



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 12:39 AM UTC

PDB ID : 9OVV / pdb_00009ovv
EMDB ID : EMD-70920
Title : Heteromeric GluA1/A2-CNIH1 in the activated state, composite map of LBD-TMD
Authors : Yen, L.Y.; Newton, T.P.; Gangwar, S.P.; Sobolevsky, A.I.
Deposited on : 2025-05-31
Resolution : 3.76 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

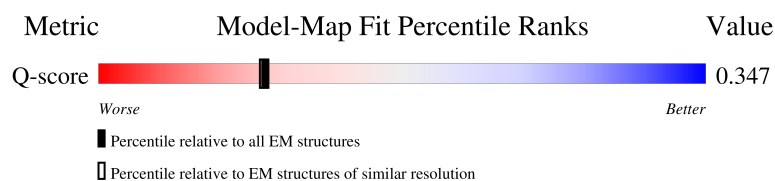
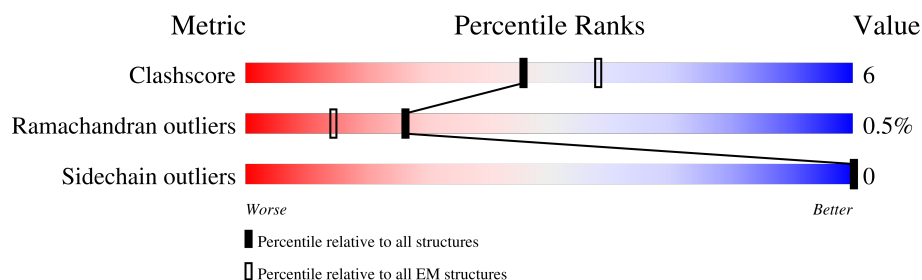
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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





The reported resolution of this entry is 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	A	431	
1	C	431	
2	B	428	
2	D	428	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	142	 51% 89% 11%
3	F	142	 44% 85% 15%
3	G	142	 42% 88% 11%
3	H	142	 39% 87% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35769 atoms, of which 17516 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 Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	404	Total	C	H	N	O	S	0	0
			6383	2064	3202	517	582	18		
1	C	404	Total	C	H	N	O	S	0	0
			6383	2064	3202	517	582	18		

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	403	Total	C	H	N	O	S	0	0
			6363	2047	3208	512	575	21		
2	D	403	Total	C	H	N	O	S	0	0
			6363	2047	3208	512	575	21		

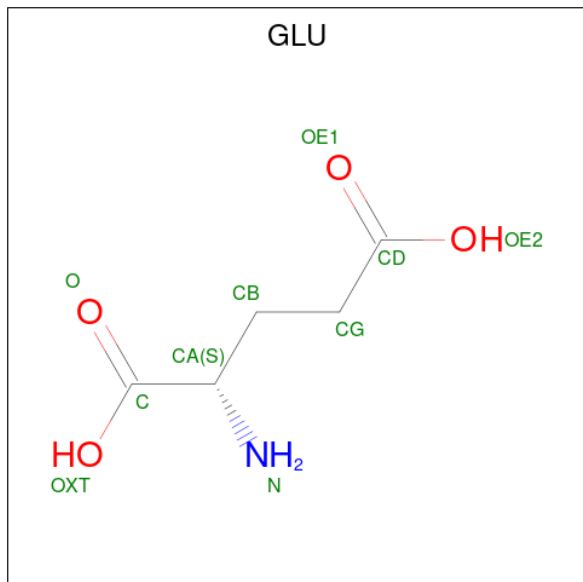
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLN	ASN	conflict	UNP P19491
B	586	ARG	GLN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491

- Molecule 3 is a protein called Protein cornichon homolog 1.

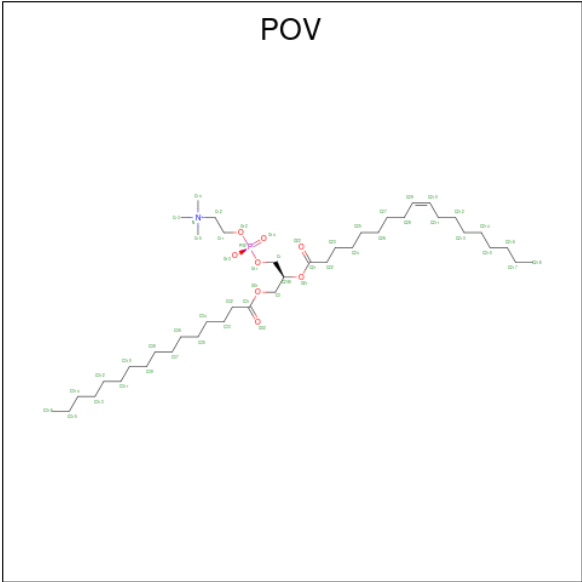
Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	142	Total	C	H	N	O	S	0	0
			2317	790	1156	169	189	13		
3	F	142	Total	C	H	N	O	S	0	0
			2317	790	1156	169	189	13		
3	G	142	Total	C	H	N	O	S	0	0
			2317	790	1156	169	189	13		
3	H	142	Total	C	H	N	O	S	0	0
			2317	790	1156	169	189	13		

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			10	5	1	4	
4	B	1	Total	C	N	O	0
			10	5	1	4	
4	C	1	Total	C	N	O	0
			10	5	1	4	
4	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



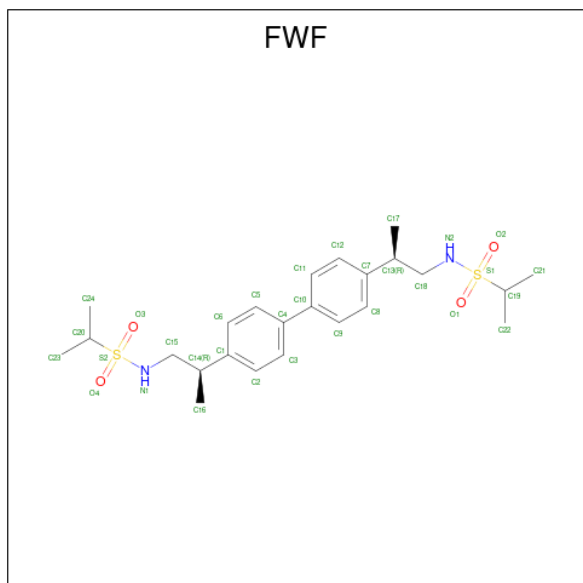
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is N,N'-[biphenyl-4,4'-diyl]di(2R)propane-2,1-diyl]dipropyl-2-sulfonamide (CCD ID: FWF) (formula: $C_{24}H_{36}N_2O_4S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
6	A	1	Total	C	H	N	O	S	0
			68	24	36	2	4	2	
6	B	1	Total	C	H	N	O	S	0
			68	24	36	2	4	2	

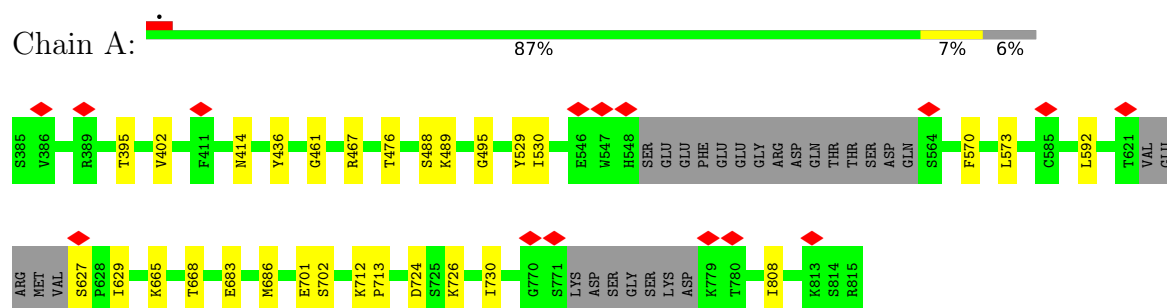
- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Na	0
			1	1	

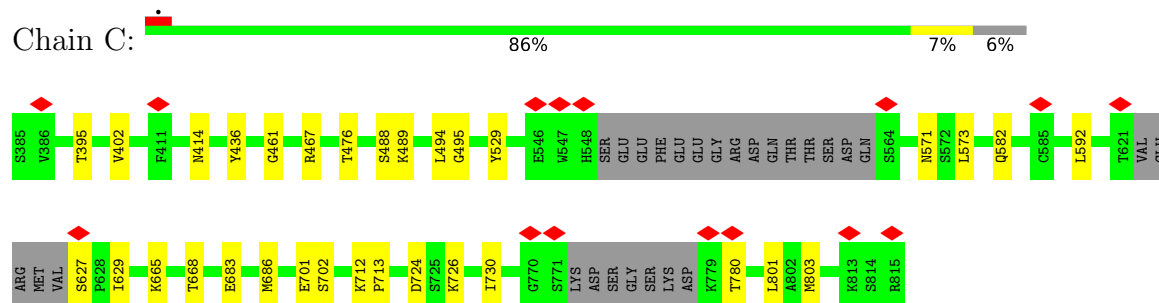
3 Residue-property plots [i](#)

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.

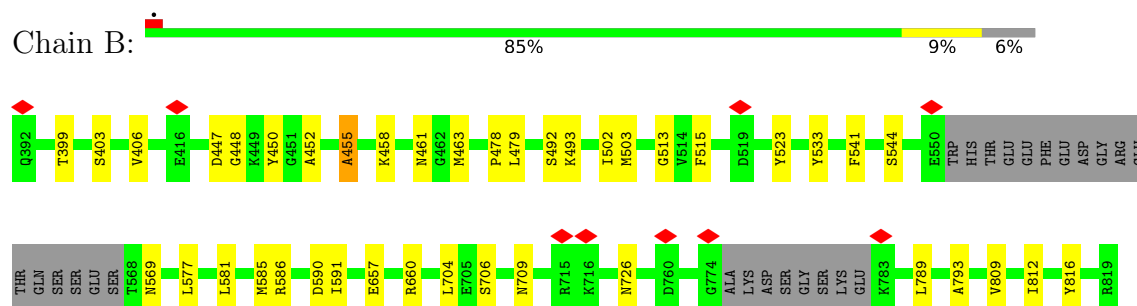
- Molecule 1: Isoform Flip of Glutamate receptor 1



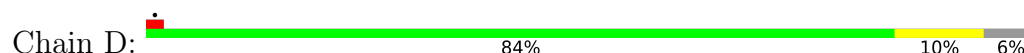
- Molecule 1: Isoform Flip of Glutamate receptor 1

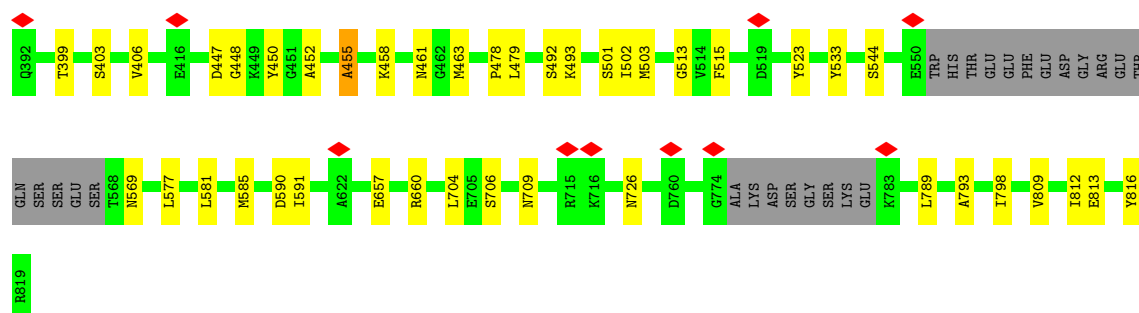


- Molecule 2: Isoform Flip of Glutamate receptor 2

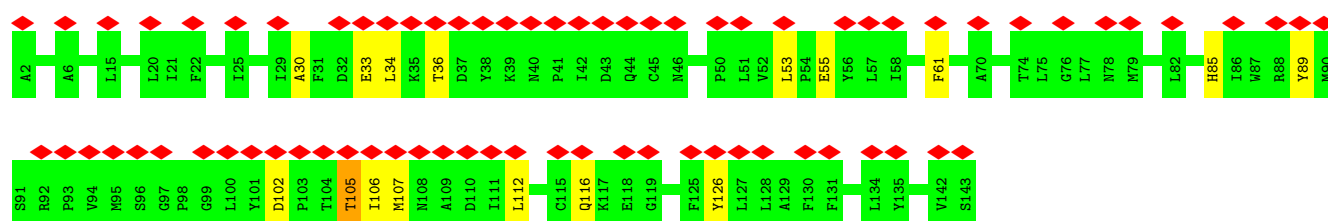
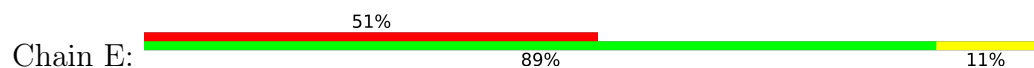


- Molecule 2: Isoform Flip of Glutamate receptor 2

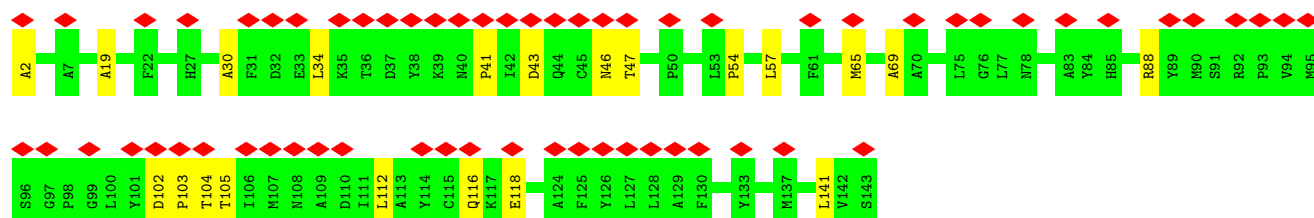
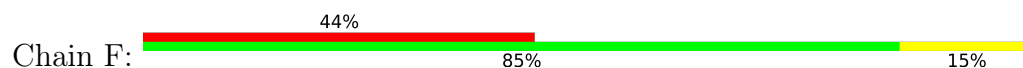




