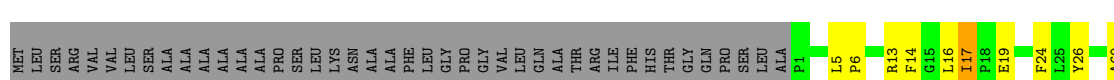
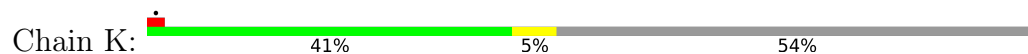
- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial

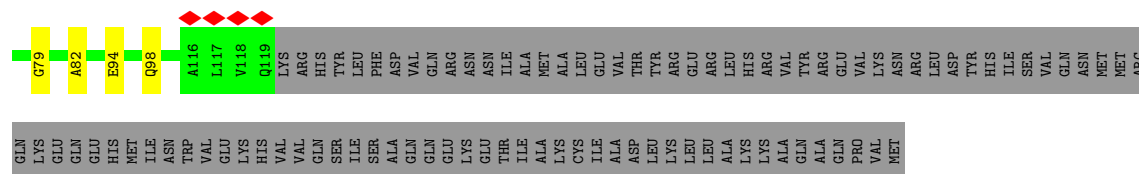


- Molecule 1: ATP synthase F(0) complex subunit C1, mitochondrial

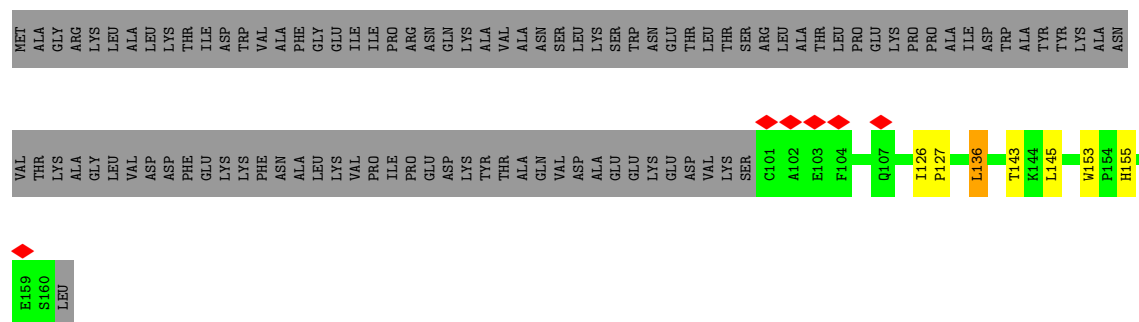


- Molecule 2: ATP synthase subunit b

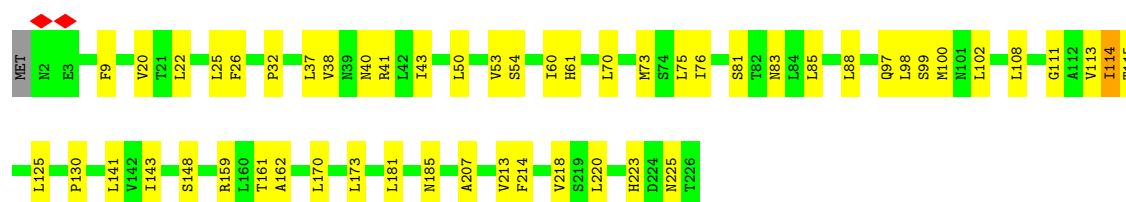
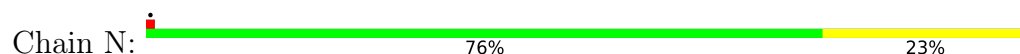




- Molecule 3: ATP synthase subunit d, mitochondrial



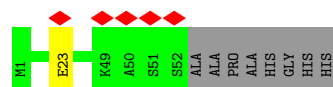
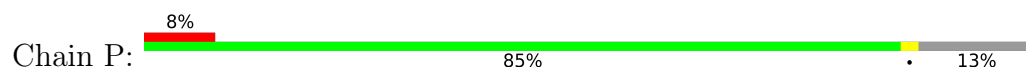
- Molecule 4: ATP synthase subunit a



- Molecule 5: ATP synthase membrane subunit DAPIT

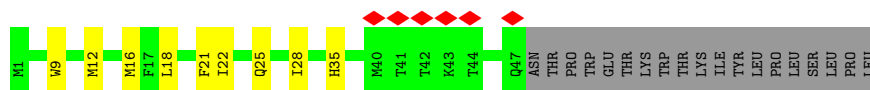


- Molecule 6: ATP synthase membrane subunit 6.8PL

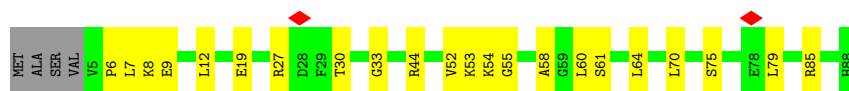


- Molecule 7: ATP synthase protein 8





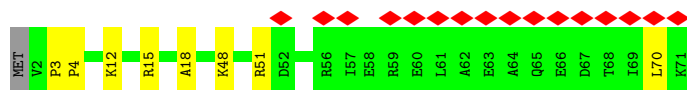
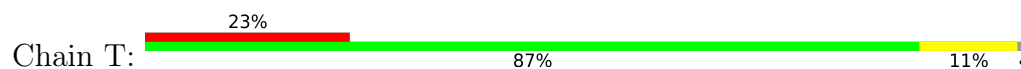
- Molecule 8: ATP synthase membrane subunit f



- Molecule 9: ATP synthase subunit



- Molecule 10: ATP synthase subunit e, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	217266	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 ($e^-/\text{\AA}^2$)	106	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	131951	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.329	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	106.1, 122.015, 129.442	wwPDB
Map dimensions	122, 115, 100	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CDL, S12

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	1	0.31	0/535	0.58	0/722
1	2	0.31	0/535	0.61	0/722
1	3	0.33	0/535	0.64	0/722
1	4	0.30	0/535	0.63	0/722
1	5	0.28	0/535	0.59	0/722
1	6	0.31	0/535	0.61	0/722
1	7	0.30	0/535	0.55	0/722
1	8	0.28	0/535	0.56	0/722
2	K	0.28	0/954	0.61	0/1292
3	M	0.27	0/532	0.57	0/716
4	N	0.38	0/1772	0.64	0/2421
5	O	0.21	0/335	0.50	0/450
6	P	0.29	0/435	0.54	0/585
7	Q	0.34	0/381	0.63	0/518
8	R	0.37	0/719	0.68	0/963
9	S	0.31	0/691	0.63	0/940
10	T	0.28	0/585	0.62	0/780
All	All	0.32	0/10684	0.61	0/14441

There are no bond length outliers.

There are no bond angle outliers.

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	1	526	0	544	6	0
1	2	526	0	544	6	0
1	3	526	0	544	10	0
1	4	526	0	544	4	0
1	5	526	0	544	6	0
1	6	526	0	544	6	0
1	7	526	0	544	6	0
1	8	526	0	544	8	0
2	K	933	0	962	12	0
3	M	519	0	515	5	0
4	N	1734	0	1856	44	0
5	O	327	0	337	2	0
6	P	425	0	455	1	0
7	Q	371	0	357	11	0
8	R	701	0	726	17	0
9	S	673	0	701	14	0
10	T	577	0	601	6	0
11	2	45	0	63	0	0
11	K	92	0	133	0	0
11	R	49	0	74	2	0
11	S	98	0	148	4	0
12	N	92	0	137	6	0
12	R	188	0	285	11	0
13	T	35	0	44	0	0
All	All	11067	0	11746	134	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 6.

All (134) 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)
1:5:70:LEU:O	1:5:74:ALA:HB3	1.90	0.70
1:6:70:LEU:O	1:6:74:ALA:HB3	1.92	0.70
12:R:301:CDL:H851	12:R:301:CDL:H381	1.75	0.68
1:1:70:LEU:O	1:1:74:ALA:HB3	1.94	0.67
1:2:70:LEU:O	1:2:74:ALA:HB3	1.98	0.64
2:K:79:GLY:O	4:N:41:ARG:NH2	2.29	0.63
9:S:87:PHE:HB2	10:T:18:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:PRO:HG2	8:R:52:VAL:HG12	1.82	0.62
4:N:97:GLN:HG3	7:Q:12:MET:HE3	1.82	0.61
1:7:19:ALA:HB2	1:8:17:GLY:HA2	1.81	0.61
7:Q:21:PHE:O	7:Q:25:GLN:CB	2.49	0.60
1:4:31:SER:HA	1:4:34:ILE:HG22	1.82	0.59
4:N:41:ARG:NE	8:R:54:LYS:O	2.32	0.59
4:N:25:LEU:HD21	7:Q:18:LEU:HD12	1.84	0.59
9:S:41:PRO:HG3	10:T:12:LYS:HE2	1.85	0.59
1:6:31:SER:HA	1:6:34:ILE:HG22	1.83	0.59
1:1:31:SER:HA	1:1:34:ILE:HG22	1.83	0.59
12:R:301:CDL:H552	12:R:301:CDL:H422	1.83	0.59
2:K:16:LEU:HD12	2:K:17:ILE:HG23	1.85	0.59
5:O:23:THR:HG23	5:O:26:GLY:H	1.69	0.58
1:7:31:SER:HA	1:7:34:ILE:HG22	1.85	0.58
1:1:19:ALA:HB2	1:2:17:GLY:HA2	1.86	0.58
1:2:31:SER:HA	1:2:34:ILE:HG22	1.86	0.58
4:N:25:LEU:HB3	12:N:401:CDL:H341	1.85	0.58
1:5:31:SER:HA	1:5:34:ILE:HG22	1.85	0.58
4:N:98:LEU:O	4:N:102:LEU:HB2	2.05	0.57
7:Q:21:PHE:O	7:Q:25:GLN:HB2	2.05	0.57
12:N:401:CDL:H181	12:R:302:CDL:H601	1.87	0.56
1:4:66:MET:HG2	4:N:170:LEU:HD13	1.87	0.56
4:N:37:LEU:HD23	4:N:38:VAL:HG13	1.85	0.56
8:R:75:SER:O	8:R:79:LEU:N	2.39	0.56
8:R:7:LEU:HD21	8:R:19:GLU:HB3	1.88	0.56
8:R:60:LEU:HD22	12:R:301:CDL:H731	1.87	0.56
1:4:19:ALA:HB2	1:5:17:GLY:HA2	1.89	0.55
1:8:7:LYS:NZ	1:8:72:LEU:O	2.40	0.55
2:K:14:PHE:HD2	2:K:17:ILE:HD11	1.72	0.55
1:3:31:SER:HA	1:3:34:ILE:HG22	1.89	0.55
4:N:50:LEU:HD21	7:Q:28:ILE:HG23	1.88	0.54
9:S:92:ILE:HD12	9:S:95:LYS:HD3	1.89	0.54
8:R:30:THR:HG23	8:R:33:GLY:H	1.72	0.54
1:3:59:ALA:HB1	4:N:159:ARG:HB2	1.89	0.54
1:3:70:LEU:O	1:3:74:ALA:HB3	2.07	0.53
2:K:94:GLU:HG3	2:K:98:GLN:HE22	1.73	0.53
12:R:302:CDL:H322	12:R:302:CDL:H531	1.90	0.53
4:N:9:PHE:O	4:N:97:GLN:NE2	2.41	0.53
4:N:83:ASN:HB3	4:N:207:ALA:HB1	1.90	0.53
1:8:70:LEU:O	1:8:74:ALA:HB3	2.08	0.53
12:N:401:CDL:H621	7:Q:22:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:22:LEU:HD12	12:N:401:CDL:H372	1.91	0.53
12:N:401:CDL:H442	8:R:70:LEU:HB3	1.91	0.52
1:7:65:LEU:HD11	1:8:67:VAL:HG21	1.92	0.52
1:5:37:ALA:O	1:6:39:ASN:ND2	2.43	0.51
4:N:111:GLY:O	4:N:115:THR:OG1	2.25	0.51
8:R:8:LYS:O	8:R:27:ARG:NH2	2.44	0.50
4:N:54:SER:HA	4:N:73:MET:HE3	1.92	0.50
4:N:26:PHE:HD2	4:N:85:LEU:HD21	1.75	0.50
2:K:13:ARG:NH1	2:K:19:GLU:OE1	2.45	0.50
7:Q:21:PHE:O	7:Q:25:GLN:HB3	2.11	0.50
9:S:92:ILE:HD11	9:S:98:ILE:HA	1.94	0.50
4:N:73:MET:HA	4:N:76:ILE:HG22	1.95	0.49
12:N:401:CDL:H382	12:N:401:CDL:H211	1.93	0.49
1:1:17:GLY:HA2	1:8:19:ALA:HB2	1.94	0.49
1:8:31:SER:HA	1:8:34:ILE:HG22	1.95	0.49
12:R:301:CDL:H132	12:R:301:CDL:H312	1.94	0.49
4:N:100:MET:HG3	7:Q:16:MET:HG3	1.94	0.49
8:R:44:ARG:NH2	11:R:303:LHG:O8	2.46	0.49
9:S:58:ASN:O	9:S:62:THR:OG1	2.29	0.48
2:K:26:TYR:OH	10:T:3:PRO:O	2.28	0.48
4:N:81:SER:O	4:N:85:LEU:HB2	2.13	0.48
1:5:12:GLY:HA2	1:6:14:ALA:HB2	1.96	0.48
4:N:75:LEU:HD21	4:N:214:PHE:HD2	1.79	0.48
8:R:75:SER:HB3	8:R:79:LEU:HD13	1.95	0.48
3:M:145:LEU:HB3	3:M:155:HIS:HB2	1.95	0.47
9:S:64:SER:HB2	9:S:66:LYS:HG2	1.96	0.47
10:T:48:LYS:HD2	10:T:51:ARG:HD2	1.97	0.47
1:7:59:ALA:O	1:7:63:PHE:HB2	2.15	0.47
8:R:58:ALA:HA	8:R:61:SER:HB3	1.97	0.47
1:2:19:ALA:HB2	1:3:17:GLY:HA2	1.96	0.47
8:R:12:LEU:H	11:R:303:LHG:HC11	1.80	0.47
1:5:65:LEU:HD11	1:6:67:VAL:HG21	1.97	0.46
3:M:143:THR:HA	7:Q:35:HIS:HB2	1.97	0.46
4:N:20:VAL:HG21	7:Q:12:MET:HE1	1.96	0.46
12:R:301:CDL:H602	12:R:301:CDL:H762	1.98	0.46
1:3:62:LEU:HD13	1:3:62:LEU:HA	1.75	0.46
4:N:108:LEU:HD23	4:N:218:VAL:HG11	1.98	0.46
4:N:181:LEU:O	4:N:185:ASN:N	2.44	0.46
2:K:60:ALA:HB1	12:R:301:CDL:H232	1.98	0.46
2:K:82:ALA:HB3	4:N:41:ARG:HH21	1.80	0.46
9:S:33:TYR:HD1	10:T:4:PRO:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:130:PRO:HD2	4:N:141:LEU:HD11	1.97	0.45
9:S:58:ASN:HA	9:S:61:LYS:HG2	1.98	0.45
1:3:21:SER:HB2	1:3:61:GLY:HA3	1.98	0.45
3:M:153:TRP:HB3	4:N:70:LEU:HB2	1.98	0.45
9:S:61:LYS:HG3	9:S:62:THR:HG23	2.00	0.44
12:R:302:CDL:H211	12:R:302:CDL:H351	2.00	0.44
1:6:19:ALA:HB2	1:7:17:GLY:HA2	2.00	0.43
1:3:62:LEU:HD13	1:3:65:LEU:HB3	2.01	0.43
4:N:98:LEU:HA	4:N:161:THR:HG21	2.00	0.43
3:M:126:ILE:HA	3:M:127:PRO:HD3	1.88	0.43
4:N:40:ASN:N	4:N:40:ASN:OD1	2.51	0.43
1:1:6:ALA:HB1	1:8:9:ILE:HG13	2.00	0.42
4:N:60:ILE:HG13	4:N:61:HIS:CD2	2.54	0.42
4:N:125:LEU:HD21	5:O:32:LEU:HD21	2.01	0.42
4:N:32:PRO:HG2	4:N:43:ILE:HD11	2.01	0.42
4:N:114:ILE:HD11	6:P:23:GLU:HA	2.02	0.42
8:R:52:VAL:HG23	8:R:55:GLY:H	1.85	0.42
8:R:6:PRO:HG2	8:R:9:GLU:HB2	2.02	0.42
2:K:5:LEU:HB2	8:R:53:LYS:HG3	2.01	0.42
4:N:99:SER:HB3	7:Q:9:TRP:CD1	2.55	0.42
4:N:113:VAL:HA	4:N:225:ASN:HD21	1.85	0.42
9:S:56:ILE:HD11	11:S:202:LHG:H101	2.02	0.42
4:N:53:VAL:HG12	4:N:73:MET:HE1	2.02	0.42
1:4:70:LEU:HD12	4:N:173:LEU:HD11	2.01	0.41
4:N:88:LEU:HD23	4:N:88:LEU:HA	1.86	0.41
11:S:202:LHG:H142	11:S:202:LHG:H112	1.80	0.41
1:1:59:ALA:O	1:1:63:PHE:HB2	2.21	0.41
1:7:54:PHE:CE1	1:8:56:LEU:HD23	2.56	0.41
9:S:83:VAL:HG13	10:T:15:ARG:HA	2.03	0.41
11:S:201:LHG:HC62	11:S:201:LHG:H242	1.72	0.41
2:K:14:PHE:HD1	12:R:301:CDL:H122	1.86	0.41
2:K:24:PHE:HE1	9:S:71:LYS:HG3	1.85	0.41
4:N:50:LEU:HD11	4:N:73:MET:HB3	2.03	0.41
1:2:21:SER:HB2	1:2:61:GLY:HA3	2.03	0.41
1:3:55:ALA:HB3	4:N:213:VAL:HG21	2.02	0.41
4:N:88:LEU:HD11	8:R:64:LEU:HD22	2.02	0.41
12:R:301:CDL:H751	12:R:301:CDL:H781	1.83	0.41
9:S:76:ASN:HB3	11:S:202:LHG:H111	2.03	0.41
4:N:61:HIS:NE2	4:N:223:HIS:HB2	2.36	0.40
1:2:59:ALA:HB2	4:N:148:SER:HB2	2.02	0.40
1:3:18:VAL:HG21	1:3:65:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:136:LEU:HD13	3:M:143:THR:HG21	2.03	0.40
8:R:85:ARG:NH2	9:S:99:ILE:O	2.54	0.40
1:3:62:LEU:HB3	4:N:162:ALA:HB1	2.03	0.40
4:N:143:ILE:HD13	4:N:143:ILE:HA	1.96	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	1	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
1	2	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
1	3	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
1	4	72/136 (53%)	69 (96%)	3 (4%)	0	100	100
1	5	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
1	6	72/136 (53%)	72 (100%)	0	0	100	100
1	7	72/136 (53%)	72 (100%)	0	0	100	100
1	8	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
2	K	117/256 (46%)	107 (92%)	10 (8%)	0	100	100
3	M	58/161 (36%)	54 (93%)	4 (7%)	0	100	100
4	N	223/226 (99%)	213 (96%)	10 (4%)	0	100	100
5	O	38/58 (66%)	37 (97%)	1 (3%)	0	100	100
6	P	50/60 (83%)	49 (98%)	1 (2%)	0	100	100
7	Q	45/66 (68%)	41 (91%)	4 (9%)	0	100	100
8	R	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
9	S	83/103 (81%)	76 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	T	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	1340/2177 (62%)	1287 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1	50/105 (48%)	49 (98%)	1 (2%)	48	64
1	2	50/105 (48%)	50 (100%)	0	100	100
1	3	50/105 (48%)	50 (100%)	0	100	100
1	4	50/105 (48%)	49 (98%)	1 (2%)	48	64
1	5	50/105 (48%)	49 (98%)	1 (2%)	48	64
1	6	50/105 (48%)	50 (100%)	0	100	100
1	7	50/105 (48%)	50 (100%)	0	100	100
1	8	50/105 (48%)	50 (100%)	0	100	100
2	K	102/218 (47%)	101 (99%)	1 (1%)	68	73
3	M	59/144 (41%)	58 (98%)	1 (2%)	53	67
4	N	197/198 (100%)	195 (99%)	2 (1%)	68	73
5	O	35/47 (74%)	35 (100%)	0	100	100
6	P	45/49 (92%)	45 (100%)	0	100	100
7	Q	39/66 (59%)	39 (100%)	0	100	100
8	R	73/76 (96%)	73 (100%)	0	100	100
9	S	71/84 (84%)	71 (100%)	0	100	100
10	T	59/60 (98%)	58 (98%)	1 (2%)	53	67
All	All	1080/1782 (61%)	1072 (99%)	8 (1%)	73	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	25	ILE
1	4	25	ILE
1	5	25	ILE
2	K	17	ILE
3	M	136	LEU
4	N	114	ILE
4	N	220	LEU
10	T	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	98	GLN
2	K	115	GLN
4	N	225	ASN
10	T	6	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
11	LHG	K	301	-	42,42,48	0.63	0	45,48,54	1.22	4 (8%)
11	LHG	2	101	-	44,44,48	0.64	0	47,50,54	1.32	6 (12%)
11	LHG	S	201	-	48,48,48	0.67	0	51,54,54	1.32	6 (11%)
11	LHG	S	202	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
13	S12	T	201	-	33,34,34	0.70	1 (3%)	34,40,40	0.42	0
12	CDL	R	302	-	87,87,99	1.08	6 (6%)	93,99,111	1.02	13 (13%)
11	LHG	R	303	-	48,48,48	0.72	2 (4%)	51,54,54	1.26	6 (11%)
11	LHG	K	302	-	48,48,48	0.65	1 (2%)	51,54,54	1.30	7 (13%)
12	CDL	N	401	-	91,91,99	1.08	7 (7%)	97,103,111	0.98	12 (12%)
12	CDL	R	301	-	99,99,99	1.15	8 (8%)	105,111,111	1.02	16 (15%)

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
11	LHG	K	301	-	-	30/47/47/53	-
11	LHG	2	101	-	-	27/49/49/53	-
11	LHG	S	201	-	-	26/53/53/53	-
11	LHG	S	202	-	-	28/53/53/53	-
13	S12	T	201	-	-	12/38/38/38	-
12	CDL	R	302	-	2/2/9/9	38/98/98/110	-
11	LHG	R	303	-	-	32/53/53/53	-
11	LHG	K	302	-	-	20/53/53/53	-
12	CDL	N	401	-	1/1/9/9	38/102/102/110	-
12	CDL	R	301	-	1/1/9/9	39/110/110/110	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	301	CDL	C39-C38	-4.04	1.31	1.51
12	R	302	CDL	C62-C61	-4.01	1.31	1.51
12	R	301	CDL	C42-C41	-3.99	1.31	1.51
12	N	401	CDL	C59-C58	-3.98	1.32	1.51
12	N	401	CDL	C42-C41	-3.98	1.32	1.51
12	R	301	CDL	C22-C21	-3.97	1.32	1.51
12	R	302	CDL	C19-C18	-3.96	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	302	CDL	C59-C58	-3.94	1.32	1.51
12	N	401	CDL	C22-C21	-3.92	1.32	1.51
12	R	301	CDL	C59-C58	-3.91	1.32	1.51
12	R	301	CDL	C19-C18	-3.91	1.32	1.51
12	R	301	CDL	C82-C81	-3.90	1.32	1.51
12	N	401	CDL	C39-C38	-3.90	1.32	1.51
12	R	302	CDL	C42-C41	-3.90	1.32	1.51
12	R	302	CDL	C22-C21	-3.89	1.32	1.51
12	N	401	CDL	C19-C18	-3.89	1.32	1.51
12	R	301	CDL	C79-C78	-3.89	1.32	1.51
12	R	301	CDL	C62-C61	-3.89	1.32	1.51
12	R	302	CDL	C39-C38	-3.87	1.32	1.51
12	N	401	CDL	C62-C61	-3.86	1.32	1.51
13	T	201	S12	C14-C13	3.72	1.52	1.31
11	R	303	LHG	O7-C5	-2.77	1.40	1.46
12	N	401	CDL	C79-C78	-2.55	1.32	1.50
11	K	302	LHG	O7-C5	-2.38	1.41	1.46
11	R	303	LHG	P-O6	2.35	1.68	1.59
11	S	202	LHG	O7-C5	-2.35	1.41	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	101	LHG	O4-P-O5	4.47	133.26	112.44
11	K	301	LHG	O4-P-O5	4.44	133.11	112.44
11	K	302	LHG	O4-P-O5	4.43	133.03	112.44
11	S	202	LHG	O4-P-O5	4.41	132.98	112.44
11	S	201	LHG	O4-P-O5	4.40	132.89	112.44
11	R	303	LHG	O4-P-O5	4.25	132.22	112.44
11	S	201	LHG	O8-C23-C24	3.30	121.89	111.83
11	K	302	LHG	O8-C23-C24	2.99	120.94	111.83
11	S	201	LHG	C11-C10-C9	-2.82	100.13	114.37
11	S	202	LHG	O8-C23-C24	2.80	120.38	111.83
11	2	101	LHG	O8-C23-C24	2.67	119.96	111.83
11	R	303	LHG	O8-C23-C24	2.64	119.89	111.83
12	R	302	CDL	C62-C61-C60	2.64	127.72	114.37
12	R	301	CDL	C62-C61-C60	2.63	127.65	114.37
12	N	401	CDL	C40-C39-C38	2.62	127.59	114.37
12	R	302	CDL	C40-C39-C38	2.61	127.56	114.37
12	N	401	CDL	C22-C21-C20	2.60	127.52	114.37
12	N	401	CDL	C23-C22-C21	2.59	127.47	114.37
12	R	302	CDL	C22-C21-C20	2.58	127.41	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	301	LHG	O8-C23-C24	2.57	119.69	111.83
11	R	303	LHG	C11-C10-C9	-2.55	101.48	114.37
12	R	301	CDL	C60-C59-C58	2.54	127.22	114.37
12	R	302	CDL	C60-C59-C58	2.54	127.19	114.37
11	2	101	LHG	C11-C10-C9	-2.52	101.61	114.37
12	R	302	CDL	C20-C19-C18	2.50	127.01	114.37
12	R	301	CDL	C22-C21-C20	2.49	126.97	114.37
12	N	401	CDL	C63-C62-C61	2.48	126.89	114.37
12	N	401	CDL	C39-C38-C37	2.48	126.89	114.37
12	N	401	CDL	C62-C61-C60	2.45	126.77	114.37
11	2	101	LHG	C20-C19-C18	-2.45	101.97	114.37
12	R	301	CDL	C79-C78-C77	2.45	126.76	114.37
12	R	301	CDL	C19-C18-C17	2.45	126.75	114.37
12	R	302	CDL	C42-C41-C40	2.45	126.74	114.37
12	R	301	CDL	C80-C79-C78	2.44	126.72	114.37
12	R	301	CDL	C40-C39-C38	2.44	126.72	114.37
12	R	301	CDL	C42-C41-C40	2.44	126.70	114.37
12	N	401	CDL	C19-C18-C17	2.44	126.69	114.37
11	K	302	LHG	C11-C10-C9	-2.43	102.07	114.37
12	N	401	CDL	C20-C19-C18	2.43	126.66	114.37
12	R	301	CDL	C82-C81-C80	2.43	126.65	114.37
11	R	303	LHG	C20-C19-C18	-2.41	102.19	114.37
12	R	301	CDL	C20-C19-C18	2.41	126.53	114.37
11	K	301	LHG	C11-C10-C9	-2.40	102.23	114.37
12	N	401	CDL	C42-C41-C40	2.40	126.50	114.37
12	R	302	CDL	C19-C18-C17	2.39	126.47	114.37
12	N	401	CDL	C60-C59-C58	2.36	126.31	114.37
12	R	301	CDL	C59-C58-C57	2.35	126.25	114.37
11	S	201	LHG	C20-C19-C18	-2.35	102.50	114.37
11	K	302	LHG	C20-C19-C18	-2.35	102.50	114.37
12	R	302	CDL	C43-C42-C41	2.35	126.23	114.37
11	S	202	LHG	C20-C19-C18	-2.32	102.62	114.37
12	R	301	CDL	C23-C22-C21	2.32	126.10	114.37
12	R	302	CDL	C59-C58-C57	2.31	126.05	114.37
11	S	202	LHG	C11-C10-C9	-2.31	102.70	114.37
12	R	302	CDL	C63-C62-C61	2.29	125.93	114.37
12	N	401	CDL	C59-C58-C57	2.27	125.84	114.37
11	S	201	LHG	C27-C26-C25	-2.26	102.94	114.37
12	R	301	CDL	C43-C42-C41	2.24	125.70	114.37
12	R	302	CDL	C23-C22-C21	2.24	125.70	114.37
11	K	301	LHG	C27-C26-C25	-2.24	103.07	114.37
11	K	302	LHG	C18-C17-C16	-2.23	103.10	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	302	LHG	C5-O7-C7	-2.23	112.46	117.80
11	2	101	LHG	C18-C17-C16	-2.22	103.15	114.37
12	R	301	CDL	C63-C62-C61	2.22	125.58	114.37
11	R	303	LHG	C18-C17-C16	-2.21	103.18	114.37
11	S	202	LHG	C18-C17-C16	-2.21	103.21	114.37
11	S	201	LHG	C18-C17-C16	-2.19	103.28	114.37
12	N	401	CDL	C43-C42-C41	2.19	125.43	114.37
12	R	301	CDL	C83-C82-C81	2.17	125.32	114.37
11	S	202	LHG	C27-C26-C25	-2.16	103.43	114.37
12	R	302	CDL	C39-C38-C37	2.16	125.29	114.37
11	R	303	LHG	C27-C26-C25	-2.16	103.45	114.37
12	R	301	CDL	C39-C38-C37	2.15	125.24	114.37
11	2	101	LHG	C27-C26-C25	-2.05	103.98	114.37
12	R	302	CDL	CB4-OB6-CB5	2.05	122.70	117.80
11	K	302	LHG	C27-C26-C25	-2.02	104.18	114.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	N	401	CDL	CB4
12	R	301	CDL	CB4
12	R	302	CDL	CA4
12	R	302	CDL	CB4