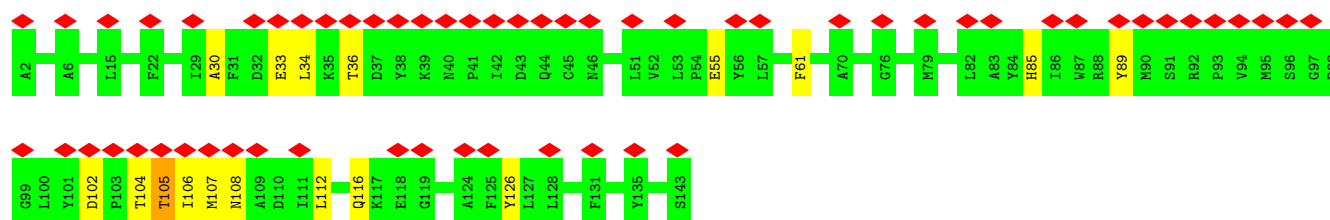
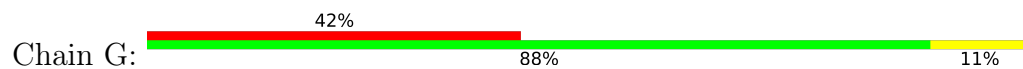
• Molecule 3: Protein cornichon homolog 1



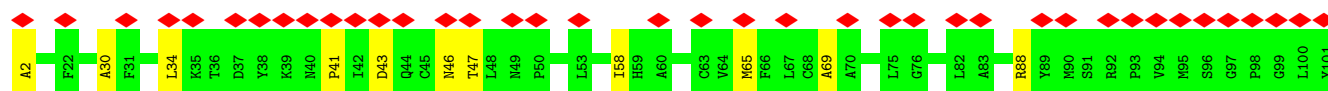
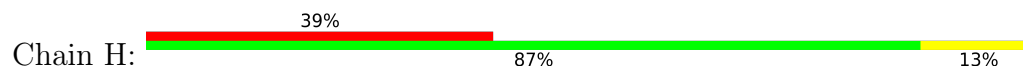
• Molecule 3: Protein cornichon homolog 1



• Molecule 3: Protein cornichon homolog 1



• Molecule 3: Protein cornichon homolog 1



D102	P103	T104	T105	I106	M107	N108	A109	D110	I111	L112	A113	Y114	C115	Q116	K117	E118	A124	F125	Y126	L127	L128	Y135	L141	V142	S143
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	76183	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.03	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	48.769	Depositor
Minimum map value	-30.522	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.947	Depositor
Recommended contour level	4.7	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FWF, NA, POV

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	0.32	0/3253	0.53	0/4392
1	C	0.32	0/3253	0.53	0/4392
2	B	0.30	0/3223	0.52	1/4348 (0.0%)
2	D	0.30	0/3223	0.52	1/4348 (0.0%)
3	E	0.20	0/1202	0.45	0/1642
3	F	0.23	0/1202	0.51	0/1642
3	G	0.20	0/1202	0.45	0/1642
3	H	0.23	0/1202	0.51	0/1642
All	All	0.29	0/17760	0.51	2/24048 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
3	E	0	1
3	G	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	SER	N-CA-C	-5.33	102.09	110.14
2	D	403	SER	N-CA-C	-5.32	102.11	110.14

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	712	LYS	Peptide
1	C	712	LYS	Peptide
3	E	105	THR	Peptide
3	G	105	THR	Peptide

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	3181	3202	3196	20	0
1	C	3181	3202	3196	22	0
2	B	3155	3208	3203	31	0
2	D	3155	3208	3203	30	0
3	E	1161	1156	1153	10	0
3	F	1161	1156	1153	14	0
3	G	1161	1156	1153	9	0
3	H	1161	1156	1153	10	0
4	A	10	0	5	0	0
4	B	10	0	5	1	0
4	C	10	0	5	0	0
4	D	10	0	5	1	0
5	A	156	0	246	21	0
5	B	208	0	328	41	0
5	C	208	0	328	22	0
5	D	208	0	328	34	0
5	E	52	0	82	12	0
6	A	32	36	36	0	0
6	B	32	36	36	0	0
7	A	1	0	0	0	0
All	All	18253	17516	18814	230	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 (230) 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)
5:A:904:POV:H36A	5:E:201:POV:H24A	1.47	0.95
5:B:905:POV:H26A	5:B:905:POV:H32	1.47	0.92
5:A:904:POV:H21D	5:A:904:POV:H315	1.54	0.89
5:A:904:POV:H23A	5:A:904:POV:H28	1.57	0.87
5:C:904:POV:H25A	5:C:904:POV:H211	1.58	0.83
5:D:905:POV:H24	5:D:905:POV:H29	1.61	0.81
5:C:904:POV:H215	5:C:904:POV:H313	1.63	0.80
2:B:492:SER:O	1:C:489:LYS:NZ	2.20	0.74
2:B:493:LYS:NZ	1:C:488:SER:O	2.22	0.73
2:B:544:SER:O	2:B:569:ASN:ND2	2.22	0.72
2:D:544:SER:O	2:D:569:ASN:ND2	2.22	0.72
5:A:902:POV:H31A	5:A:903:POV:H31C	1.71	0.72
3:H:2:ALA:N	3:H:141:LEU:O	2.24	0.71
1:C:461:GLY:O	1:C:467:ARG:NH1	2.24	0.70
3:F:2:ALA:N	3:F:141:LEU:O	2.24	0.70
1:A:489:LYS:NZ	2:D:492:SER:O	2.25	0.70
1:A:461:GLY:O	1:A:467:ARG:NH1	2.24	0.69
5:A:904:POV:H313	5:A:904:POV:H215	1.74	0.69
5:B:904:POV:H28	5:B:905:POV:H24A	1.75	0.69
5:D:902:POV:H12A	5:D:902:POV:H32A	1.74	0.69
2:B:399:THR:HG21	2:B:406:VAL:HG11	1.75	0.69
2:D:399:THR:HG21	2:D:406:VAL:HG11	1.75	0.69
1:C:495:GLY:O	1:C:702:SER:OG	2.11	0.68
3:G:55:GLU:OE2	3:G:126:TYR:OH	2.12	0.67
3:H:30:ALA:O	3:H:34:LEU:N	2.28	0.67
3:E:55:GLU:OE2	3:E:126:TYR:OH	2.12	0.66
3:F:30:ALA:O	3:F:34:LEU:N	2.28	0.66
5:B:902:POV:H32A	5:B:902:POV:H12A	1.77	0.66
5:C:904:POV:H36A	5:C:905:POV:H26	1.77	0.65
2:B:455:ALA:O	2:B:458:LYS:NZ	2.27	0.64
2:B:706:SER:OG	2:B:726:ASN:ND2	2.32	0.63
2:D:706:SER:OG	2:D:726:ASN:ND2	2.32	0.63
1:A:495:GLY:O	1:A:702:SER:OG	2.11	0.62
5:B:902:POV:H21C	5:B:902:POV:H31H	1.81	0.62
2:D:455:ALA:O	2:D:458:LYS:NZ	2.26	0.61
5:B:903:POV:H31E	5:B:904:POV:H21F	1.80	0.61
3:F:43:ASP:O	3:F:47:THR:OG1	2.19	0.61
3:H:43:ASP:O	3:H:47:THR:OG1	2.19	0.60
3:E:33:GLU:OE1	3:E:36:THR:OG1	2.19	0.60
3:G:33:GLU:OE1	3:G:36:THR:OG1	2.19	0.60
1:A:665:LYS:O	1:A:668:THR:OG1	2.18	0.60
1:A:414:ASN:ND2	1:A:436:TYR:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:46:ASN:O	3:H:47:THR:OG1	2.17	0.59
5:B:905:POV:C31	5:B:905:POV:H23A	2.33	0.59
3:F:46:ASN:O	3:F:47:THR:OG1	2.18	0.58
5:A:904:POV:C23	5:A:904:POV:H211	2.35	0.57
1:C:665:LYS:O	1:C:668:THR:OG1	2.18	0.57
3:E:53:LEU:HG	5:E:201:POV:H3	1.87	0.57
1:A:529:TYR:OH	1:A:573:LEU:O	2.23	0.57
2:B:523:TYR:CE1	5:B:902:POV:H3A	2.41	0.56
1:C:414:ASN:ND2	1:C:436:TYR:O	2.35	0.56
2:D:523:TYR:CE1	5:D:902:POV:H3A	2.39	0.56
2:D:523:TYR:HE1	5:D:902:POV:H3A	1.71	0.56
1:C:529:TYR:OH	1:C:573:LEU:O	2.23	0.55
2:B:523:TYR:HE1	5:B:902:POV:H3A	1.72	0.55
5:B:905:POV:H28	3:F:57:LEU:CD1	2.37	0.55
5:D:905:POV:H313	5:D:905:POV:H214	1.89	0.55
5:D:904:POV:O14	5:D:904:POV:H33	2.07	0.55
5:A:904:POV:H26	5:A:904:POV:O21	2.06	0.54
5:D:902:POV:H1A	5:D:902:POV:H33A	1.89	0.54
5:E:201:POV:H27	5:E:201:POV:H38A	1.89	0.54
3:G:112:LEU:O	3:G:116:GLN:N	2.41	0.54
1:A:627:SER:OG	1:A:629:ILE:O	2.16	0.54
5:B:904:POV:H33	5:B:904:POV:O14	2.08	0.53
5:C:904:POV:H21D	5:C:904:POV:H31E	1.89	0.53
3:E:112:LEU:O	3:E:116:GLN:N	2.41	0.53
5:B:904:POV:H27A	5:B:905:POV:H24A	1.89	0.53
1:A:488:SER:N	1:A:730:ILE:O	2.41	0.53
5:B:904:POV:H211	5:B:905:POV:H213	1.89	0.53
1:C:488:SER:N	1:C:730:ILE:O	2.41	0.53
3:G:102:ASP:O	3:G:105:THR:OG1	2.25	0.53
2:B:515:PHE:CZ	5:B:902:POV:H35A	2.44	0.52
2:D:513:GLY:HA3	5:D:903:POV:H14B	1.91	0.52
3:E:102:ASP:O	3:E:105:THR:OG1	2.25	0.52
5:B:902:POV:H21C	5:B:902:POV:C316	2.39	0.52
3:H:88:ARG:NH1	3:H:118:GLU:OE1	2.42	0.52
5:D:905:POV:H23A	5:D:905:POV:O32	2.10	0.51
3:E:61:PHE:HD1	5:E:201:POV:H31C	1.75	0.51
2:B:541:PHE:CE2	5:B:905:POV:H37	2.46	0.51
1:A:488:SER:O	2:D:493:LYS:NZ	2.43	0.51
2:B:541:PHE:CE2	5:B:905:POV:H35A	2.45	0.51
3:F:88:ARG:NH1	3:F:118:GLU:OE1	2.42	0.51
2:B:452:ALA:N	2:B:461:ASN:OD1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:902:POV:H35A	5:C:902:POV:H21B	1.92	0.51
3:E:105:THR:O	3:E:107:MET:N	2.44	0.51
3:G:105:THR:O	3:G:107:MET:N	2.44	0.51
2:D:813:GLU:HG2	5:D:904:POV:H37A	1.93	0.50
1:C:476:THR:OG1	1:C:701:GLU:OE2	2.29	0.50
1:C:724:ASP:OD2	1:C:726:LYS:NZ	2.44	0.50
1:C:801:LEU:HD12	5:C:903:POV:H21G	1.92	0.50
3:G:85:HIS:O	3:G:89:TYR:N	2.44	0.50
1:A:724:ASP:OD2	1:A:726:LYS:NZ	2.44	0.50
2:D:452:ALA:N	2:D:461:ASN:OD1	2.44	0.50
5:C:904:POV:C36	5:C:905:POV:H26	2.41	0.50
2:D:478:PRO:O	4:D:901:GLU:N	2.45	0.50
5:A:904:POV:H33	5:E:201:POV:H24A	1.94	0.49
2:D:447:ASP:OD1	2:D:448:GLY:N	2.46	0.49
1:C:803:MET:CE	3:F:19:ALA:HB2	2.42	0.49
3:E:85:HIS:O	3:E:89:TYR:N	2.44	0.49
3:E:30:ALA:O	3:E:34:LEU:N	2.45	0.49
1:A:592:LEU:HD12	2:B:809:VAL:HG11	1.93	0.49
3:G:30:ALA:O	3:G:34:LEU:N	2.45	0.49
5:A:902:POV:H31A	5:A:903:POV:C312	2.41	0.49
1:A:476:THR:OG1	1:A:701:GLU:OE2	2.29	0.49
1:C:395:THR:HG21	1:C:402:VAL:HG21	1.95	0.49
5:D:902:POV:C315	5:D:903:POV:H312	2.42	0.48
2:B:447:ASP:OD1	2:B:448:GLY:N	2.46	0.48
2:B:478:PRO:O	4:B:901:GLU:N	2.45	0.48
2:D:515:PHE:CZ	5:D:902:POV:H35A	2.48	0.48
2:D:450:TYR:O	2:D:463:MET:N	2.46	0.48
2:B:450:TYR:O	2:B:463:MET:N	2.46	0.48
2:D:581:LEU:HD11	5:D:902:POV:H316	1.95	0.48
5:D:905:POV:H212	5:D:905:POV:H31D	1.96	0.48
5:E:201:POV:H35	5:E:201:POV:H32A	1.52	0.48
2:B:541:PHE:CZ	5:B:905:POV:H35A	2.49	0.48
5:A:904:POV:H32A	5:E:201:POV:O22	2.14	0.47
2:B:513:GLY:HA3	5:B:903:POV:H14B	1.96	0.47
1:A:395:THR:HG21	1:A:402:VAL:HG21	1.95	0.47
5:A:904:POV:H211	5:A:904:POV:H23	1.96	0.47
5:C:903:POV:H28A	5:C:903:POV:H32A	1.97	0.47
5:C:905:POV:H31C	3:G:61:PHE:HD1	1.79	0.47
2:B:502:ILE:O	2:B:709:ASN:ND2	2.48	0.47
5:B:903:POV:H23A	5:B:903:POV:H26A	1.56	0.47
2:D:503:MET:SD	2:D:704:LEU:HD21	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:GLU:OE2	2:B:660:ARG:NH1	2.48	0.47
5:B:902:POV:H25A	5:B:902:POV:H22A	1.84	0.47
1:C:592:LEU:HD12	2:D:809:VAL:HG11	1.97	0.47
1:A:530:ILE:HG21	3:E:61:PHE:CE1	2.50	0.47
5:B:904:POV:H33A	5:B:904:POV:H36A	1.61	0.47
5:B:905:POV:H39	3:F:57:LEU:HB2	1.97	0.47
5:B:905:POV:H34A	5:B:905:POV:H28A	1.98	0.47
5:B:904:POV:C28	5:B:905:POV:H24A	2.42	0.46
5:B:904:POV:H210	5:B:904:POV:H26	1.96	0.46
5:C:904:POV:H26	5:C:904:POV:O21	2.15	0.46
2:B:503:MET:SD	2:B:704:LEU:HD21	2.55	0.46
2:B:515:PHE:CE2	5:B:902:POV:H33	2.50	0.46
5:B:905:POV:H35	3:F:54:PRO:HD3	1.96	0.46
5:C:904:POV:H25A	5:C:904:POV:H28	1.44	0.46
5:C:905:POV:H35	5:C:905:POV:H32A	1.62	0.46
5:B:904:POV:C27	5:B:905:POV:H24A	2.45	0.46
5:E:201:POV:H31C	5:E:201:POV:H39	1.59	0.46
2:B:590:ASP:OD1	2:B:591:ILE:N	2.49	0.46
2:D:502:ILE:O	2:D:709:ASN:ND2	2.48	0.46
2:D:657:GLU:OE2	2:D:660:ARG:NH1	2.48	0.46
2:D:515:PHE:CE2	5:D:902:POV:H33	2.51	0.46
2:D:585:MET:HE1	5:D:902:POV:H29	1.97	0.46
5:D:904:POV:H33A	5:D:904:POV:H36A	1.60	0.45
2:B:581:LEU:HD11	5:B:902:POV:H316	1.97	0.45
2:D:590:ASP:OD1	2:D:591:ILE:N	2.49	0.45
5:D:903:POV:H11	5:D:903:POV:H15A	1.44	0.45
1:A:808:ILE:CD1	5:A:904:POV:H216	2.47	0.45
5:D:903:POV:H310	5:D:904:POV:C218	2.47	0.45
2:D:463:MET:HE3	2:D:479:LEU:HD11	1.98	0.45
2:B:463:MET:HE3	2:B:479:LEU:HD11	1.98	0.45
5:B:905:POV:H36	3:F:57:LEU:HD12	1.98	0.45
5:D:903:POV:O22	5:D:903:POV:H24	2.17	0.45
5:C:905:POV:H31C	5:C:905:POV:H39	1.64	0.45
5:D:902:POV:H31F	5:D:903:POV:H312	1.99	0.45
3:F:102:ASP:HB2	3:F:103:PRO:HD2	1.98	0.44
1:A:570:PHE:CD1	5:A:904:POV:H34	2.53	0.44
1:A:395:THR:CG2	1:A:402:VAL:HG21	2.47	0.44
1:C:395:THR:CG2	1:C:402:VAL:HG21	2.47	0.44
5:C:904:POV:H210	5:C:904:POV:H21C	1.81	0.44
2:B:789:LEU:O	2:B:793:ALA:N	2.50	0.44
1:C:627:SER:OG	1:C:629:ILE:O	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:ASP:HB2	3:H:103:PRO:HD2	1.98	0.44
1:A:529:TYR:CE2	5:E:201:POV:H214	2.53	0.44
5:A:904:POV:H23A	5:A:904:POV:H211	1.99	0.44
2:B:812:ILE:O	2:B:816:TYR:N	2.51	0.44
5:A:904:POV:H36	5:A:904:POV:H39A	1.63	0.44
5:A:904:POV:H21C	5:A:904:POV:H210	1.86	0.44
2:D:812:ILE:O	2:D:816:TYR:N	2.51	0.44
5:D:905:POV:H214	5:D:905:POV:C313	2.48	0.44
5:B:905:POV:H31C	5:B:905:POV:H39A	1.43	0.44
5:B:904:POV:H13B	5:B:904:POV:H11A	1.72	0.43
5:B:905:POV:H214	5:B:905:POV:H313	2.00	0.43
3:F:103:PRO:O	3:F:105:THR:N	2.51	0.43
3:H:103:PRO:O	3:H:105:THR:N	2.51	0.43
1:A:570:PHE:CD1	5:A:904:POV:H37A	2.53	0.43
5:C:904:POV:H25	5:C:904:POV:H33A	2.00	0.43
5:A:904:POV:C29	5:A:904:POV:H25A	2.48	0.43
5:B:903:POV:H210	5:B:903:POV:H21C	1.77	0.43
2:D:704:LEU:HD11	2:D:709:ASN:HB2	2.00	0.43
5:C:904:POV:H211	5:C:904:POV:C25	2.40	0.43
2:D:789:LEU:O	2:D:793:ALA:N	2.50	0.43
3:F:112:LEU:O	3:F:116:GLN:N	2.47	0.43
2:D:798:ILE:HD12	5:D:902:POV:H31A	2.00	0.43
5:B:902:POV:H315	5:B:903:POV:H312	2.00	0.43
5:B:904:POV:H36	5:B:904:POV:H39	1.34	0.43
5:B:905:POV:H23A	5:B:905:POV:C32	2.49	0.43
5:C:905:POV:H11	5:C:905:POV:H15A	1.59	0.43
5:C:905:POV:H27	5:C:905:POV:H38A	1.99	0.43
5:C:904:POV:H215	5:C:904:POV:C313	2.40	0.43
5:D:903:POV:H21C	5:D:903:POV:H210	1.70	0.42
1:C:571:ASN:O	1:C:571:ASN:ND2	2.51	0.42
5:D:905:POV:H23A	5:D:905:POV:C31	2.49	0.42
2:B:533:TYR:OH	2:B:577:LEU:O	2.34	0.42
3:G:104:THR:O	3:G:108:ASN:ND2	2.48	0.42
5:D:904:POV:H13B	5:D:904:POV:H11A	1.71	0.42
5:E:201:POV:H21F	5:E:201:POV:H213	1.90	0.42
2:B:704:LEU:HD11	2:B:709:ASN:HB2	2.00	0.42
5:D:905:POV:H13A	5:D:905:POV:H11	1.75	0.42
1:A:683:GLU:O	1:A:686:MET:N	2.53	0.42
5:D:902:POV:H315	5:D:903:POV:H312	2.02	0.42
5:B:903:POV:H11	5:B:903:POV:H15A	1.46	0.42
5:B:905:POV:H13A	5:B:905:POV:H11	1.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:GLU:O	1:C:686:MET:N	2.53	0.42
5:D:905:POV:H31A	3:H:58:ILE:HG13	2.02	0.42
3:F:65:MET:O	3:F:69:ALA:N	2.53	0.42
2:B:585:MET:HE1	5:B:902:POV:H29	2.02	0.41
5:D:904:POV:H214	5:D:905:POV:H217	2.02	0.41
3:H:65:MET:O	3:H:69:ALA:N	2.53	0.41
5:B:902:POV:H21J	5:B:902:POV:H21E	1.85	0.41
1:C:592:LEU:HB2	5:D:904:POV:H24	2.03	0.41
2:D:533:TYR:OH	2:D:577:LEU:O	2.34	0.41
5:A:904:POV:H28	5:A:904:POV:H211	1.80	0.41
1:C:780:THR:HG22	1:C:780:THR:O	2.21	0.41
5:D:904:POV:H212	5:D:905:POV:H215	2.03	0.41
5:E:201:POV:O22	5:E:201:POV:H1	2.15	0.41
5:C:902:POV:O21	5:C:902:POV:H24	2.19	0.41
3:H:112:LEU:O	3:H:116:GLN:N	2.47	0.41
5:A:904:POV:H36A	5:E:201:POV:H26	2.03	0.40
5:A:902:POV:O21	5:A:902:POV:H24	2.20	0.40
5:C:902:POV:H312	5:C:903:POV:H314	2.03	0.40
5:D:903:POV:H310	5:D:904:POV:H21J	2.02	0.40
5:C:903:POV:H34A	5:C:903:POV:H37A	1.77	0.40
2:B:586:ARG:NH2	1:C:582:GLN:OE1	2.55	0.40
1:C:494:LEU:HD12	1:C:495:GLY:N	2.37	0.40
2:D:501:SER:OG	2:D:502:ILE:N	2.55	0.40
5:D:902:POV:H25A	5:D:902:POV:H22A	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	396/431 (92%)	342 (86%)	53 (13%)	1 (0%)	36 66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	396/431 (92%)	342 (86%)	53 (13%)	1 (0%)	36	66
2	B	397/428 (93%)	361 (91%)	35 (9%)	1 (0%)	36	66
2	D	397/428 (93%)	362 (91%)	34 (9%)	1 (0%)	36	66
3	E	140/142 (99%)	122 (87%)	17 (12%)	1 (1%)	18	50
3	F	140/142 (99%)	117 (84%)	21 (15%)	2 (1%)	9	36
3	G	140/142 (99%)	122 (87%)	17 (12%)	1 (1%)	18	50
3	H	140/142 (99%)	117 (84%)	21 (15%)	2 (1%)	9	36
All	All	2146/2286 (94%)	1885 (88%)	251 (12%)	10 (0%)	26	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	104	THR
3	H	104	THR
1	A	713	PRO
2	B	455	ALA
1	C	713	PRO
2	D	455	ALA
3	F	41	PRO
3	H	41	PRO
3	E	106	ILE
3	G	106	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	341/366 (93%)	341 (100%)	0	100	100
1	C	341/366 (93%)	341 (100%)	0	100	100
2	B	341/363 (94%)	341 (100%)	0	100	100
2	D	341/363 (94%)	341 (100%)	0	100	100
3	E	121/121 (100%)	121 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	121/121 (100%)	121 (100%)	0	100	100
3	G	121/121 (100%)	121 (100%)	0	100	100
3	H	121/121 (100%)	121 (100%)	0	100	100
All	All	1848/1942 (95%)	1848 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	764	ASN
1	C	583	GLN
2	D	764	ASN
3	F	59	HIS
3	H	59	HIS

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](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	POV	D	902	-	51,51,51	1.09	3 (5%)	57,59,59	0.92	3 (5%)
5	POV	E	201	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	C	903	-	51,51,51	1.10	3 (5%)	57,59,59	0.95	3 (5%)
5	POV	A	903	-	51,51,51	1.10	3 (5%)	57,59,59	0.95	3 (5%)
4	GLU	C	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.17	1 (12%)
5	POV	C	904	-	51,51,51	1.09	3 (5%)	57,59,59	0.87	3 (5%)
4	GLU	B	901	-	8,9,9	1.11	1 (12%)	8,11,11	1.22	1 (12%)
4	GLU	D	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.22	1 (12%)
6	FWF	A	905	-	31,33,33	0.29	0	40,48,48	0.30	0
5	POV	D	905	-	51,51,51	1.09	3 (5%)	57,59,59	0.95	3 (5%)
5	POV	C	902	-	51,51,51	1.10	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	B	903	-	51,51,51	1.10	3 (5%)	57,59,59	0.92	3 (5%)
5	POV	D	903	-	51,51,51	1.10	3 (5%)	57,59,59	0.94	3 (5%)
5	POV	B	904	-	51,51,51	1.10	3 (5%)	57,59,59	0.91	3 (5%)
5	POV	A	904	-	51,51,51	1.09	3 (5%)	57,59,59	0.91	3 (5%)
6	FWF	B	906	-	31,33,33	0.29	0	40,48,48	0.33	0
5	POV	B	905	-	51,51,51	1.09	3 (5%)	57,59,59	0.96	3 (5%)
4	GLU	A	901	-	8,9,9	1.11	1 (12%)	8,11,11	1.18	1 (12%)
5	POV	B	902	-	51,51,51	1.09	3 (5%)	57,59,59	0.92	3 (5%)
5	POV	A	902	-	51,51,51	1.10	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	D	904	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	C	905	-	51,51,51	1.09	3 (5%)	57,59,59	0.95	3 (5%)