All (290) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	2	101	LHG	O1-C1-C2-C3
11	2	101	LHG	C3-O3-P-O6
11	2	101	LHG	C4-O6-P-O3
11	2	101	LHG	C8-C7-O7-C5
11	K	301	LHG	C1-C2-C3-O3
11	K	301	LHG	C3-O3-P-O4
11	K	301	LHG	C3-O3-P-O5
11	K	301	LHG	C3-O3-P-O6
11	K	301	LHG	C4-O6-P-O3
11	K	301	LHG	C4-O6-P-O4
11	K	302	LHG	O1-C1-C2-C3
11	K	302	LHG	C8-C7-O7-C5
11	K	302	LHG	C24-C23-O8-C6
11	R	303	LHG	O1-C1-C2-C3
11	R	303	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
11	R	303	LHG	C3-O3-P-O6
11	R	303	LHG	C4-O6-P-O4
11	R	303	LHG	C4-O6-P-O5
11	S	201	LHG	C3-O3-P-O5
11	S	201	LHG	C3-O3-P-O6
11	S	201	LHG	O7-C5-C6-O8
11	S	201	LHG	O9-C7-O7-C5
11	S	201	LHG	O10-C23-O8-C6
11	S	201	LHG	C24-C23-O8-C6
11	S	202	LHG	O2-C2-C3-O3
11	S	202	LHG	C4-O6-P-O3
12	N	401	CDL	CA3-OA5-PA1-OA2
12	N	401	CDL	CA3-OA5-PA1-OA3
12	N	401	CDL	CA3-OA5-PA1-OA4
12	N	401	CDL	OA6-CA4-CA6-OA8
12	R	301	CDL	O1-C1-CB2-OB2
12	R	301	CDL	CA2-OA2-PA1-OA3
12	R	301	CDL	CA2-OA2-PA1-OA4
12	R	301	CDL	CA2-OA2-PA1-OA5
12	R	301	CDL	CA3-OA5-PA1-OA2
12	R	301	CDL	CA3-OA5-PA1-OA3
12	R	301	CDL	CA3-OA5-PA1-OA4
12	R	301	CDL	CB2-OB2-PB2-OB5
12	R	301	CDL	CB3-OB5-PB2-OB2
12	R	301	CDL	CB3-OB5-PB2-OB3
12	R	302	CDL	CB2-C1-CA2-OA2
12	R	302	CDL	CA2-OA2-PA1-OA4
12	R	302	CDL	CA3-OA5-PA1-OA2
12	R	302	CDL	CA3-OA5-PA1-OA3
12	R	302	CDL	CB2-OB2-PB2-OB4
12	R	302	CDL	CB2-OB2-PB2-OB5
12	R	302	CDL	CB3-OB5-PB2-OB3
12	R	302	CDL	CB3-OB5-PB2-OB4
13	T	201	S12	CB-OG-P-O3
13	T	201	S12	O2-C2-C3-O11
13	T	201	S12	C-CA-CB-OG
13	T	201	S12	N-CA-CB-OG
11	K	302	LHG	O10-C23-O8-C6
11	S	202	LHG	O10-C23-O8-C6
11	2	101	LHG	O9-C7-O7-C5
11	K	301	LHG	O9-C7-O7-C5
11	S	201	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
11	2	101	LHG	O10-C23-O8-C6
11	2	101	LHG	C24-C23-O8-C6
11	S	202	LHG	C24-C23-O8-C6
12	R	301	CDL	C20-C21-C22-C23
12	R	302	CDL	C57-C58-C59-C60
12	N	401	CDL	C40-C41-C42-C43
12	N	401	CDL	C20-C21-C22-C23
12	N	401	CDL	C57-C58-C59-C60
12	R	301	CDL	C37-C38-C39-C40
12	R	301	CDL	C40-C41-C42-C43
12	R	301	CDL	C80-C81-C82-C83
12	N	401	CDL	C37-C38-C39-C40
12	R	302	CDL	O1-C1-CA2-OA2
12	R	302	CDL	C61-C62-C63-C64
11	2	101	LHG	C1-C2-C3-O3
11	S	202	LHG	C1-C2-C3-O3
12	R	301	CDL	CA2-C1-CB2-OB2
11	K	301	LHG	C24-C23-O8-C6
11	K	301	LHG	O2-C2-C3-O3
13	T	201	S12	C12-C13-C14-C15
11	S	202	LHG	O1-C1-C2-O2
12	N	401	CDL	CA5-C11-C12-C13
12	R	301	CDL	C61-C62-C63-C64
11	R	303	LHG	O2-C2-C3-O3
11	S	201	LHG	O2-C2-C3-O3
11	K	301	LHG	C23-C24-C25-C26
12	R	301	CDL	CA7-C31-C32-C33
11	K	301	LHG	C7-C8-C9-C10
11	K	302	LHG	O9-C7-O7-C5
11	R	303	LHG	C1-C2-C3-O3
11	S	201	LHG	C1-C2-C3-O3
11	2	101	LHG	O2-C2-C3-O3
11	S	202	LHG	O1-C1-C2-C3
11	K	301	LHG	C8-C7-O7-C5
11	R	303	LHG	C11-C10-C9-C8
12	R	301	CDL	C36-C37-C38-C39
12	R	302	CDL	C38-C39-C40-C41
12	N	401	CDL	C36-C37-C38-C39
11	S	201	LHG	C32-C33-C34-C35
12	R	302	CDL	C21-C22-C23-C24
12	N	401	CDL	C61-C62-C63-C64
12	R	301	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
11	2	101	LHG	O1-C1-C2-O2
11	K	302	LHG	O1-C1-C2-O2
12	N	401	CDL	C59-C60-C61-C62
12	R	301	CDL	C41-C42-C43-C44
11	S	201	LHG	C7-C8-C9-C10
11	K	302	LHG	C9-C10-C11-C12
11	S	201	LHG	C15-C16-C17-C18
12	R	301	CDL	C39-C40-C41-C42
12	R	302	CDL	C16-C17-C18-C19
11	K	301	LHG	O10-C23-O8-C6
11	K	302	LHG	C32-C33-C34-C35
11	K	302	LHG	C33-C34-C35-C36
11	R	303	LHG	C7-C8-C9-C10
11	2	101	LHG	C9-C10-C11-C12
11	S	202	LHG	C28-C29-C30-C31
11	2	101	LHG	C27-C28-C29-C30
12	N	401	CDL	C16-C17-C18-C19
12	N	401	CDL	C18-C19-C20-C21
11	R	303	LHG	C10-C11-C12-C13
11	K	301	LHG	C31-C32-C33-C34
12	N	401	CDL	C39-C40-C41-C42
11	R	303	LHG	C12-C13-C14-C15
11	S	202	LHG	C23-C24-C25-C26
11	R	303	LHG	C15-C16-C17-C18
11	S	202	LHG	C18-C19-C20-C21
12	N	401	CDL	C62-C63-C64-C65
13	T	201	S12	C6-C7-C8-C9
12	R	302	CDL	C18-C19-C20-C21
12	N	401	CDL	CB5-C51-C52-C53
11	S	201	LHG	C24-C25-C26-C27
11	S	202	LHG	C27-C28-C29-C30
11	S	202	LHG	C8-C7-O7-C5
12	N	401	CDL	C51-CB5-OB6-CB4
11	K	302	LHG	C7-C8-C9-C10
11	R	303	LHG	C24-C25-C26-C27
12	R	302	CDL	C51-C52-C53-C54
11	K	302	LHG	C18-C19-C20-C21
11	R	303	LHG	C29-C30-C31-C32
12	N	401	CDL	C75-C76-C77-C78
11	K	302	LHG	C30-C31-C32-C33
11	R	303	LHG	C27-C28-C29-C30
12	N	401	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
11	S	201	LHG	O6-C4-C5-O7
11	K	301	LHG	C30-C31-C32-C33
11	S	202	LHG	C7-C8-C9-C10
12	R	301	CDL	OA6-CA4-CA6-OA8
13	T	201	S12	C10-C11-C12-C13
11	S	201	LHG	C27-C28-C29-C30
12	R	301	CDL	C56-C57-C58-C59
11	K	301	LHG	C28-C29-C30-C31
11	S	202	LHG	C17-C18-C19-C20
11	R	303	LHG	O1-C1-C2-O2
12	N	401	CDL	OB7-CB5-OB6-CB4
11	S	202	LHG	C11-C10-C9-C8
12	R	302	CDL	CB7-C71-C72-C73
11	K	301	LHG	C4-C5-C6-O8
12	N	401	CDL	CA3-CA4-CA6-OA8
11	K	301	LHG	C26-C27-C28-C29
11	2	101	LHG	C23-C24-C25-C26
11	K	302	LHG	C24-C25-C26-C27
11	S	202	LHG	C9-C10-C11-C12
11	K	302	LHG	C27-C28-C29-C30
11	K	301	LHG	C11-C12-C13-C14
11	S	201	LHG	C10-C11-C12-C13
12	R	302	CDL	C34-C35-C36-C37
11	K	301	LHG	C4-C5-O7-C7
11	R	303	LHG	C28-C29-C30-C31
11	S	202	LHG	C12-C13-C14-C15
12	R	301	CDL	C21-C22-C23-C24
11	R	303	LHG	C30-C31-C32-C33
11	2	101	LHG	C18-C19-C20-C21
11	K	301	LHG	C24-C25-C26-C27
11	K	301	LHG	C27-C28-C29-C30
11	S	202	LHG	C24-C25-C26-C27
11	K	301	LHG	O7-C5-C6-O8
12	N	401	CDL	OB6-CB4-CB6-OB8
11	R	303	LHG	C23-C24-C25-C26
12	R	302	CDL	C58-C59-C60-C61
11	K	301	LHG	C2-C3-O3-P
12	R	302	CDL	C1-CB2-OB2-PB2
11	S	201	LHG	C26-C27-C28-C29
11	R	303	LHG	O6-C4-C5-C6
11	S	201	LHG	O6-C4-C5-C6
12	R	302	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
12	N	401	CDL	C76-C77-C78-C79
11	2	101	LHG	C19-C20-C21-C22
11	R	303	LHG	C16-C17-C18-C19
12	R	301	CDL	C59-C60-C61-C62
13	T	201	S12	O2-C2-C3-C4
12	R	301	CDL	CA3-CA4-CA6-OA8
12	N	401	CDL	C11-C12-C13-C14
12	N	401	CDL	OB5-CB3-CB4-OB6
12	R	302	CDL	OA5-CA3-CA4-OA6
12	R	301	CDL	C35-C36-C37-C38
11	R	303	LHG	C11-C12-C13-C14
11	K	301	LHG	C32-C33-C34-C35
11	K	302	LHG	C19-C20-C21-C22
13	T	201	S12	C11-C12-C13-C14
11	R	303	LHG	C13-C14-C15-C16
11	S	201	LHG	C30-C31-C32-C33
12	R	301	CDL	C81-C82-C83-C84
12	N	401	CDL	C52-C53-C54-C55
12	R	301	CDL	C11-C12-C13-C14
11	K	301	LHG	O6-C4-C5-O7
11	R	303	LHG	O6-C4-C5-O7
11	K	302	LHG	C15-C16-C17-C18
11	S	201	LHG	C4-C5-C6-O8
12	R	302	CDL	C32-C33-C34-C35
11	2	101	LHG	O6-C4-C5-C6
12	N	401	CDL	OB5-CB3-CB4-CB6
11	R	303	LHG	C33-C34-C35-C36
12	R	301	CDL	CB4-CB3-OB5-PB2
11	2	101	LHG	O6-C4-C5-O7
12	R	302	CDL	OB5-CB3-CB4-OB6
11	R	303	LHG	C14-C15-C16-C17
11	S	201	LHG	C11-C10-C9-C8
12	N	401	CDL	CB3-CB4-CB6-OB8
11	R	303	LHG	C19-C20-C21-C22
11	S	201	LHG	C34-C35-C36-C37
11	2	101	LHG	C3-O3-P-O5
11	2	101	LHG	C4-O6-P-O5
11	K	301	LHG	C4-O6-P-O5
11	R	303	LHG	C4-O6-P-O3
11	S	202	LHG	C4-O6-P-O5
12	N	401	CDL	CA2-OA2-PA1-OA3
12	N	401	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
12	N	401	CDL	CA2-OA2-PA1-OA5
12	R	301	CDL	CB2-OB2-PB2-OB3
12	R	302	CDL	CA2-OA2-PA1-OA3
12	R	302	CDL	CA2-OA2-PA1-OA5
12	R	302	CDL	CA3-OA5-PA1-OA4
12	R	302	CDL	CB3-OB5-PB2-OB2
11	S	201	LHG	C29-C30-C31-C32
11	2	101	LHG	C2-C3-O3-P
11	R	303	LHG	C2-C3-O3-P
11	K	301	LHG	O6-C4-C5-C6
11	S	202	LHG	C29-C30-C31-C32
12	R	301	CDL	C84-C85-C86-C87
12	R	301	CDL	C14-C15-C16-C17
12	R	301	CDL	C78-C79-C80-C81
12	N	401	CDL	C71-CB7-OB8-CB6
11	K	302	LHG	C29-C30-C31-C32
12	R	301	CDL	C1-CB2-OB2-PB2
12	R	302	CDL	OB6-CB4-CB6-OB8
11	S	202	LHG	C19-C20-C21-C22
12	R	302	CDL	C41-C42-C43-C44
12	R	302	CDL	C59-C60-C61-C62
12	R	302	CDL	C52-C53-C54-C55
12	R	301	CDL	C79-C80-C81-C82
12	R	301	CDL	C62-C63-C64-C65
11	K	301	LHG	C9-C10-C11-C12
12	N	401	CDL	CA2-C1-CB2-OB2
11	K	302	LHG	C16-C17-C18-C19
11	S	201	LHG	C13-C14-C15-C16
11	S	202	LHG	C16-C17-C18-C19
11	2	101	LHG	C24-C25-C26-C27
13	T	201	S12	C13-C14-C15-C16
12	N	401	CDL	C22-C23-C24-C25
11	S	202	LHG	C15-C16-C17-C18
11	2	101	LHG	C14-C15-C16-C17
11	2	101	LHG	C29-C30-C31-C32
12	R	302	CDL	CA6-CA4-OA6-CA5
11	K	302	LHG	C28-C29-C30-C31
12	N	401	CDL	O1-C1-CB2-OB2
11	R	303	LHG	C25-C26-C27-C28
11	K	302	LHG	O6-C4-C5-C6
12	R	302	CDL	OA5-CA3-CA4-CA6
12	N	401	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
13	T	201	S12	O52-C5-C6-C7
12	N	401	CDL	OB9-CB7-OB8-CB6
11	S	202	LHG	C25-C26-C27-C28
12	R	302	CDL	OA6-CA4-CA6-OA8
11	S	201	LHG	O8-C23-C24-C25
12	R	301	CDL	OA5-CA3-CA4-CA6
12	R	302	CDL	CB6-CB4-OB6-CB5
11	2	101	LHG	C26-C27-C28-C29
11	2	101	LHG	O7-C7-C8-C9
13	T	201	S12	O51-C5-C6-C7
11	S	202	LHG	O8-C23-C24-C25
11	R	303	LHG	C26-C27-C28-C29
11	R	303	LHG	O7-C7-C8-C9
11	2	101	LHG	O9-C7-C8-C9
11	K	301	LHG	O9-C7-C8-C9
11	S	201	LHG	O10-C23-C24-C25
11	S	202	LHG	O9-C7-C8-C9
12	R	302	CDL	C12-C13-C14-C15
12	R	302	CDL	C36-C37-C38-C39
11	S	202	LHG	O10-C23-C24-C25
11	S	202	LHG	O9-C7-O7-C5
11	2	101	LHG	C30-C31-C32-C33
12	R	301	CDL	C52-C51-CB5-OB6

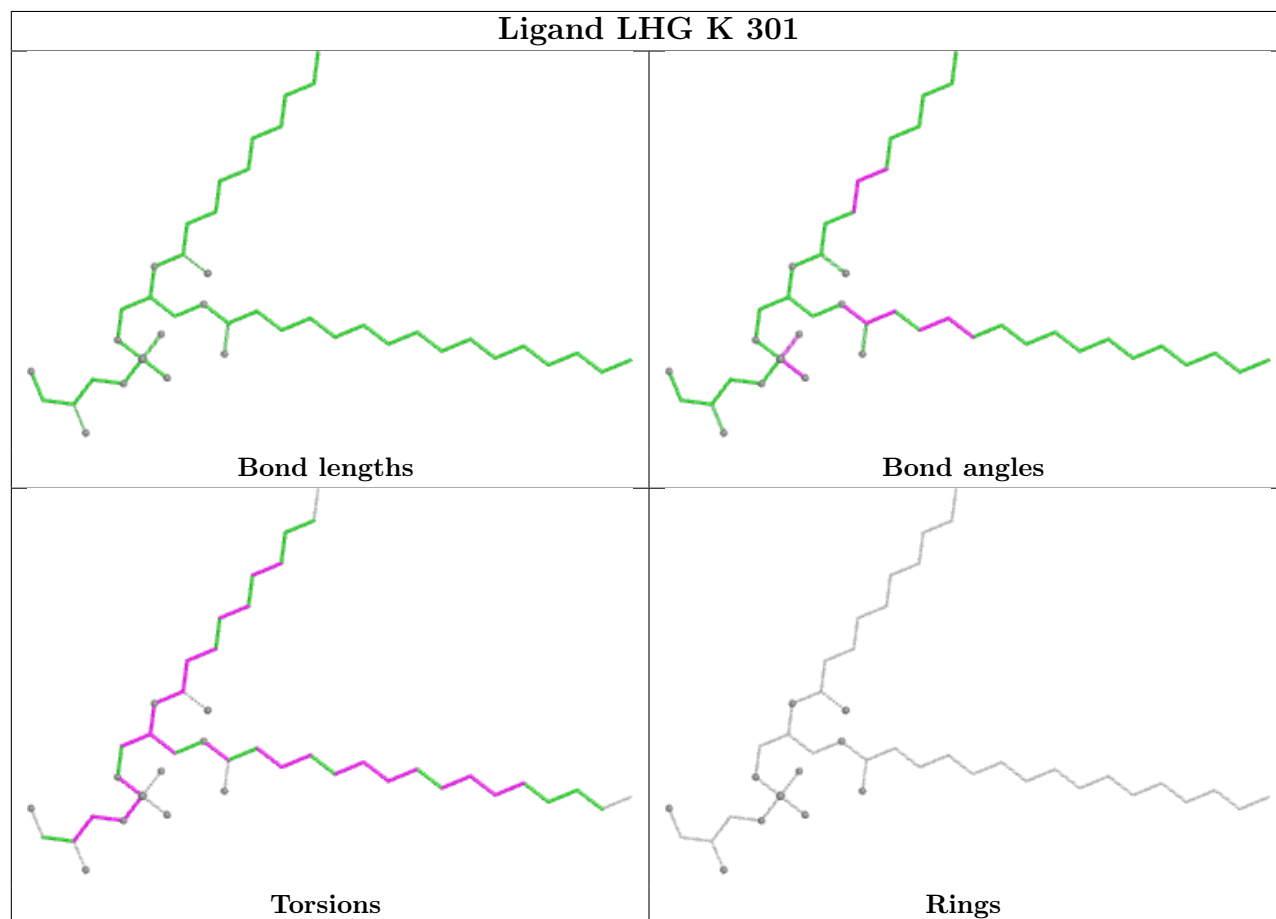
There are no ring outliers.

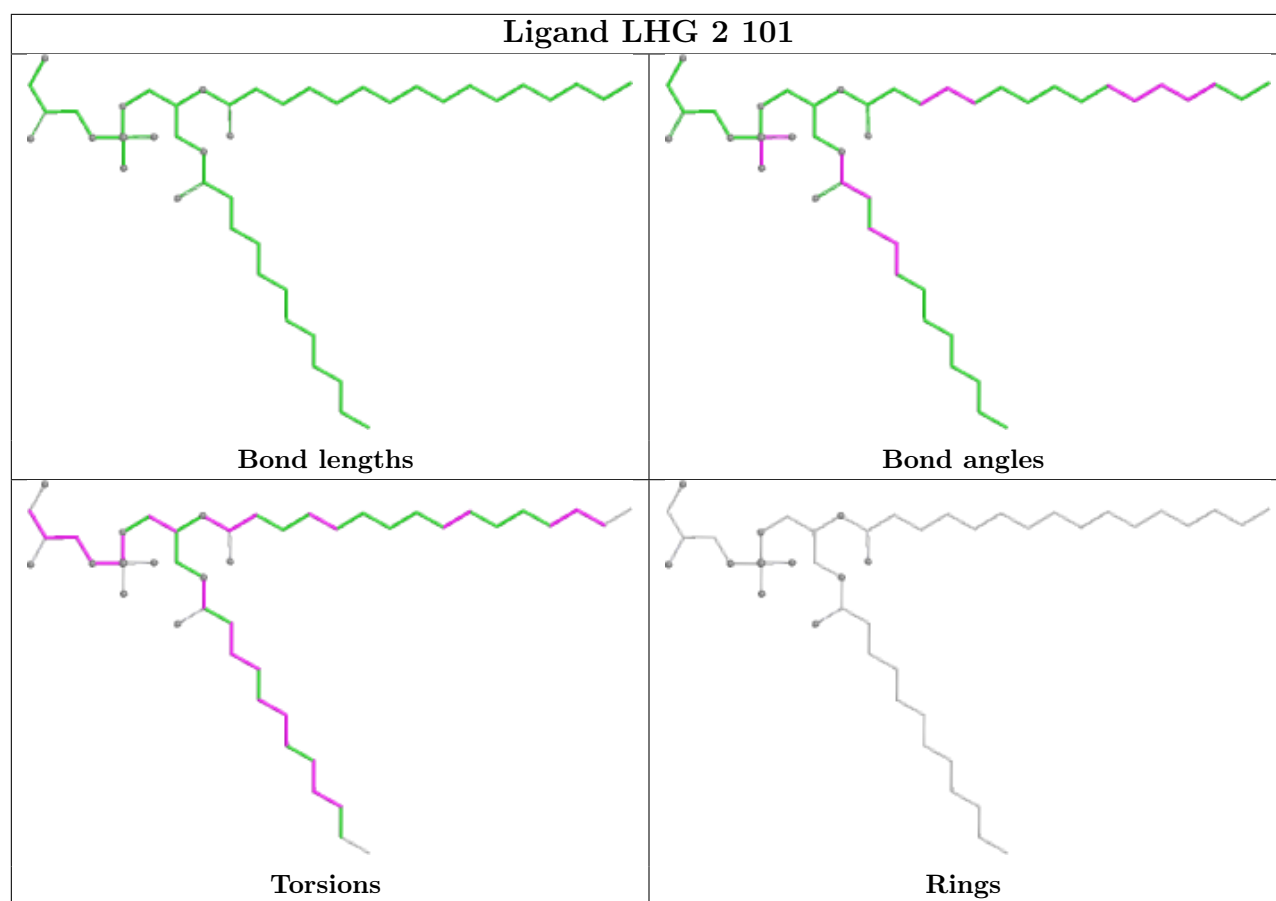
6 monomers are involved in 22 short contacts:

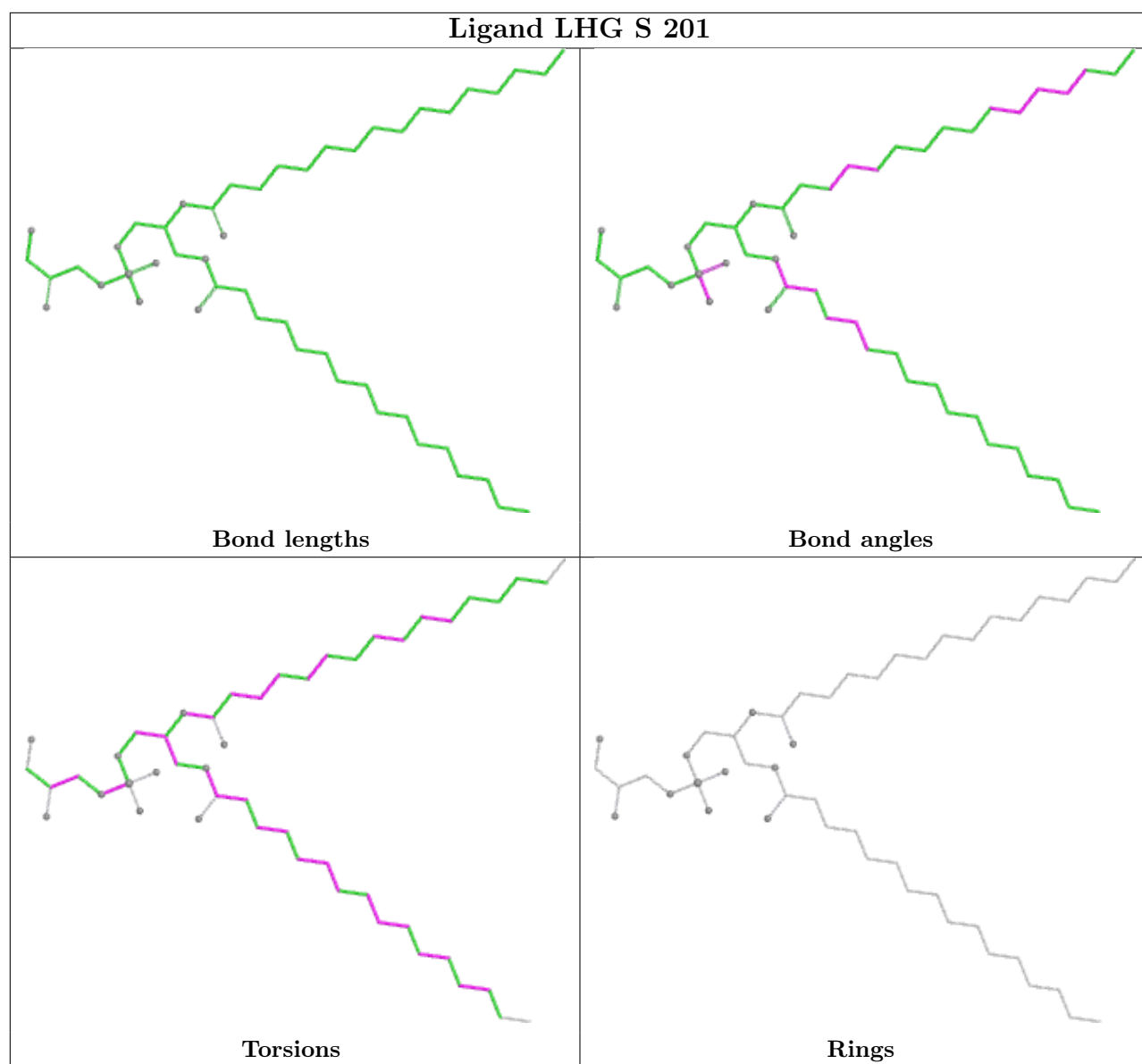
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	201	LHG	1	0
11	S	202	LHG	3	0
12	R	302	CDL	3	0
11	R	303	LHG	2	0
12	N	401	CDL	6	0
12	R	301	CDL	8	0

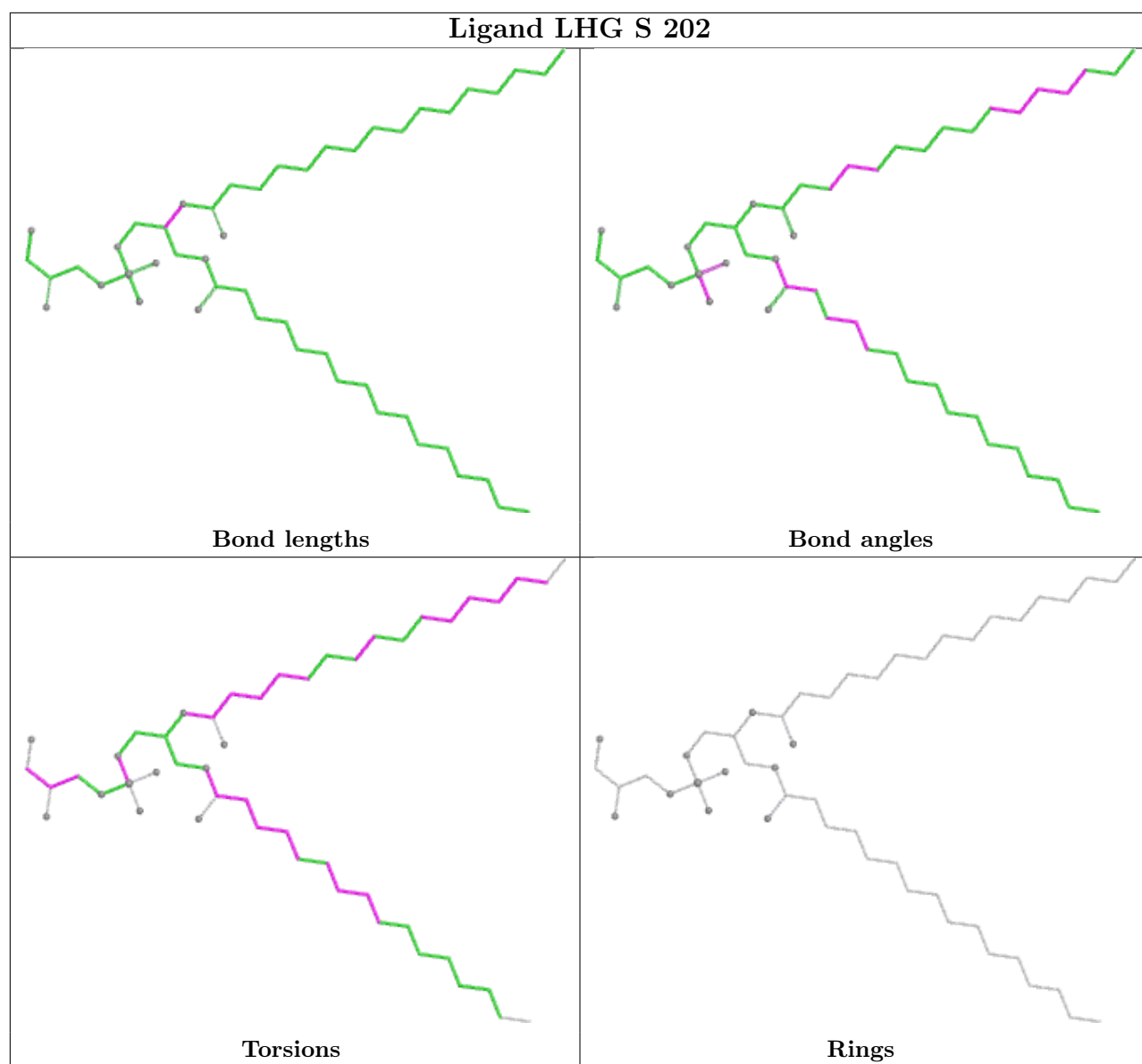
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

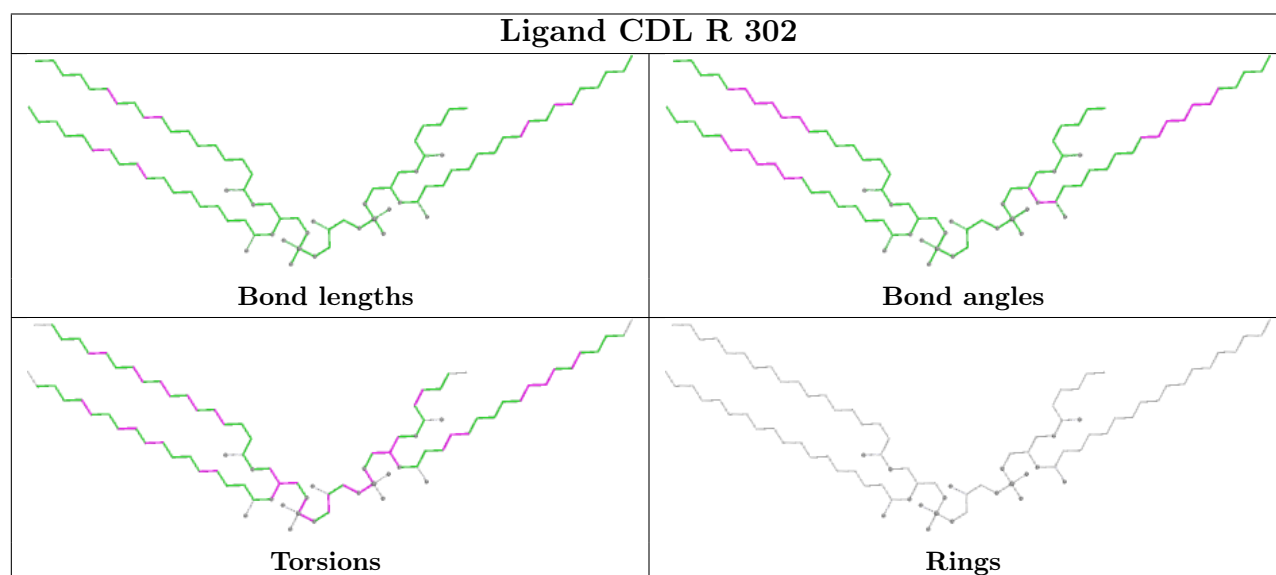
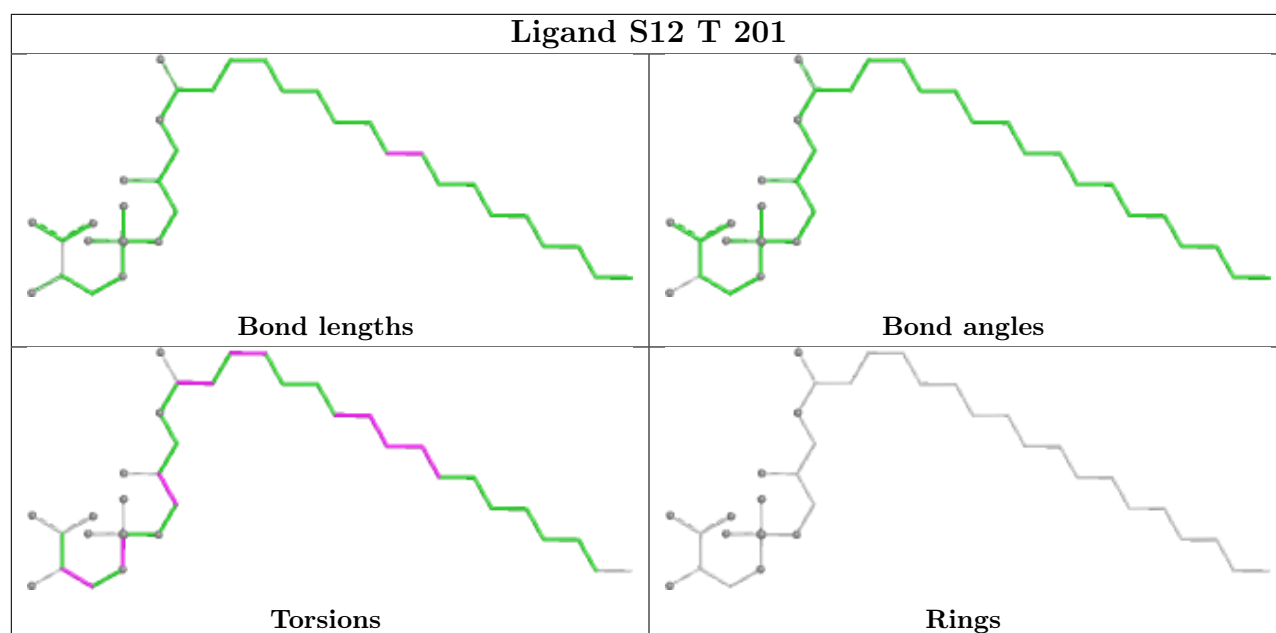
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