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
5	POV	D	902	-	-	18/55/55/55	-
5	POV	E	201	-	-	25/55/55/55	-
5	POV	C	903	-	-	28/55/55/55	-
5	POV	A	903	-	-	26/55/55/55	-
4	GLU	C	901	-	-	0/9/9/9	-
5	POV	C	904	-	-	26/55/55/55	-
4	GLU	B	901	-	-	1/9/9/9	-
4	GLU	D	901	-	-	1/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FWF	A	905	-	-	6/32/36/36	0/2/2/2
5	POV	D	905	-	-	26/55/55/55	-
5	POV	C	902	-	-	22/55/55/55	-
5	POV	B	903	-	-	29/55/55/55	-
5	POV	D	903	-	-	27/55/55/55	-
5	POV	B	904	-	-	24/55/55/55	-
5	POV	A	904	-	-	28/55/55/55	-
6	FWF	B	906	-	-	12/32/36/36	0/2/2/2
5	POV	B	905	-	-	32/55/55/55	-
4	GLU	A	901	-	-	0/9/9/9	-
5	POV	B	902	-	-	18/55/55/55	-
5	POV	A	902	-	-	24/55/55/55	-
5	POV	D	904	-	-	24/55/55/55	-
5	POV	C	905	-	-	24/55/55/55	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904	POV	O21-C21	2.97	1.42	1.34
5	C	902	POV	O21-C21	2.93	1.42	1.34
5	A	902	POV	O21-C21	2.93	1.42	1.34
5	E	201	POV	O21-C21	2.93	1.42	1.34
5	C	905	POV	O21-C21	2.90	1.42	1.34
5	B	903	POV	O21-C21	2.88	1.42	1.34
5	D	903	POV	O21-C21	2.87	1.42	1.34
5	B	905	POV	O21-C21	2.86	1.42	1.34
5	C	903	POV	O21-C21	2.84	1.42	1.34
5	A	904	POV	O21-C21	2.84	1.42	1.34
5	D	905	POV	O21-C21	2.84	1.42	1.34
5	A	903	POV	O21-C21	2.83	1.42	1.34
5	B	902	POV	O21-C21	2.80	1.42	1.34
5	D	904	POV	O21-C21	2.80	1.42	1.34
5	D	902	POV	O21-C21	2.80	1.42	1.34
5	A	903	POV	O31-C31	2.77	1.41	1.33
5	C	903	POV	O31-C31	2.76	1.41	1.33
5	B	904	POV	O21-C21	2.75	1.42	1.34
5	C	902	POV	O31-C31	2.74	1.41	1.33
5	A	904	POV	O31-C31	2.73	1.41	1.33
5	B	904	POV	O31-C31	2.73	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	905	POV	O31-C31	2.73	1.41	1.33
5	B	902	POV	O31-C31	2.73	1.41	1.33
5	A	902	POV	O31-C31	2.72	1.41	1.33
5	C	904	POV	O31-C31	2.72	1.41	1.33
5	D	904	POV	O31-C31	2.71	1.41	1.33
5	D	902	POV	O31-C31	2.70	1.41	1.33
5	D	903	POV	O31-C31	2.70	1.41	1.33
5	B	905	POV	O31-C31	2.69	1.41	1.33
5	D	905	POV	O31-C31	2.69	1.41	1.33
5	B	903	POV	O31-C31	2.69	1.41	1.33
5	E	201	POV	O31-C31	2.69	1.41	1.33
5	B	904	POV	O21-C2	-2.65	1.40	1.46
5	D	904	POV	O21-C2	-2.60	1.40	1.46
5	A	903	POV	O21-C2	-2.57	1.40	1.46
5	C	903	POV	O21-C2	-2.57	1.40	1.46
5	D	902	POV	O21-C2	-2.57	1.40	1.46
5	B	902	POV	O21-C2	-2.56	1.40	1.46
5	D	905	POV	O21-C2	-2.48	1.40	1.46
5	B	903	POV	O21-C2	-2.47	1.40	1.46
5	A	904	POV	O21-C2	-2.47	1.40	1.46
5	B	905	POV	O21-C2	-2.46	1.40	1.46
5	A	902	POV	O21-C2	-2.46	1.40	1.46
5	C	902	POV	O21-C2	-2.44	1.40	1.46
5	D	903	POV	O21-C2	-2.42	1.40	1.46
5	C	905	POV	O21-C2	-2.34	1.41	1.46
4	D	901	GLU	OXT-C	-2.34	1.23	1.30
4	C	901	GLU	OXT-C	-2.33	1.23	1.30
4	B	901	GLU	OXT-C	-2.32	1.23	1.30
5	E	201	POV	O21-C2	-2.31	1.41	1.46
4	A	901	GLU	OXT-C	-2.30	1.23	1.30
5	C	904	POV	O21-C2	-2.29	1.41	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	905	POV	O21-C21-C22	3.96	120.04	111.48
5	B	903	POV	O21-C21-C22	3.95	120.03	111.48
5	A	902	POV	O21-C21-C22	3.94	120.00	111.48
5	B	905	POV	O21-C21-C22	3.93	119.99	111.48
5	C	902	POV	O21-C21-C22	3.93	119.99	111.48
5	A	903	POV	O21-C21-C22	3.89	119.90	111.48
5	E	201	POV	O21-C21-C22	3.89	119.89	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	POV	O21-C21-C22	3.88	119.87	111.48
5	D	905	POV	O21-C21-C22	3.87	119.85	111.48
5	D	903	POV	O21-C21-C22	3.85	119.80	111.48
5	A	904	POV	O21-C21-C22	3.83	119.77	111.48
5	B	902	POV	O21-C21-C22	3.82	119.75	111.48
5	D	902	POV	O21-C21-C22	3.81	119.72	111.48
5	D	904	POV	O21-C21-C22	3.73	119.55	111.48
5	B	904	POV	O21-C21-C22	3.53	119.13	111.48
5	C	904	POV	O21-C21-C22	3.53	119.12	111.48
4	B	901	GLU	OXT-C-O	-2.81	117.70	124.08
5	C	905	POV	O31-C31-C32	2.81	120.40	111.83
5	D	903	POV	O31-C31-C32	2.80	120.38	111.83
4	D	901	GLU	OXT-C-O	-2.80	117.73	124.08
5	B	905	POV	O31-C31-C32	2.76	120.26	111.83
5	A	902	POV	O31-C31-C32	2.76	120.25	111.83
5	D	904	POV	O31-C31-C32	2.75	120.23	111.83
5	D	905	POV	O31-C31-C32	2.75	120.21	111.83
5	C	902	POV	O31-C31-C32	2.75	120.21	111.83
5	B	904	POV	O31-C31-C32	2.70	120.07	111.83
5	B	903	POV	O31-C31-C32	2.66	119.94	111.83
5	E	201	POV	O31-C31-C32	2.66	119.94	111.83
5	C	903	POV	O31-C31-C32	2.61	119.80	111.83
5	A	903	POV	O31-C31-C32	2.61	119.78	111.83
4	A	901	GLU	OXT-C-O	-2.58	118.24	124.08
4	C	901	GLU	OXT-C-O	-2.56	118.26	124.08
5	D	902	POV	O31-C31-C32	2.54	119.57	111.83
5	A	904	POV	O31-C31-C32	2.54	119.57	111.83
5	C	904	POV	O31-C31-C32	2.54	119.57	111.83
5	B	902	POV	O31-C31-C32	2.51	119.48	111.83
5	D	903	POV	C14-N-C12	2.35	119.24	109.91
5	D	905	POV	C14-N-C12	2.34	119.21	109.91
5	B	903	POV	C14-N-C12	2.33	119.18	109.91
5	B	905	POV	C14-N-C12	2.33	119.15	109.91
5	C	904	POV	C14-N-C12	2.32	119.15	109.91
5	A	902	POV	C14-N-C12	2.32	119.14	109.91
5	A	904	POV	C14-N-C12	2.32	119.13	109.91
5	C	902	POV	C14-N-C12	2.32	119.12	109.91
5	C	905	POV	C14-N-C12	2.30	119.07	109.91
5	D	904	POV	C14-N-C12	2.30	119.07	109.91
5	A	903	POV	C14-N-C12	2.30	119.06	109.91
5	E	201	POV	C14-N-C12	2.30	119.06	109.91
5	D	902	POV	C14-N-C12	2.30	119.06	109.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	POV	C14-N-C12	2.30	119.05	109.91
5	B	904	POV	C14-N-C12	2.30	119.05	109.91
5	C	903	POV	C14-N-C12	2.29	119.02	109.91

There are no chirality outliers.

All (421) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	POV	C1-O11-P-O12
5	A	902	POV	C1-O11-P-O13
5	A	902	POV	C1-O11-P-O14
5	A	902	POV	O12-C11-C12-N
5	A	903	POV	C1-O11-P-O12
5	A	903	POV	C1-O11-P-O13
5	A	903	POV	C11-O12-P-O11
5	A	903	POV	C11-O12-P-O13
5	A	903	POV	C11-O12-P-O14
5	A	903	POV	O12-C11-C12-N
5	A	904	POV	C1-O11-P-O12
5	A	904	POV	C1-O11-P-O14
5	A	904	POV	C11-O12-P-O11
5	A	904	POV	C11-O12-P-O13
5	A	904	POV	C11-O12-P-O14
5	A	904	POV	O12-C11-C12-N
5	B	903	POV	C11-O12-P-O11
5	B	903	POV	C11-O12-P-O13
5	B	903	POV	O12-C11-C12-N
5	B	903	POV	C22-C21-O21-C2
5	B	904	POV	C1-O11-P-O12
5	B	904	POV	C1-O11-P-O14
5	B	904	POV	C11-O12-P-O11
5	B	904	POV	C11-O12-P-O13
5	B	904	POV	C11-O12-P-O14
5	B	904	POV	O12-C11-C12-N
5	B	905	POV	C1-O11-P-O12
5	B	905	POV	C1-O11-P-O14
5	B	905	POV	O11-C1-C2-O21
5	B	905	POV	C22-C21-O21-C2
5	C	902	POV	C1-O11-P-O12
5	C	902	POV	C1-O11-P-O13
5	C	902	POV	C1-O11-P-O14
5	C	902	POV	O12-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	903	POV	C1-O11-P-O12
5	C	903	POV	C1-O11-P-O13
5	C	903	POV	C11-O12-P-O11
5	C	903	POV	C11-O12-P-O13
5	C	903	POV	C11-O12-P-O14
5	C	903	POV	O12-C11-C12-N
5	C	904	POV	C1-O11-P-O12
5	C	904	POV	C1-O11-P-O14
5	C	904	POV	C11-O12-P-O11
5	C	904	POV	C11-O12-P-O13
5	C	904	POV	C11-O12-P-O14
5	C	904	POV	O12-C11-C12-N
5	C	905	POV	O12-C11-C12-N
5	C	905	POV	C22-C21-O21-C2
5	D	903	POV	C11-O12-P-O11
5	D	903	POV	C11-O12-P-O13
5	D	903	POV	O12-C11-C12-N
5	D	903	POV	C22-C21-O21-C2
5	D	904	POV	C1-O11-P-O12
5	D	904	POV	C1-O11-P-O14
5	D	904	POV	C11-O12-P-O11
5	D	904	POV	C11-O12-P-O13
5	D	904	POV	C11-O12-P-O14
5	D	904	POV	O12-C11-C12-N
5	D	905	POV	C1-O11-P-O12
5	D	905	POV	C1-O11-P-O14
5	D	905	POV	O11-C1-C2-O21
5	D	905	POV	C22-C21-O21-C2
5	E	201	POV	C11-O12-P-O11
5	E	201	POV	O12-C11-C12-N
5	E	201	POV	C22-C21-O21-C2
6	A	905	FWF	C23-C20-S2-O3
6	A	905	FWF	C18-N2-S1-O1
6	B	906	FWF	C23-C20-S2-O3
6	B	906	FWF	C24-C20-S2-O3
6	B	906	FWF	C15-N1-S2-O3
6	B	906	FWF	C17-C13-C18-N2
6	B	906	FWF	C18-N2-S1-O1
5	A	904	POV	O22-C21-O21-C2
5	B	903	POV	O22-C21-O21-C2
5	B	905	POV	O22-C21-O21-C2
5	D	903	POV	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	905	POV	O22-C21-O21-C2
5	E	201	POV	O22-C21-O21-C2
5	C	905	POV	O22-C21-O21-C2
5	C	904	POV	C21-C22-C23-C24
5	B	904	POV	C36-C37-C38-C39
5	A	904	POV	C39-C310-C311-C312
5	A	904	POV	C22-C21-O21-C2
5	D	902	POV	C24-C25-C26-C27
5	C	904	POV	C39-C310-C311-C312
5	C	902	POV	C21-C22-C23-C24
5	B	902	POV	C24-C25-C26-C27
5	D	904	POV	C36-C37-C38-C39
5	C	903	POV	C34-C35-C36-C37
5	D	902	POV	C22-C23-C24-C25
5	B	902	POV	C32-C31-O31-C3
5	D	902	POV	C32-C31-O31-C3
5	A	903	POV	C34-C35-C36-C37
5	A	902	POV	C21-C22-C23-C24
5	B	902	POV	C22-C23-C24-C25
5	B	905	POV	C39-C310-C311-C312
5	C	904	POV	C25-C26-C27-C28
5	B	905	POV	C21-C22-C23-C24
5	B	903	POV	C23-C24-C25-C26
5	C	905	POV	C311-C312-C313-C314
5	A	904	POV	C25-C26-C27-C28
5	D	905	POV	C32-C33-C34-C35
5	E	201	POV	C311-C312-C313-C314
5	E	201	POV	C32-C33-C34-C35
5	B	905	POV	C311-C312-C313-C314
5	B	902	POV	C21-C22-C23-C24
5	B	904	POV	C311-C312-C313-C314
5	A	903	POV	C21-C22-C23-C24
5	C	905	POV	C31-C32-C33-C34
5	D	902	POV	C21-C22-C23-C24
6	B	906	FWF	C15-N1-S2-C20
5	C	903	POV	C21-C22-C23-C24
5	D	905	POV	C21-C22-C23-C24
5	E	201	POV	C21-C22-C23-C24
5	B	902	POV	O32-C31-O31-C3
5	D	902	POV	O32-C31-O31-C3
5	C	905	POV	C39-C310-C311-C312
5	B	903	POV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	201	POV	C39-C310-C311-C312
5	D	905	POV	C34-C35-C36-C37
5	B	904	POV	C33-C34-C35-C36
5	E	201	POV	C213-C214-C215-C216
5	C	905	POV	C21-C22-C23-C24
5	A	904	POV	C36-C37-C38-C39
5	D	904	POV	C33-C34-C35-C36
6	A	905	FWF	C11-C10-C4-C3
5	B	904	POV	C39-C310-C311-C312
5	D	905	POV	C311-C312-C313-C314
5	D	903	POV	C210-C211-C212-C213
5	D	905	POV	C24-C25-C26-C27
5	A	903	POV	C213-C214-C215-C216
5	C	902	POV	C311-C310-C39-C38
5	C	905	POV	C213-C214-C215-C216
5	D	903	POV	C24-C25-C26-C27
5	D	904	POV	C24-C25-C26-C27
5	A	903	POV	C36-C37-C38-C39
5	A	904	POV	C213-C214-C215-C216
5	A	904	POV	C32-C33-C34-C35
5	B	903	POV	C311-C312-C313-C314
5	B	905	POV	C24-C25-C26-C27
5	D	903	POV	C311-C310-C39-C38
5	D	903	POV	C211-C212-C213-C214
5	C	902	POV	C22-C23-C24-C25
5	C	902	POV	C36-C37-C38-C39
5	D	903	POV	C35-C36-C37-C38
5	D	903	POV	C36-C37-C38-C39
5	A	902	POV	C214-C215-C216-C217
5	B	904	POV	C37-C38-C39-C310
5	D	902	POV	C213-C214-C215-C216
5	D	904	POV	C35-C36-C37-C38
5	A	902	POV	C22-C23-C24-C25
5	C	902	POV	C311-C312-C313-C314
5	D	903	POV	C311-C312-C313-C314
5	D	905	POV	C39-C310-C311-C312
5	E	201	POV	C34-C35-C36-C37
5	B	904	POV	C35-C36-C37-C38
5	B	902	POV	C213-C214-C215-C216
5	A	904	POV	C24-C25-C26-C27
5	A	903	POV	C31-C32-C33-C34
5	C	903	POV	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	903	POV	C25-C26-C27-C28
5	C	903	POV	C311-C312-C313-C314
5	C	903	POV	C36-C37-C38-C39
5	C	905	POV	C32-C33-C34-C35
5	B	903	POV	C36-C37-C38-C39
5	C	904	POV	C22-C23-C24-C25
5	C	904	POV	C213-C214-C215-C216
6	B	906	FWF	C18-N2-S1-C19
5	D	905	POV	C25-C26-C27-C28
5	C	905	POV	C35-C36-C37-C38
5	D	904	POV	C37-C38-C39-C310
5	A	904	POV	C35-C36-C37-C38
5	C	902	POV	C214-C215-C216-C217
5	D	902	POV	C36-C37-C38-C39
5	C	905	POV	C34-C35-C36-C37
5	A	902	POV	C37-C38-C39-C310
5	B	904	POV	C311-C310-C39-C38
5	A	903	POV	C39-C310-C311-C312
5	D	904	POV	C311-C310-C39-C38
5	E	201	POV	C35-C36-C37-C38
5	C	903	POV	C22-C23-C24-C25
5	B	902	POV	C214-C215-C216-C217
5	B	903	POV	C22-C23-C24-C25
5	B	904	POV	C24-C25-C26-C27
5	D	904	POV	C23-C24-C25-C26
5	B	905	POV	C312-C313-C314-C315
5	A	902	POV	C32-C33-C34-C35
5	C	903	POV	C39-C310-C311-C312
5	D	905	POV	C311-C310-C39-C38
5	A	903	POV	C310-C311-C312-C313
5	A	904	POV	O11-C1-C2-O21
5	B	904	POV	C211-C212-C213-C214
5	C	902	POV	C211-C212-C213-C214
5	B	903	POV	C31-C32-C33-C34
5	C	904	POV	C26-C27-C28-C29
5	A	902	POV	C213-C214-C215-C216
5	B	904	POV	C27-C28-C29-C210
5	B	903	POV	C24-C25-C26-C27
5	B	904	POV	C25-C26-C27-C28
6	A	905	FWF	C18-N2-S1-C19
5	A	902	POV	C39-C310-C311-C312
5	C	902	POV	C213-C214-C215-C216

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	902	POV	C215-C216-C217-C218
5	B	902	POV	C36-C37-C38-C39
5	E	201	POV	C22-C23-C24-C25
5	A	904	POV	C26-C27-C28-C29
5	A	902	POV	C211-C212-C213-C214
5	D	904	POV	C22-C23-C24-C25
5	A	904	POV	O11-C1-C2-C3
5	B	905	POV	O11-C1-C2-C3
6	A	905	FWF	C9-C10-C4-C3
5	C	903	POV	C311-C310-C39-C38
5	C	903	POV	C32-C33-C34-C35
5	A	902	POV	C31-C32-C33-C34
5	C	903	POV	C25-C26-C27-C28
5	A	903	POV	C22-C23-C24-C25
5	A	903	POV	C32-C31-O31-C3
5	B	902	POV	C1-C2-C3-O31
5	D	902	POV	C1-C2-C3-O31
5	D	903	POV	C1-C2-C3-O31
5	D	903	POV	C26-C27-C28-C29
5	C	905	POV	C24-C25-C26-C27
5	D	903	POV	C33-C34-C35-C36
5	D	904	POV	C310-C311-C312-C313
5	B	905	POV	C32-C31-O31-C3
5	B	905	POV	C36-C37-C38-C39
5	A	903	POV	C311-C310-C39-C38
5	D	904	POV	C34-C35-C36-C37
5	E	201	POV	C24-C25-C26-C27
6	B	906	FWF	C11-C10-C4-C3
5	E	201	POV	C1-C2-O21-C21
5	B	902	POV	C26-C27-C28-C29
5	C	904	POV	C24-C25-C26-C27
5	A	903	POV	O32-C31-O31-C3
5	B	904	POV	C34-C35-C36-C37
5	B	902	POV	C215-C216-C217-C218
5	D	903	POV	C22-C23-C24-C25
5	C	903	POV	O21-C2-C3-O31
5	C	903	POV	C32-C31-O31-C3
5	D	905	POV	C36-C37-C38-C39
5	B	903	POV	C215-C216-C217-C218
5	C	902	POV	C35-C36-C37-C38
5	E	201	POV	C36-C37-C38-C39
5	C	903	POV	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	903	POV	C34-C35-C36-C37
5	D	905	POV	O11-C1-C2-C3
5	A	903	POV	C212-C213-C214-C215
5	A	903	POV	C32-C33-C34-C35
5	D	903	POV	C310-C311-C312-C313
5	B	905	POV	C313-C314-C315-C316
5	B	905	POV	O32-C31-O31-C3
5	C	903	POV	C310-C311-C312-C313
5	A	904	POV	C22-C23-C24-C25
5	B	905	POV	C1-C2-C3-O31
5	D	905	POV	C1-C2-C3-O31
5	B	904	POV	C22-C23-C24-C25
5	E	201	POV	C33-C34-C35-C36
5	D	904	POV	C215-C216-C217-C218
5	D	904	POV	C311-C312-C313-C314
5	C	902	POV	C31-C32-C33-C34
5	C	905	POV	C22-C23-C24-C25
5	B	905	POV	C22-C23-C24-C25
5	A	902	POV	O21-C2-C3-O31
5	B	902	POV	O21-C2-C3-O31
5	B	905	POV	O21-C2-C3-O31
5	C	902	POV	O21-C2-C3-O31
5	D	902	POV	O21-C2-C3-O31
5	D	905	POV	C22-C23-C24-C25
5	B	902	POV	C35-C36-C37-C38
5	E	201	POV	C311-C310-C39-C38
5	B	905	POV	C32-C33-C34-C35
5	B	903	POV	C211-C212-C213-C214
5	E	201	POV	O11-C1-C2-C3
5	B	902	POV	C311-C310-C39-C38
5	B	904	POV	C213-C214-C215-C216
5	D	904	POV	C213-C214-C215-C216
5	C	903	POV	O32-C31-O31-C3
5	C	904	POV	C22-C21-O21-C2
5	C	904	POV	C32-C33-C34-C35
5	A	904	POV	C3-C2-O21-C21
5	B	903	POV	C1-C2-O21-C21
5	C	904	POV	C1-C2-O21-C21
5	B	903	POV	C26-C27-C28-C29
5	A	902	POV	O11-C1-C2-O21
5	C	902	POV	O11-C1-C2-O21
5	E	201	POV	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	902	POV	C1-C2-C3-O31
5	B	903	POV	C1-C2-C3-O31
5	C	902	POV	C1-C2-C3-O31
5	C	902	POV	C32-C33-C34-C35
5	B	903	POV	C33-C34-C35-C36
5	D	902	POV	C32-C33-C34-C35
5	B	903	POV	O21-C2-C3-O31
5	C	905	POV	O21-C2-C3-O31
5	D	905	POV	O21-C2-C3-O31
5	C	905	POV	C311-C310-C39-C38
5	C	905	POV	C33-C34-C35-C36
6	B	906	FWF	C9-C10-C4-C3
5	D	902	POV	C311-C310-C39-C38
5	B	902	POV	O12-C11-C12-N
5	B	905	POV	O12-C11-C12-N
5	D	902	POV	O12-C11-C12-N
5	D	905	POV	O12-C11-C12-N
5	C	904	POV	O22-C21-O21-C2
5	C	905	POV	C36-C37-C38-C39
5	D	902	POV	C34-C35-C36-C37
5	D	903	POV	C25-C26-C27-C28
5	B	905	POV	C311-C310-C39-C38
5	C	904	POV	C310-C311-C312-C313
5	A	902	POV	O11-C1-C2-C3
5	C	902	POV	O11-C1-C2-C3
5	C	904	POV	C37-C38-C39-C310
5	C	905	POV	C23-C24-C25-C26
5	A	903	POV	C24-C25-C26-C27
5	A	902	POV	C23-C24-C25-C26
5	B	903	POV	C210-C211-C212-C213
5	C	903	POV	C24-C25-C26-C27
5	A	904	POV	C310-C311-C312-C313
5	A	904	POV	C1-O11-P-O13
5	B	903	POV	C1-O11-P-O12
5	B	904	POV	C1-O11-P-O13
5	C	904	POV	C1-O11-P-O13
5	C	905	POV	C1-O11-P-O14
5	C	905	POV	C11-O12-P-O14
5	D	904	POV	C1-O11-P-O13
5	E	201	POV	C11-O12-P-O14
6	B	906	FWF	C23-C20-S2-O4
6	B	906	FWF	C24-C20-S2-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	904	POV	C2-C1-O11-P
5	D	903	POV	C37-C38-C39-C310
5	B	904	POV	C313-C314-C315-C316
5	C	902	POV	C27-C28-C29-C210
5	B	905	POV	C1-C2-O21-C21
5	C	905	POV	C1-C2-O21-C21
5	D	903	POV	C1-C2-O21-C21
5	B	905	POV	C213-C214-C215-C216
5	A	902	POV	C27-C28-C29-C210
5	D	903	POV	O21-C2-C3-O31
6	A	905	FWF	C11-C10-C4-C5
5	E	201	POV	C212-C213-C214-C215
5	D	902	POV	C26-C27-C28-C29
5	C	903	POV	C1-C2-C3-O31
5	C	905	POV	C1-C2-C3-O31
5	D	903	POV	C21-C22-C23-C24
5	C	902	POV	C23-C24-C25-C26
5	B	902	POV	C212-C213-C214-C215
5	D	903	POV	C32-C33-C34-C35
5	B	905	POV	C310-C311-C312-C313
5	B	903	POV	C27-C28-C29-C210
5	D	904	POV	C211-C212-C213-C214
5	E	201	POV	C23-C24-C25-C26
6	B	906	FWF	C11-C10-C4-C5
5	A	902	POV	C36-C37-C38-C39
5	D	902	POV	C31-C32-C33-C34
5	A	904	POV	C212-C213-C214-C215
5	B	902	POV	O31-C31-C32-C33
5	A	902	POV	C34-C35-C36-C37
5	A	904	POV	C311-C310-C39-C38
5	D	903	POV	C27-C28-C29-C210
5	D	905	POV	C2-C1-O11-P
5	A	903	POV	O21-C2-C3-O31
5	A	903	POV	C35-C36-C37-C38
5	B	905	POV	C29-C210-C211-C212
5	D	902	POV	O31-C31-C32-C33
5	C	903	POV	C29-C210-C211-C212
5	B	905	POV	C2-C1-O11-P
5	A	902	POV	C29-C210-C211-C212
5	A	903	POV	C29-C210-C211-C212
5	C	904	POV	C29-C210-C211-C212
5	D	904	POV	C27-C28-C29-C210

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	904	POV	C34-C35-C36-C37
5	B	905	POV	C3-C2-O21-C21
5	D	905	POV	C1-C2-O21-C21
5	D	905	POV	C3-C2-O21-C21
5	C	902	POV	C29-C210-C211-C212
5	C	905	POV	C27-C28-C29-C210
5	E	201	POV	C27-C28-C29-C210
5	C	905	POV	C212-C213-C214-C215
5	B	904	POV	C29-C210-C211-C212
5	B	905	POV	C35-C36-C37-C38
5	A	903	POV	C27-C28-C29-C210
5	C	903	POV	C27-C28-C29-C210
5	A	902	POV	C311-C312-C313-C314
5	B	905	POV	O31-C31-C32-C33
5	C	903	POV	O21-C21-C22-C23
5	D	904	POV	C29-C210-C211-C212
5	A	903	POV	C37-C38-C39-C310
5	D	905	POV	C29-C210-C211-C212
5	B	905	POV	O21-C21-C22-C23
5	D	905	POV	O21-C21-C22-C23
5	A	904	POV	C11-C12-N-C15
5	B	903	POV	O21-C21-C22-C23
5	E	201	POV	O31-C31-C32-C33
5	C	904	POV	C11-C12-N-C15
5	D	902	POV	C212-C213-C214-C215
5	D	903	POV	O21-C21-C22-C23
5	D	905	POV	C31-C32-C33-C34
5	B	902	POV	C34-C35-C36-C37
5	A	904	POV	C11-C12-N-C13
5	C	904	POV	C11-C12-N-C13
5	B	903	POV	C311-C310-C39-C38
5	D	904	POV	C25-C26-C27-C28
5	C	903	POV	O22-C21-C22-C23
5	B	905	POV	O22-C21-C22-C23
5	D	905	POV	O22-C21-C22-C23
5	B	904	POV	C23-C24-C25-C26
5	D	903	POV	C34-C35-C36-C37
4	B	901	GLU	OXT-C-CA-N
4	D	901	GLU	OXT-C-CA-N
5	B	903	POV	O22-C21-C22-C23
5	B	905	POV	O32-C31-C32-C33
5	D	903	POV	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	904	POV	O21-C21-C22-C23
5	E	201	POV	O32-C31-C32-C33
5	B	903	POV	O32-C31-O31-C3
5	B	903	POV	C214-C215-C216-C217
5	A	902	POV	C25-C26-C27-C28
5	C	903	POV	C215-C216-C217-C218
5	B	903	POV	C35-C36-C37-C38
5	C	904	POV	C212-C213-C214-C215
5	A	904	POV	C34-C35-C36-C37