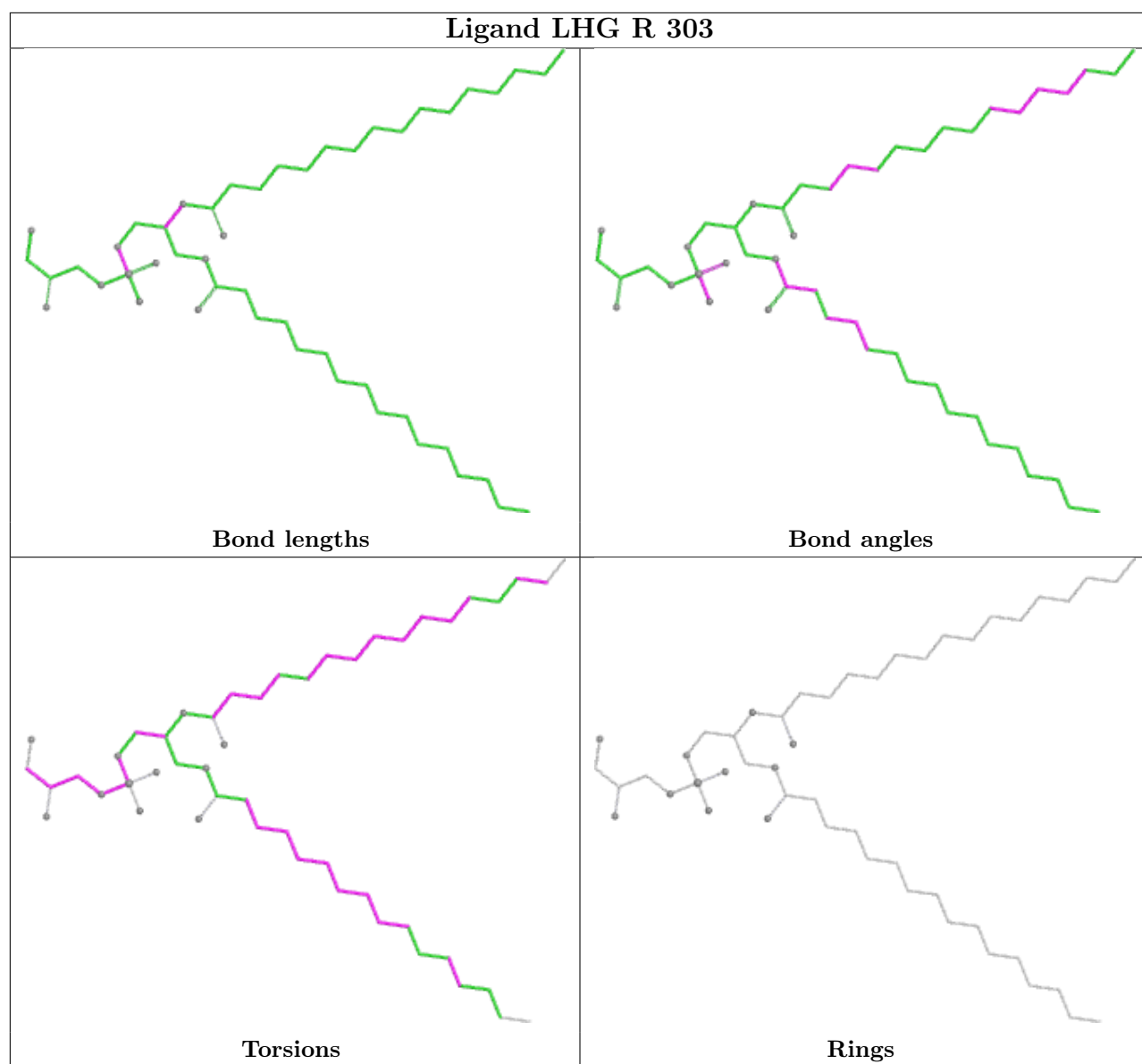


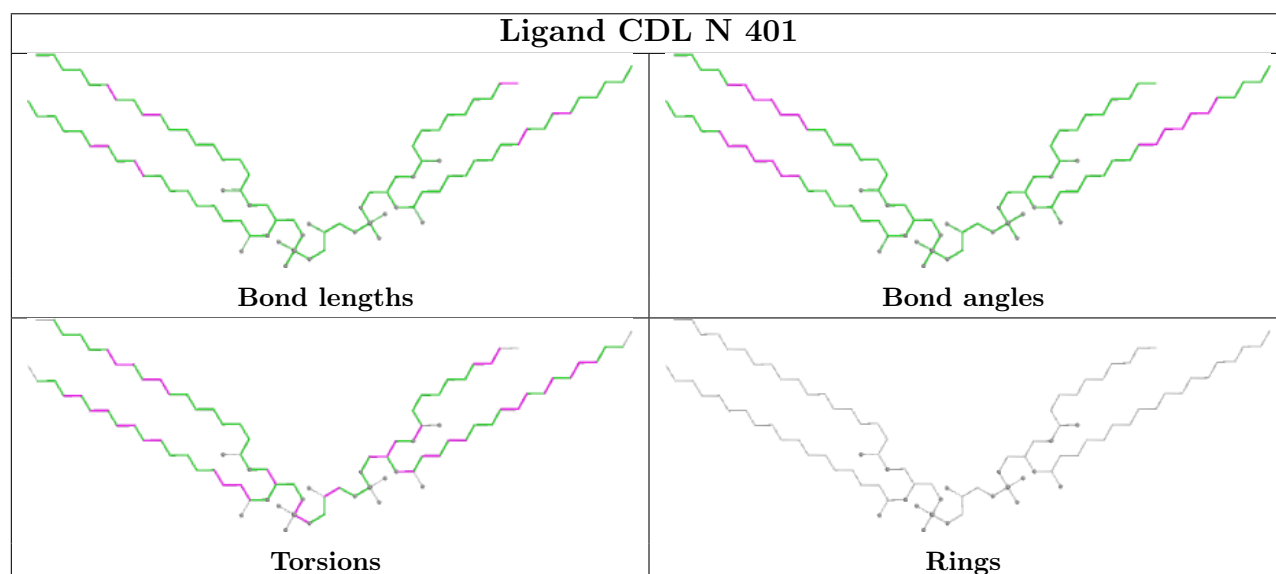
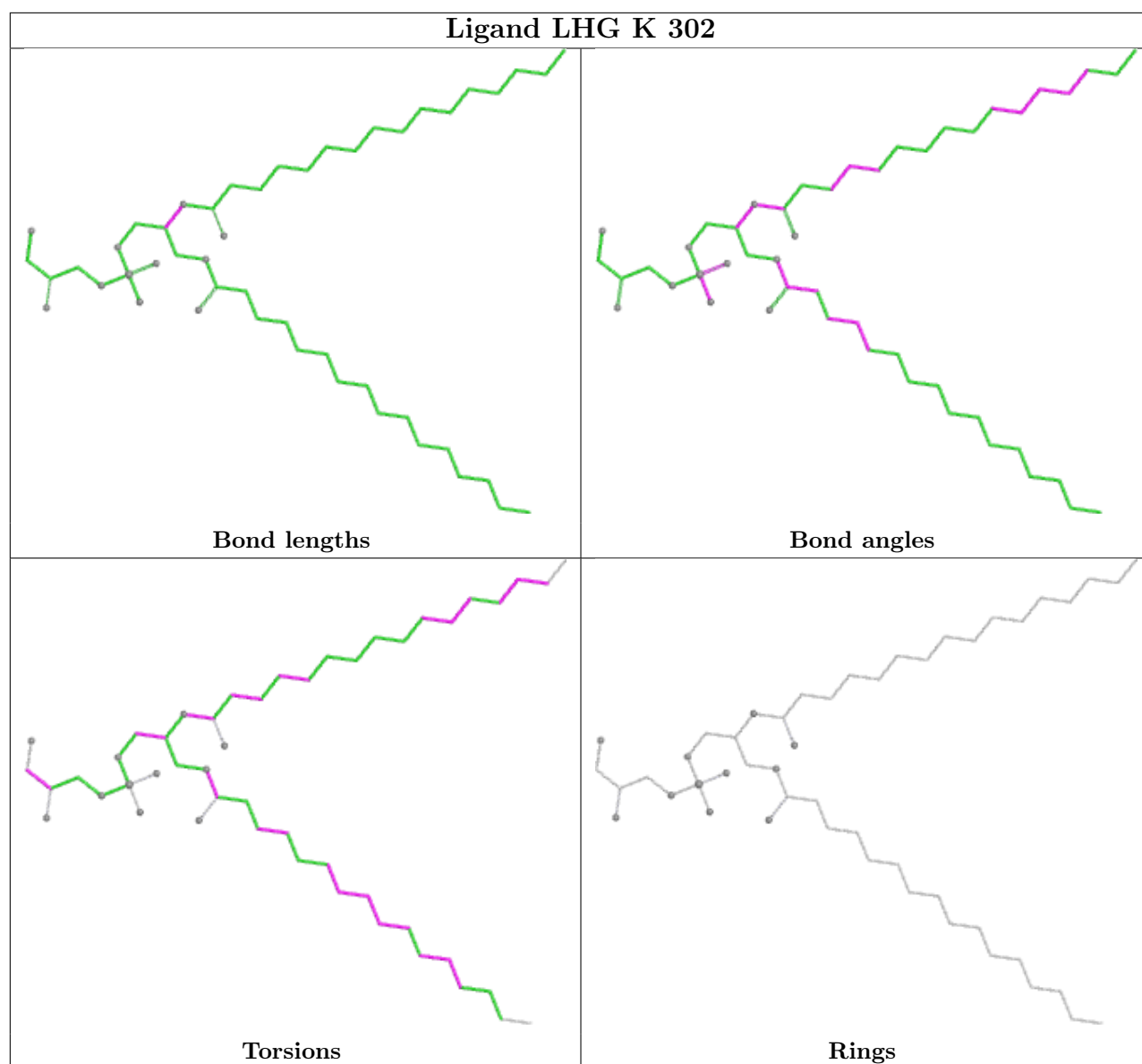


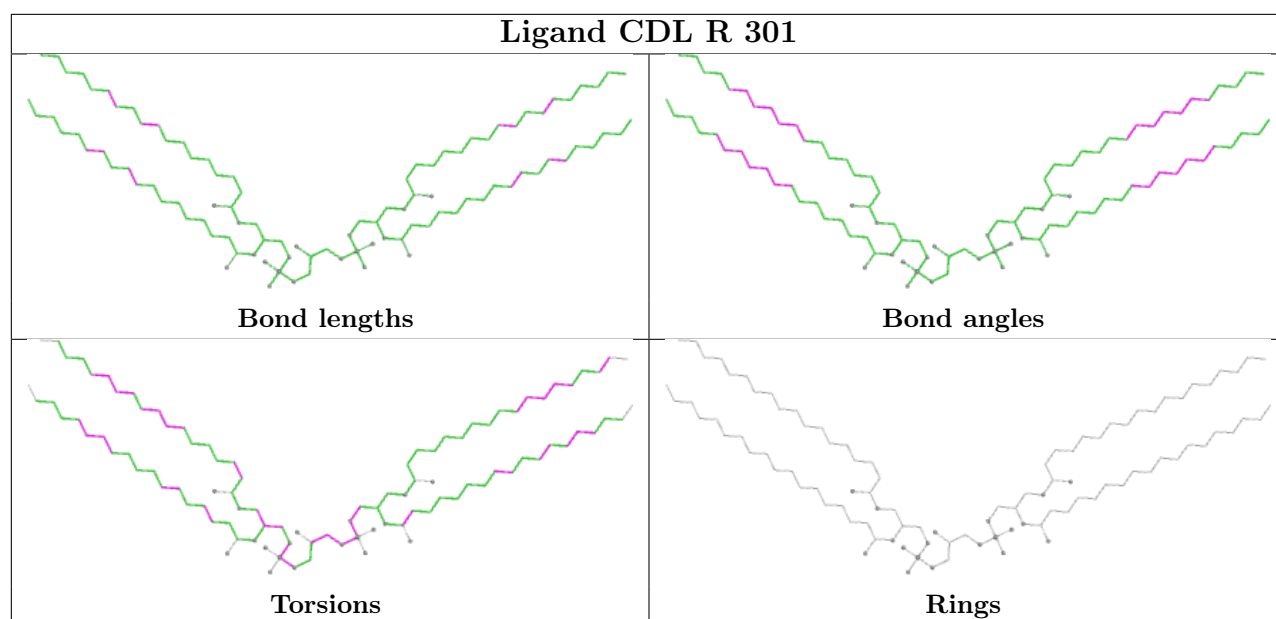












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

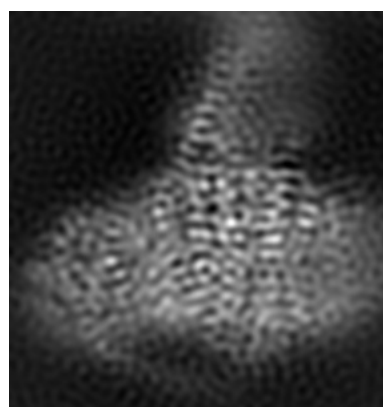
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11127. These allow visual inspection of the internal detail of the map and identification of artifacts.