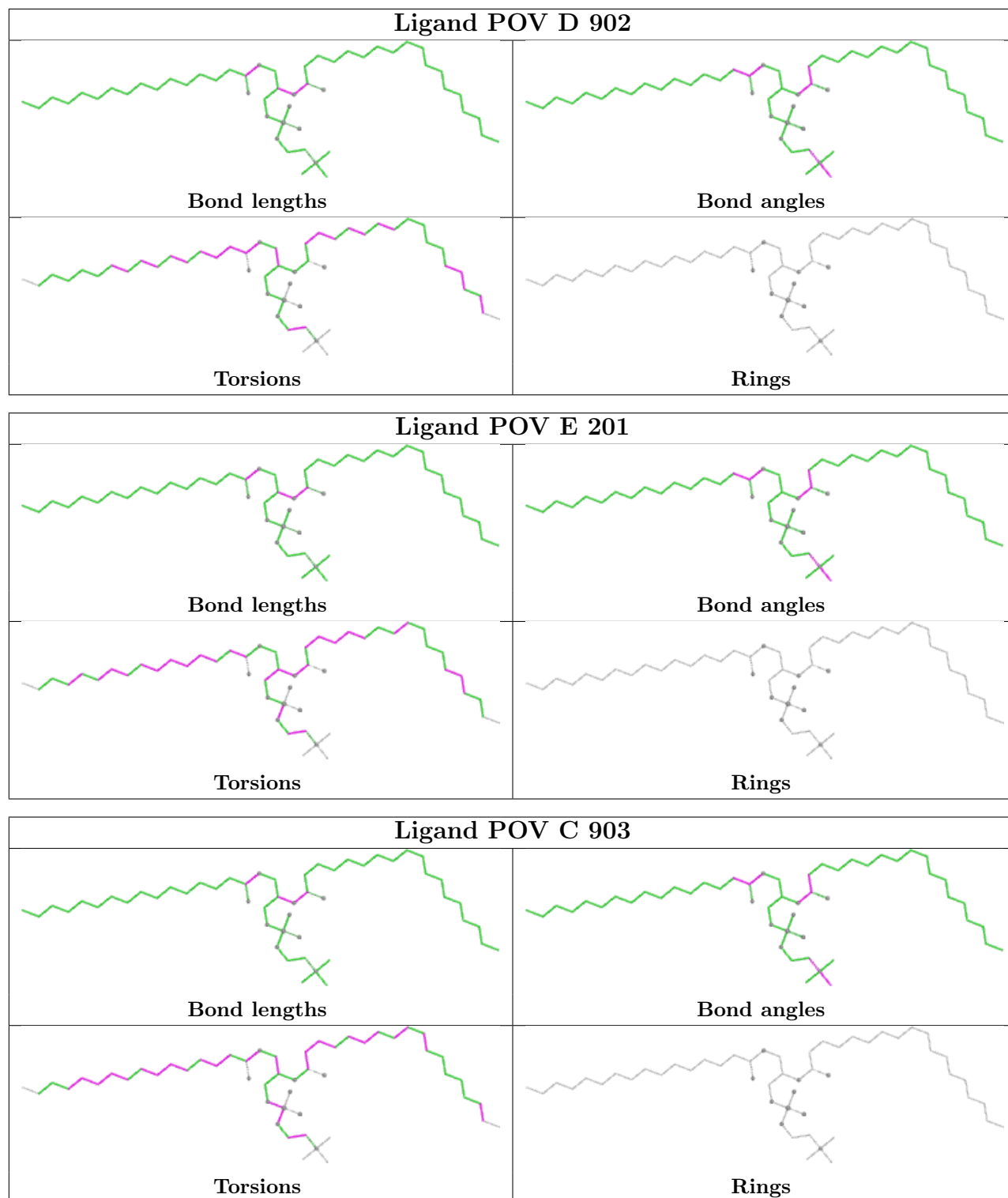
There are no ring outliers.

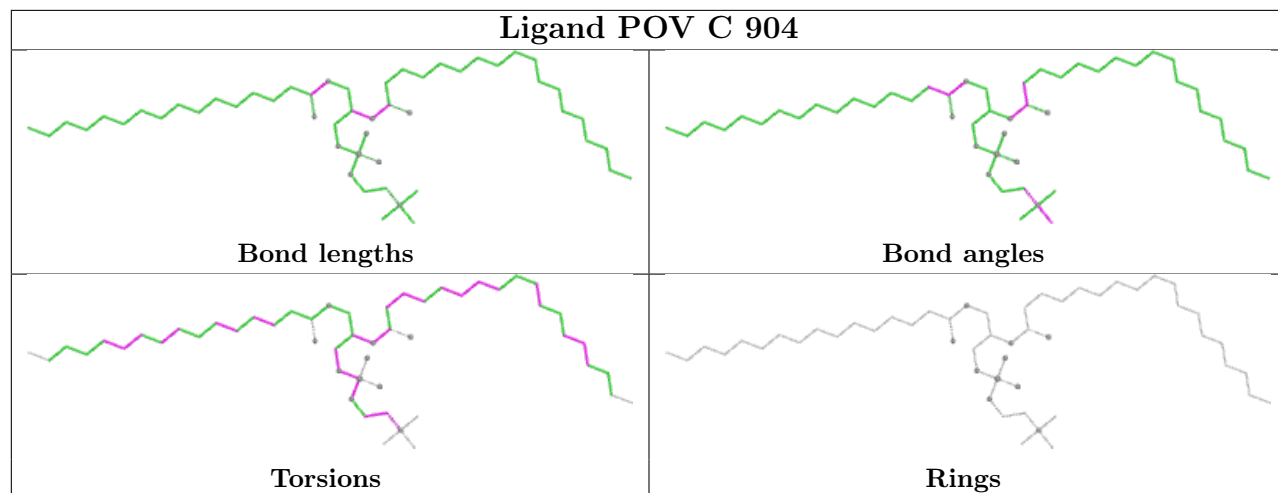
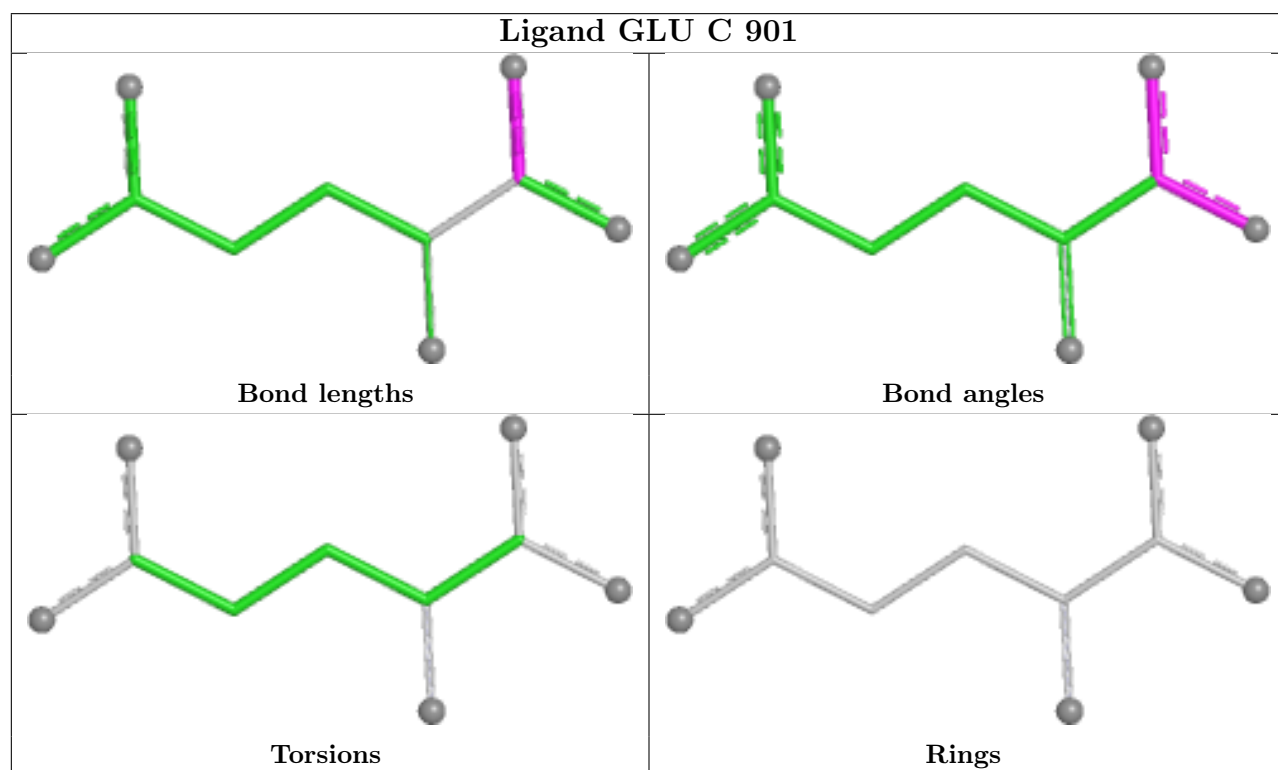
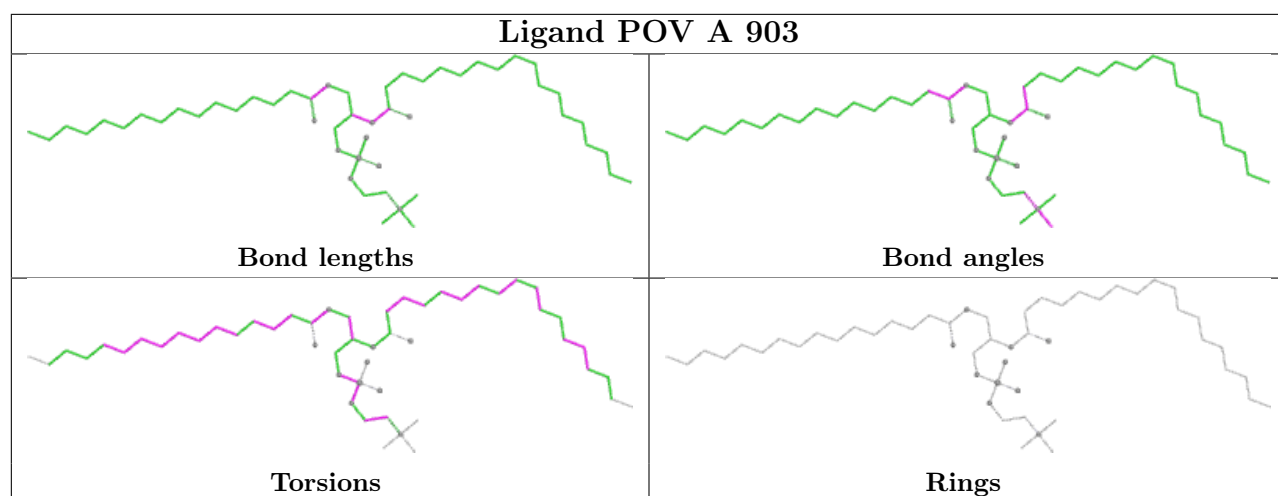
18 monomers are involved in 128 short contacts:

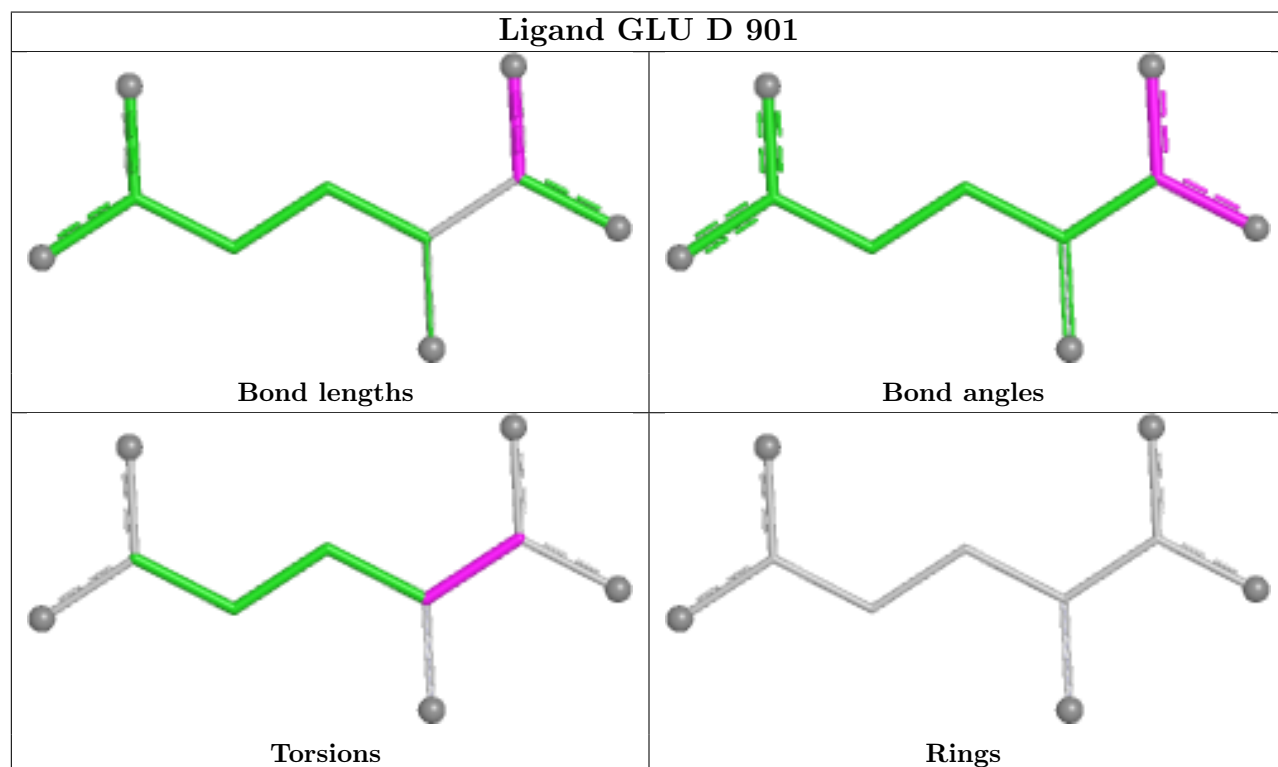
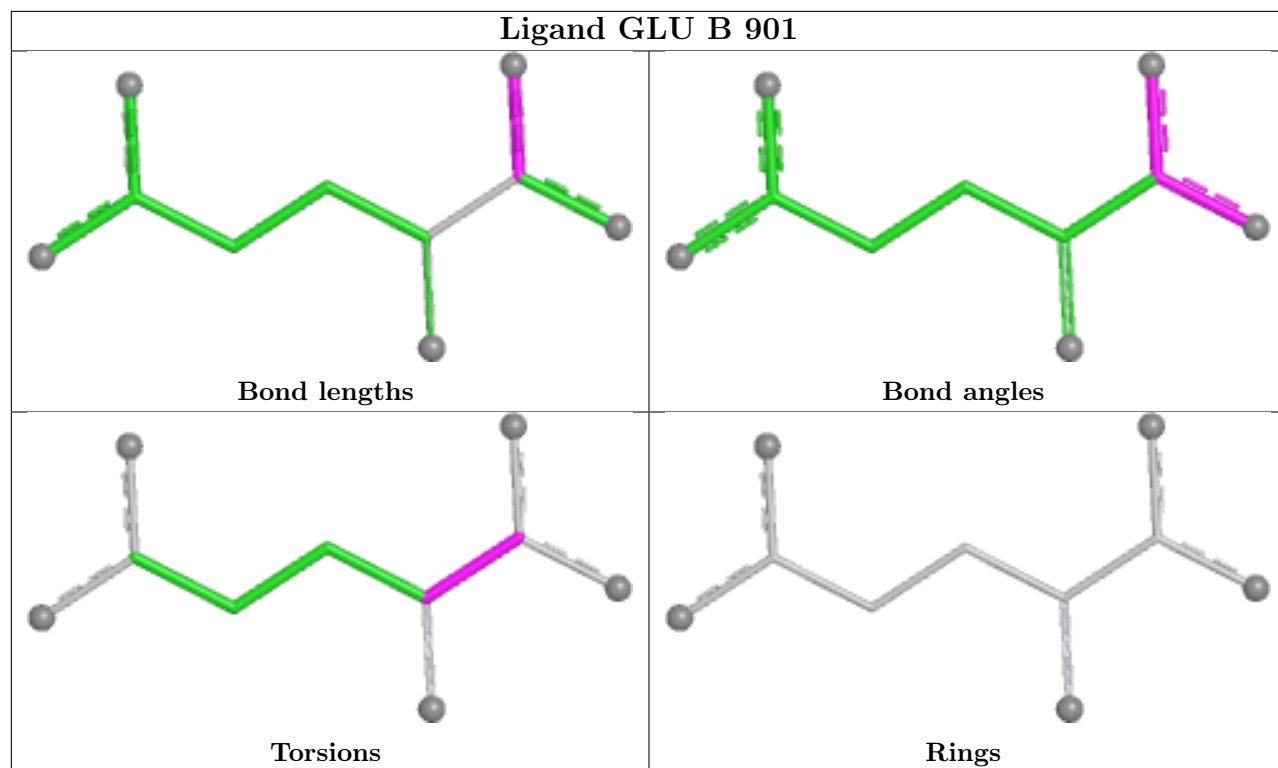
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	902	POV	13	0
5	E	201	POV	12	0
5	C	903	POV	4	0
5	A	903	POV	2	0
5	C	904	POV	11	0
4	B	901	GLU	1	0
4	D	901	GLU	1	0
5	D	905	POV	10	0
5	C	902	POV	3	0
5	B	903	POV	6	0
5	D	903	POV	9	0
5	B	904	POV	11	0
5	A	904	POV	18	0
5	B	905	POV	19	0
5	B	902	POV	12	0
5	A	902	POV	3	0
5	D	904	POV	9	0
5	C	905	POV	7	0

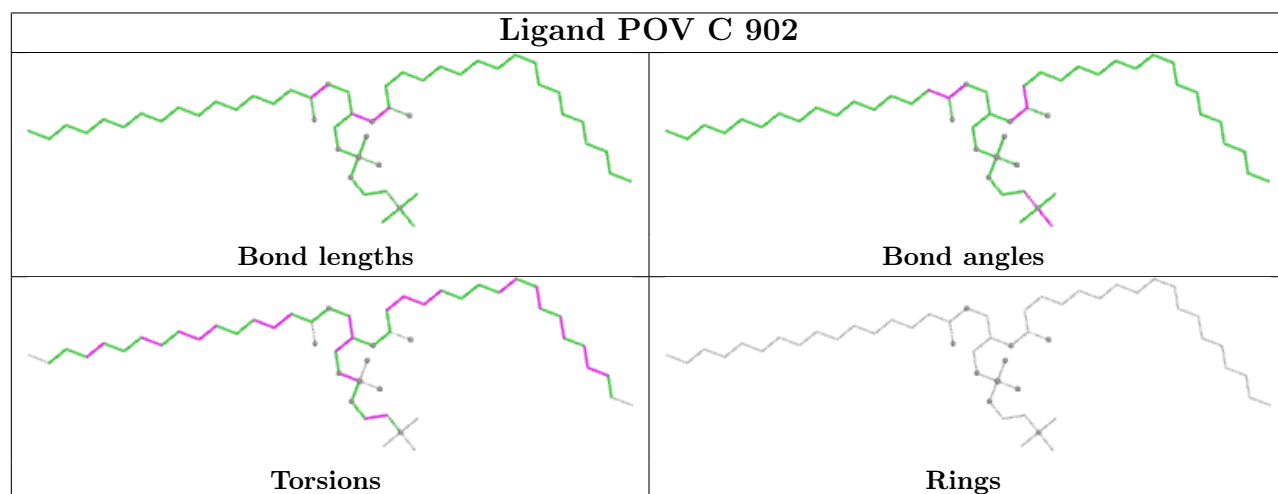
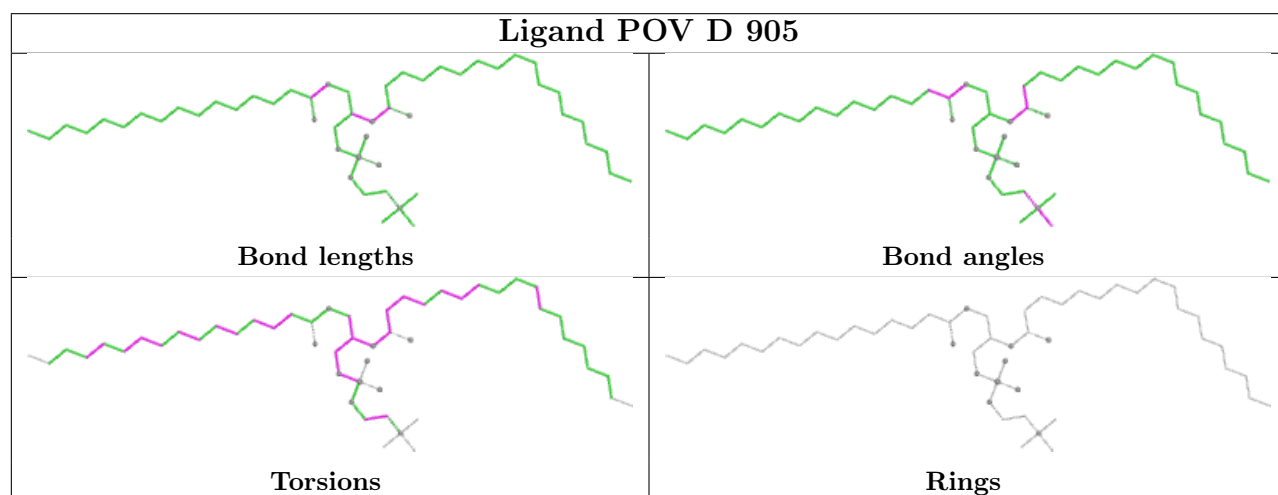
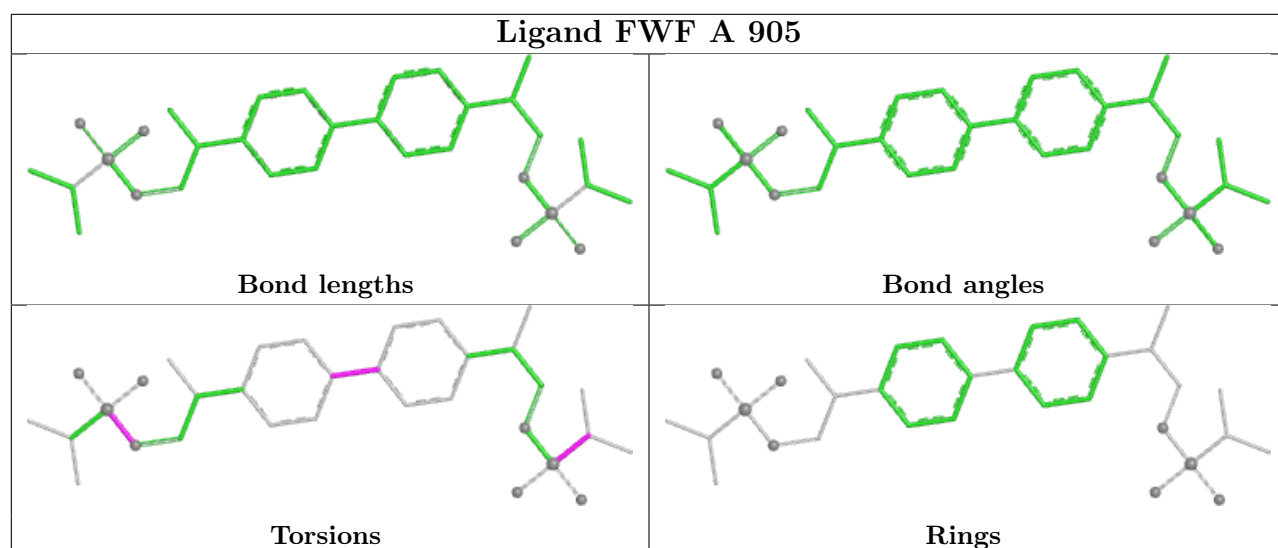
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

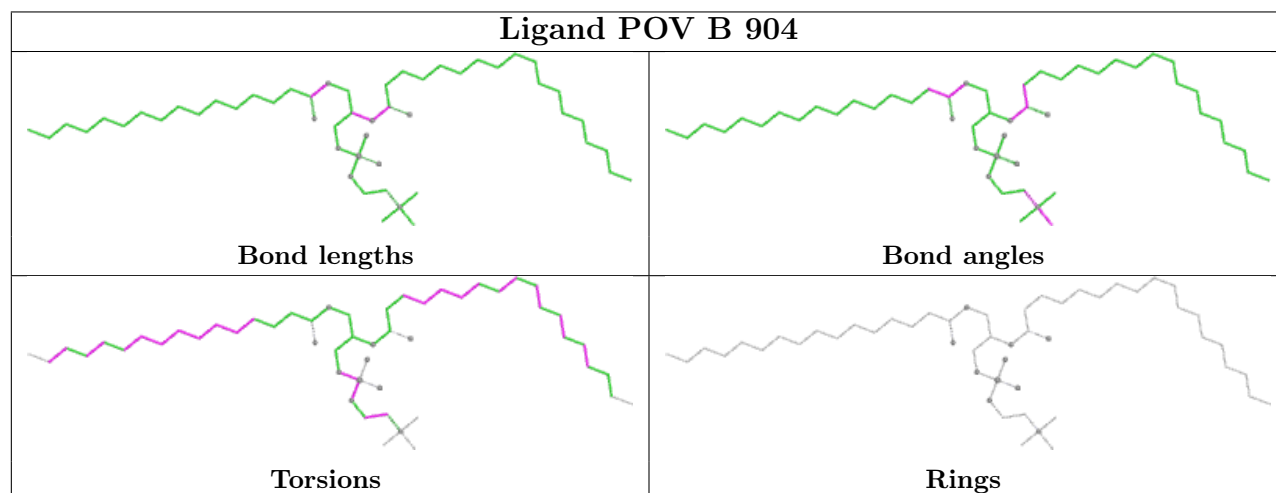
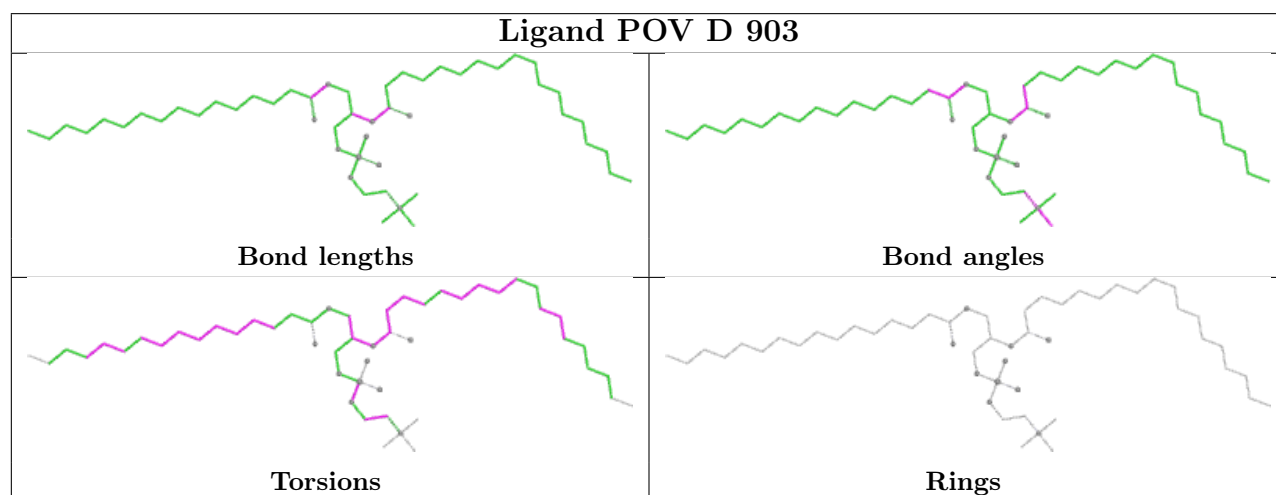
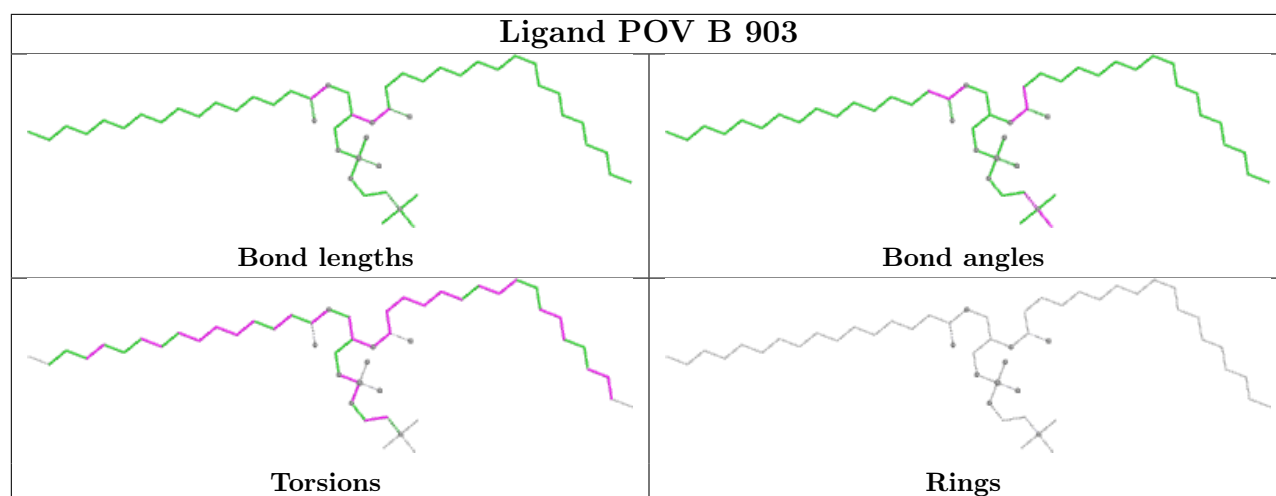
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