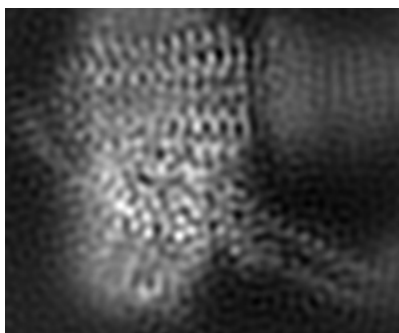
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

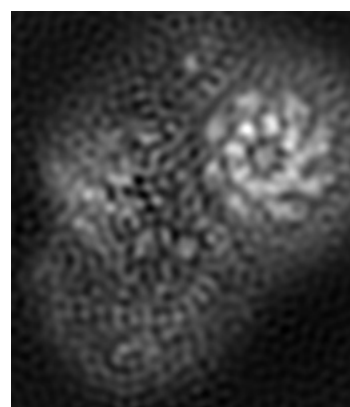
6.1.1 Primary map



X



Y

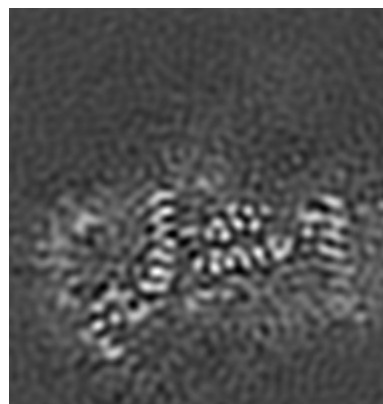


Z

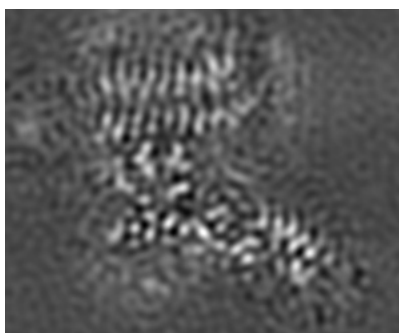
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

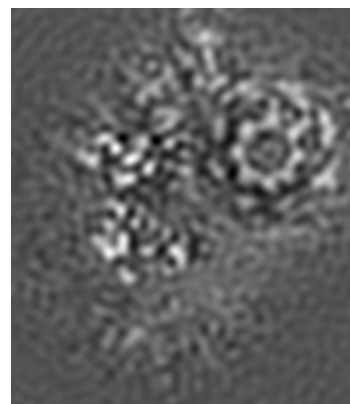
6.2.1 Primary map



X Index: 50



Y Index: 57

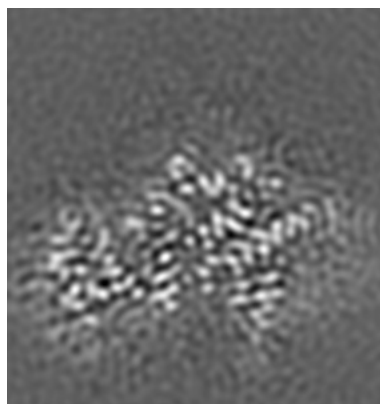


Z Index: 61

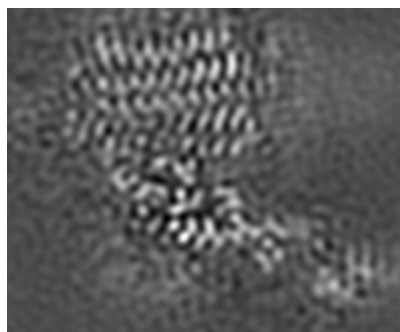
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

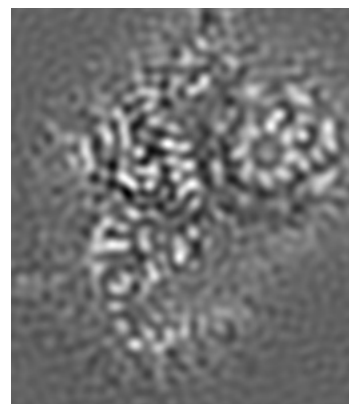
6.3.1 Primary map



X Index: 40



Y Index: 65

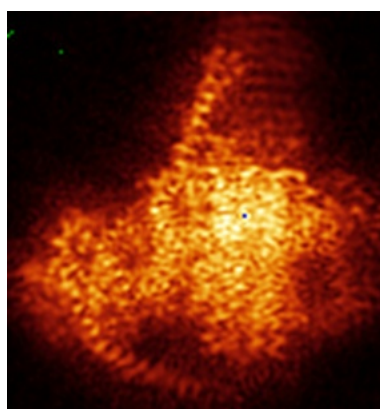


Z Index: 56

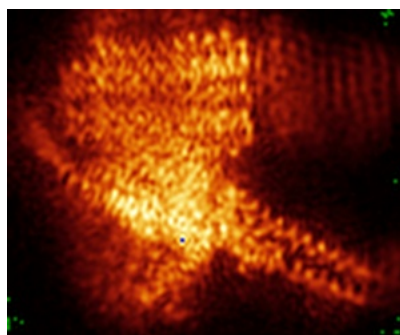
The images above show the largest variance slices of the map in three orthogonal directions.

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

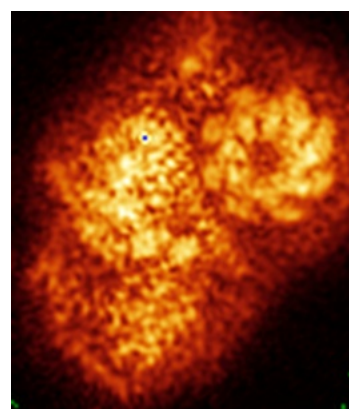
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

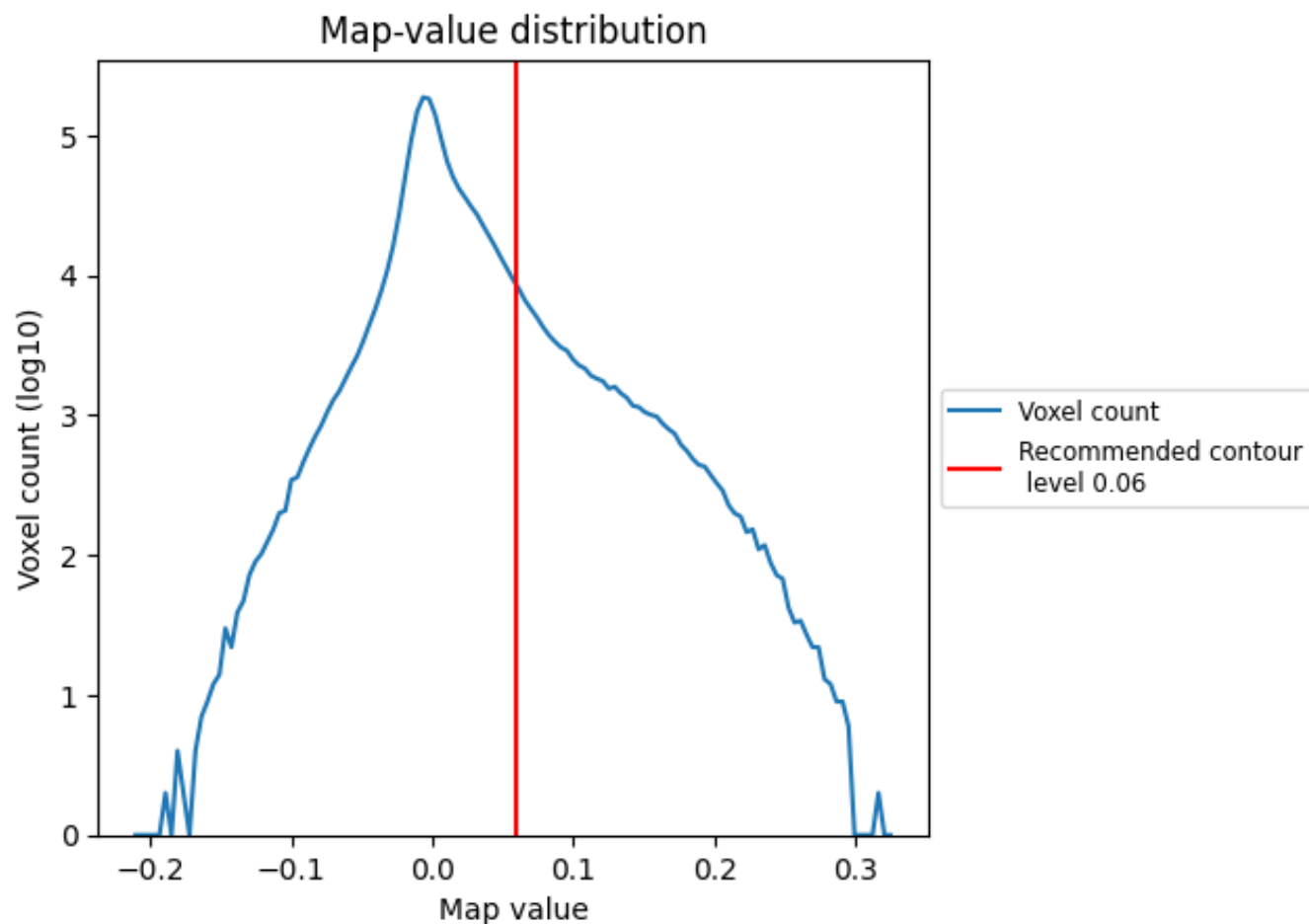
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

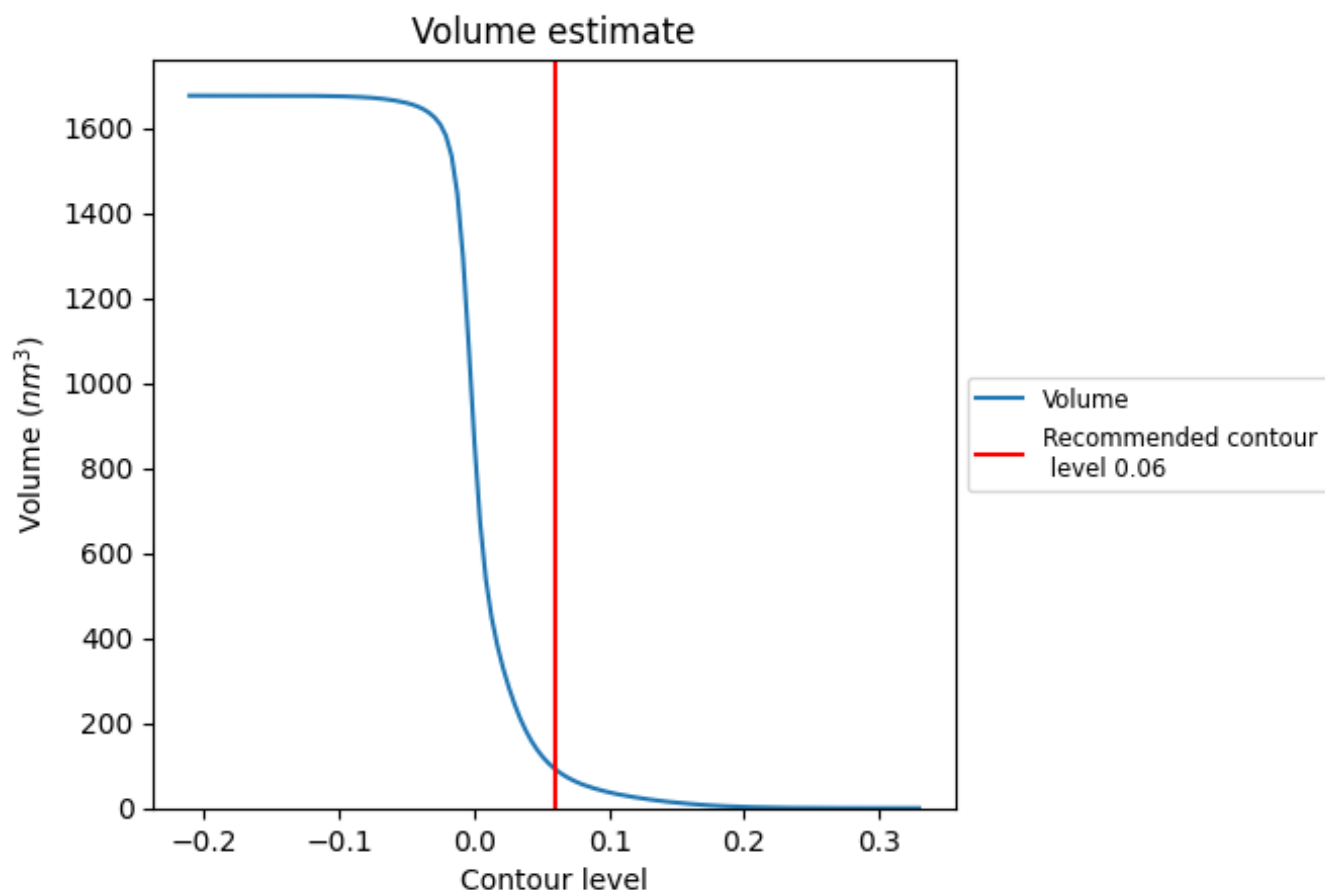
This section contains the results of statistical analysis of the map.

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 92 nm³; this corresponds to an approximate mass of 83 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.

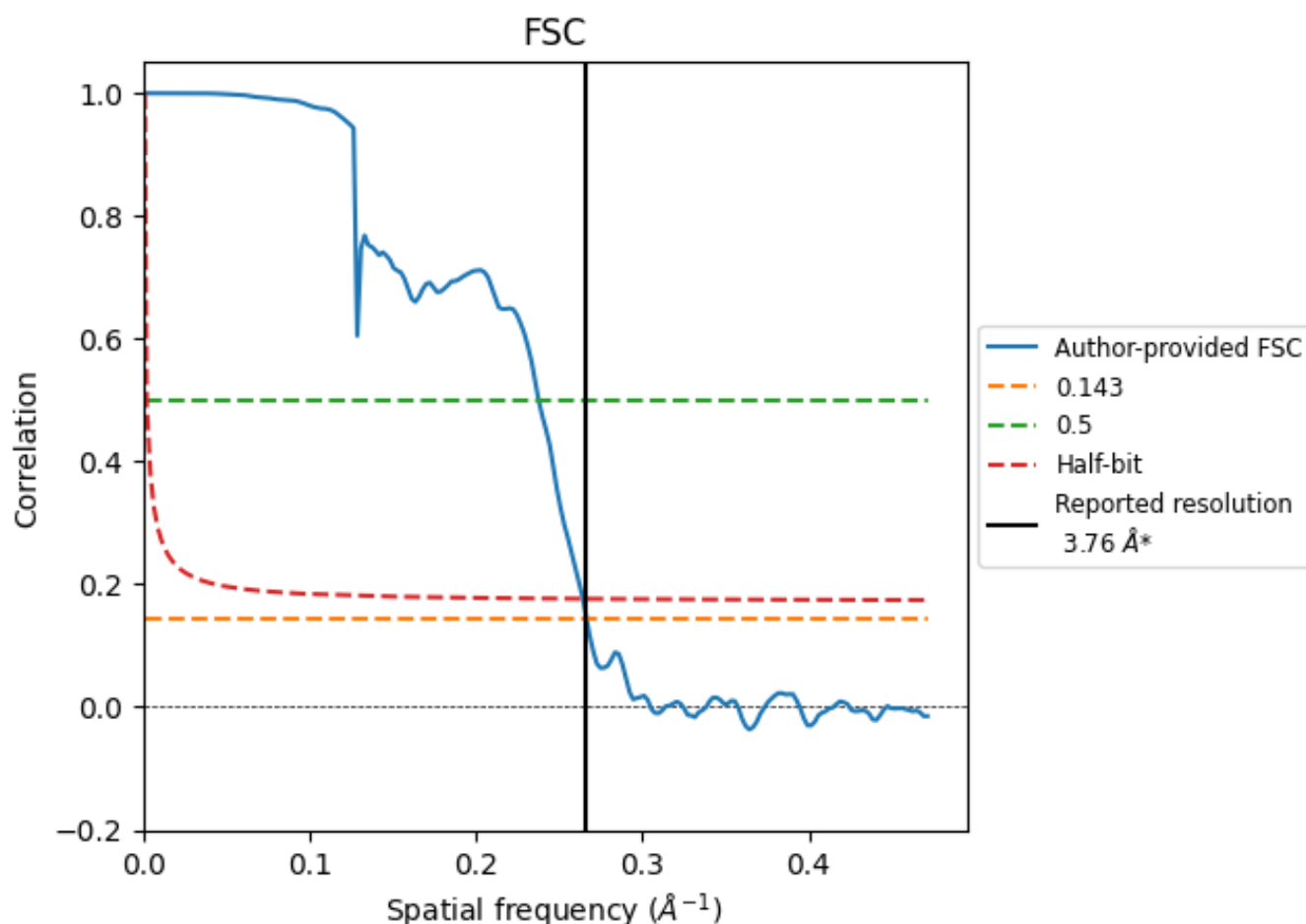
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.266 Å⁻¹

8.2 Resolution estimates [i](#)

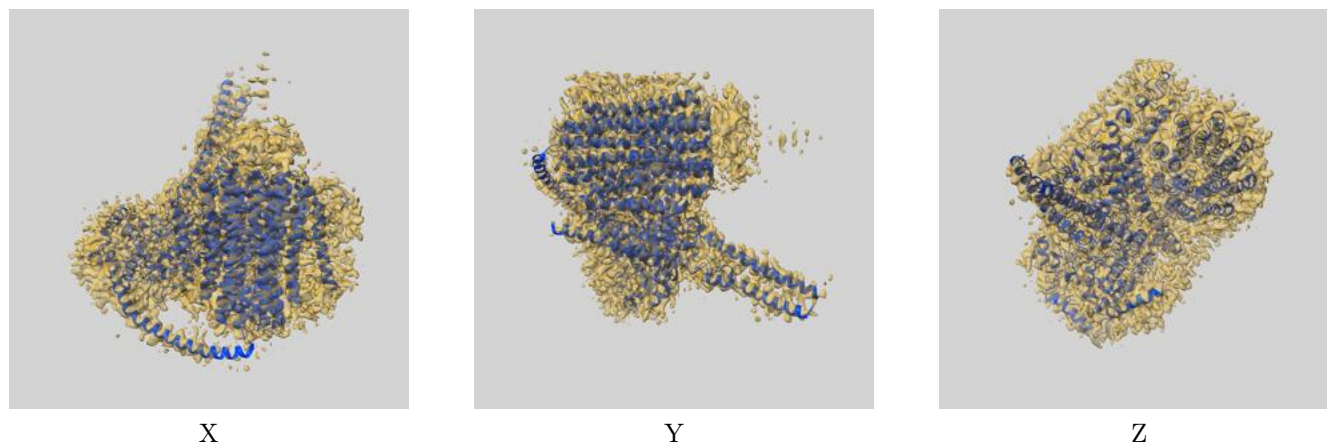
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.75	4.21	3.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

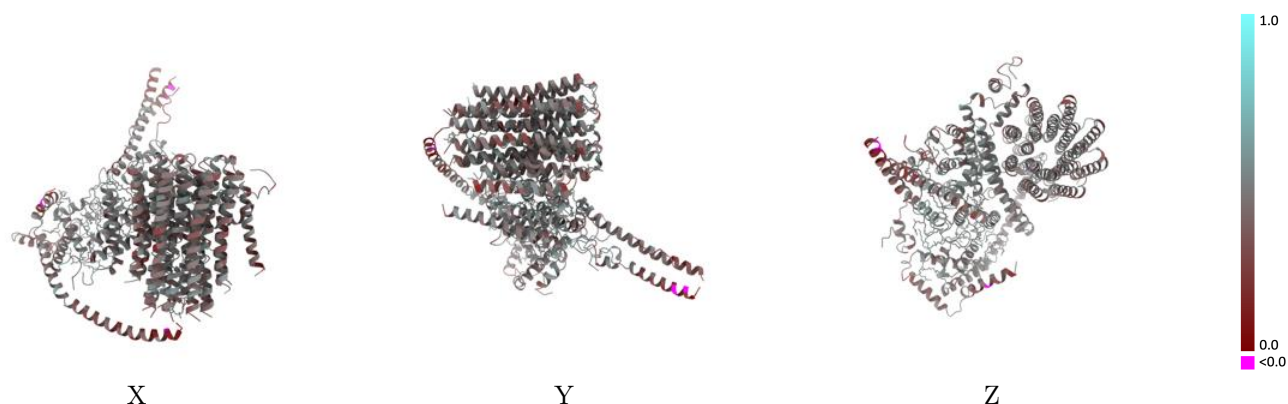
This section contains information regarding the fit between EMDB map EMD-11127 and PDB model 6ZA9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



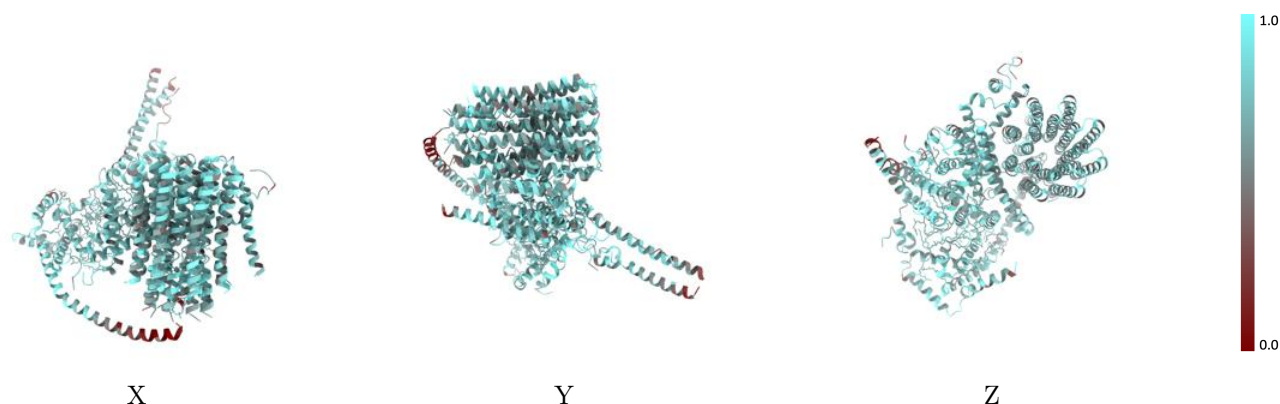
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



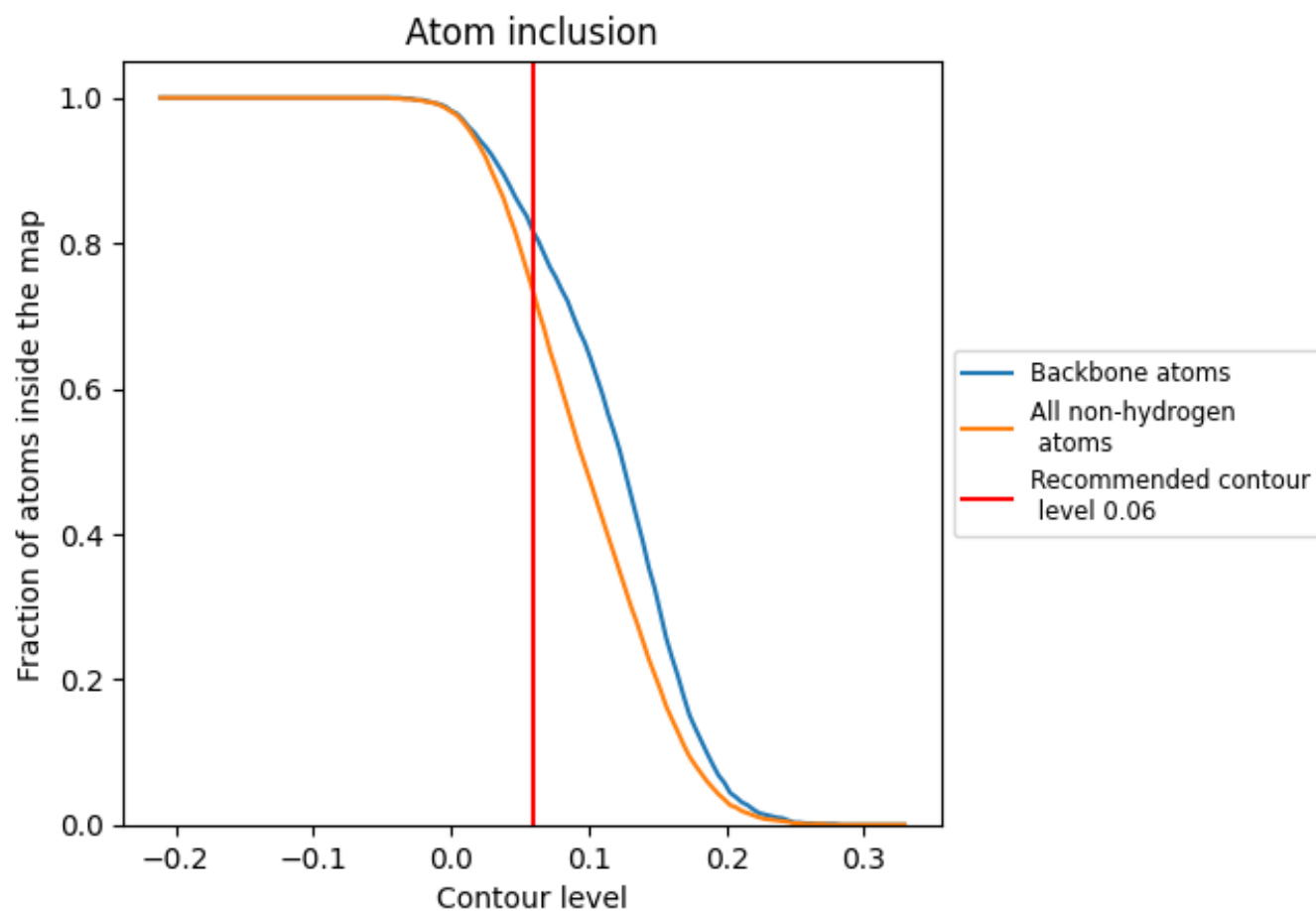
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.4360
1	0.7110	0.4280
2	0.7090	0.4420
3	0.7200	0.4430
4	0.7010	0.4250
5	0.6940	0.4130
6	0.7380	0.4250
7	0.7410	0.4340
8	0.7110	0.4320
K	0.7460	0.4510
M	0.7050	0.3890
N	0.7790	0.4720
O	0.7090	0.4030
P	0.7510	0.4440
Q	0.7860	0.4660
R	0.7620	0.4690
S	0.7480	0.4030
T	0.5980	0.3670

1.0

0.0

<0.0