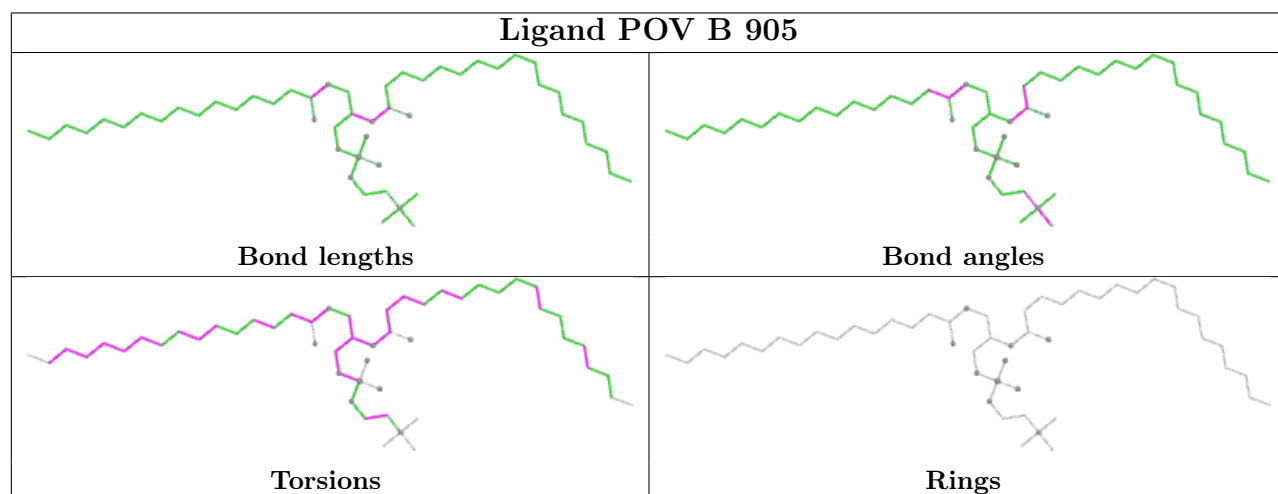
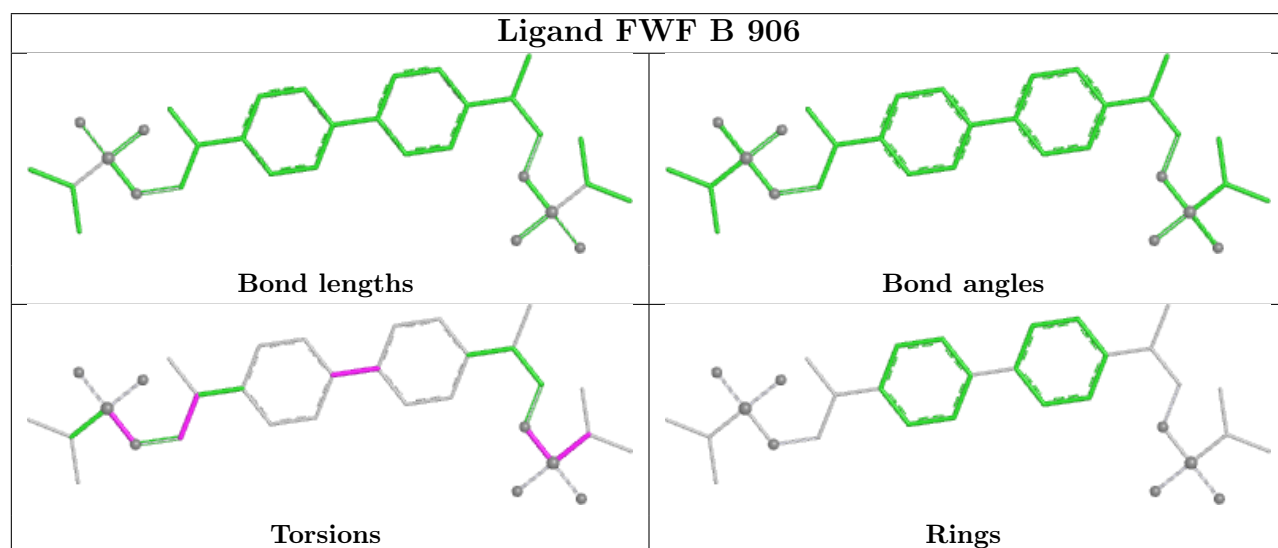
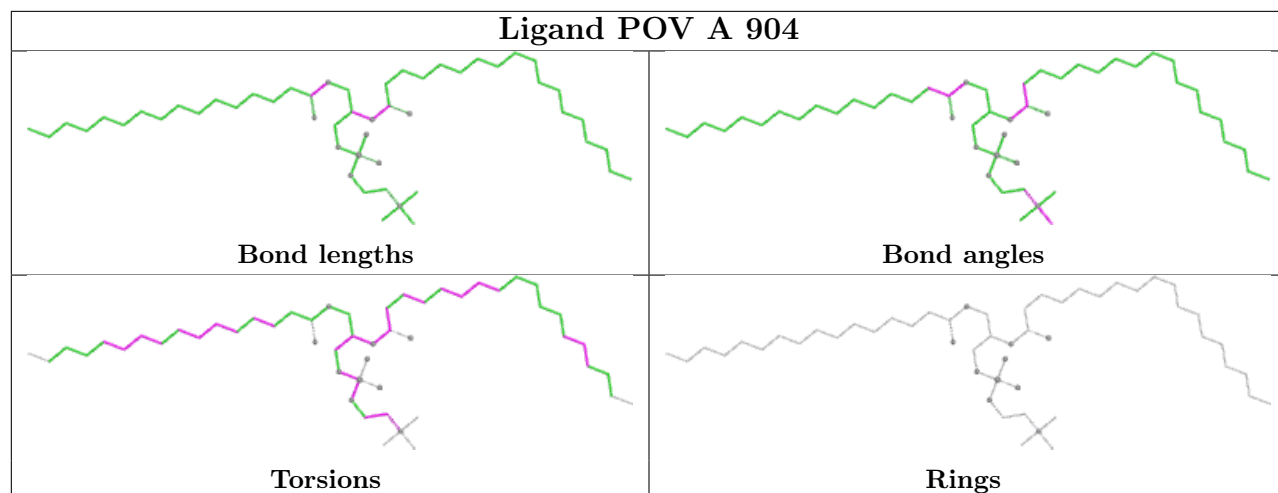


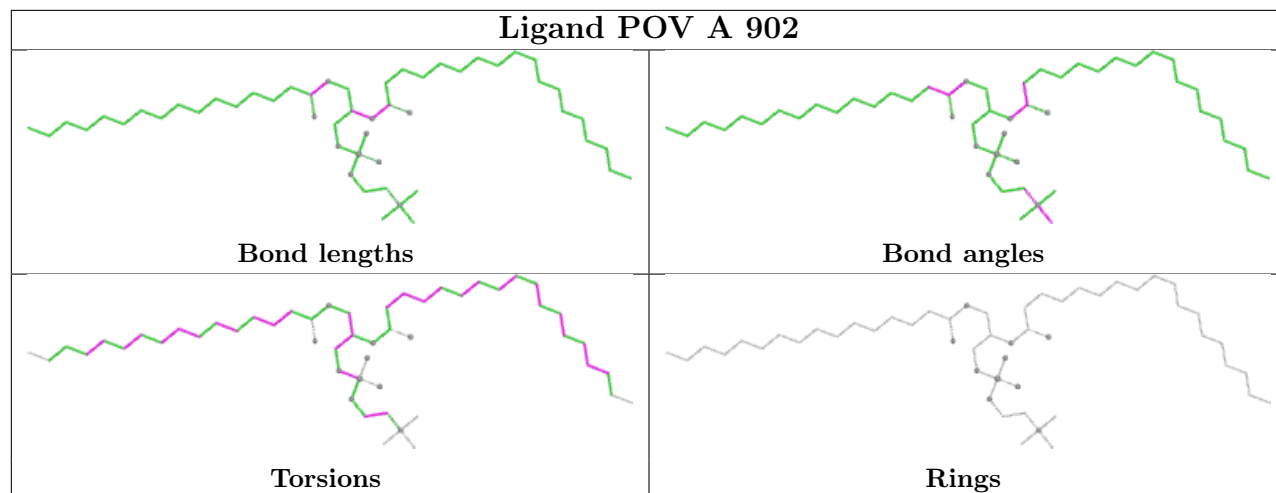
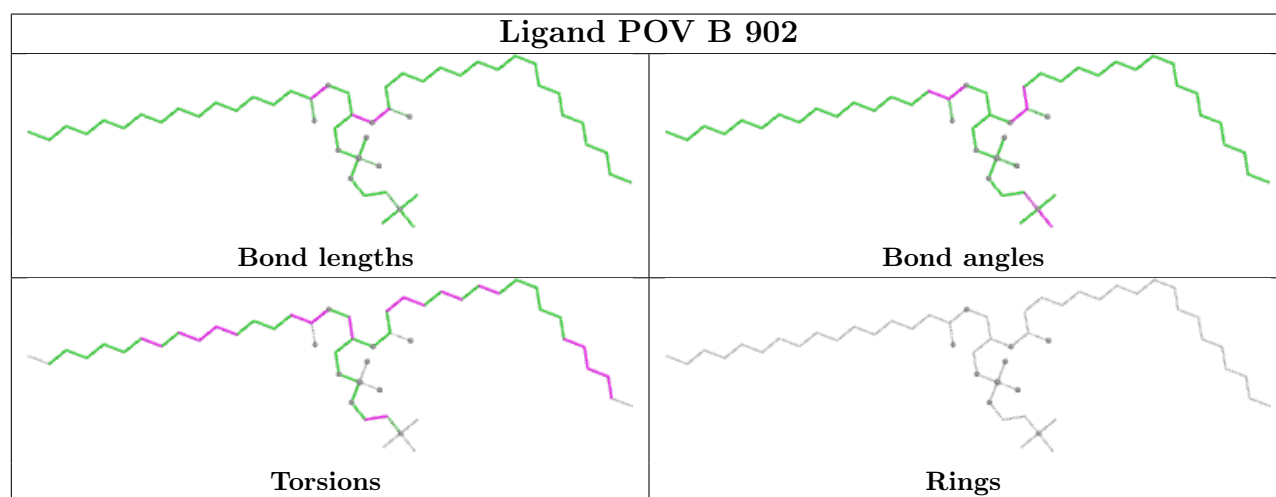
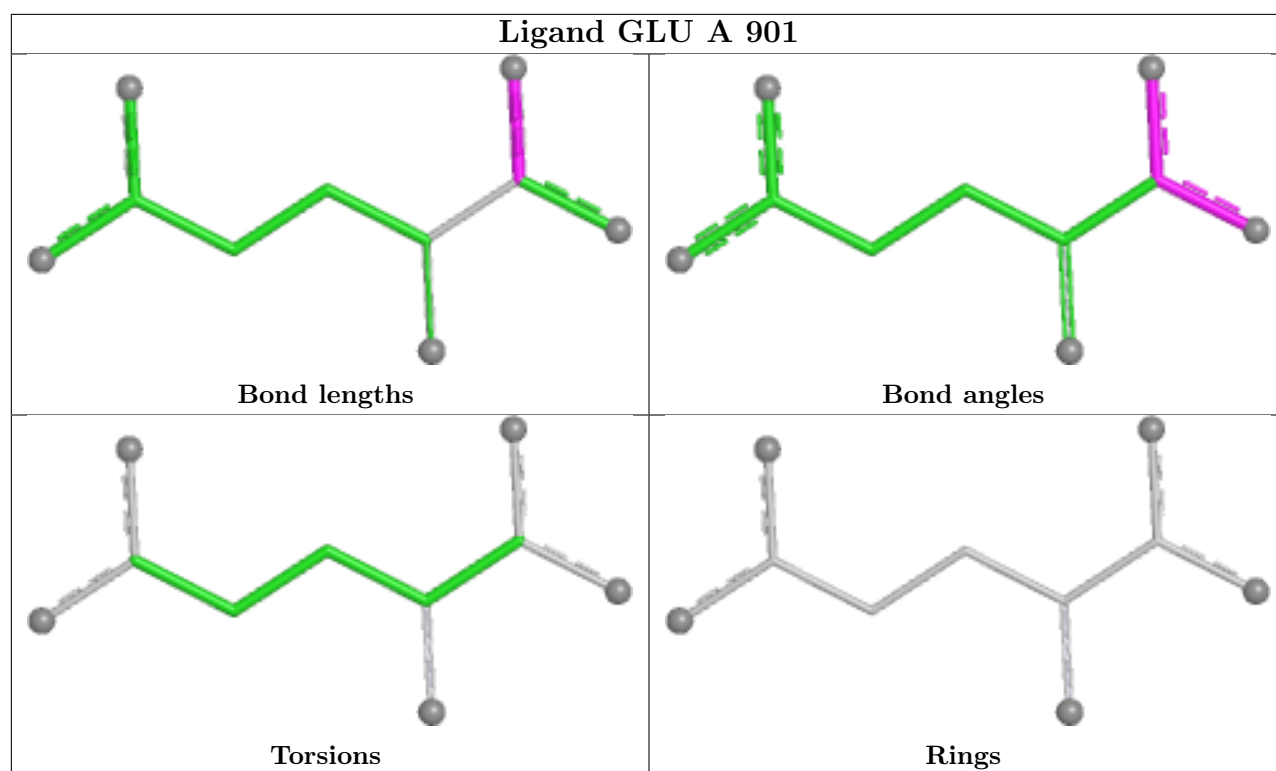


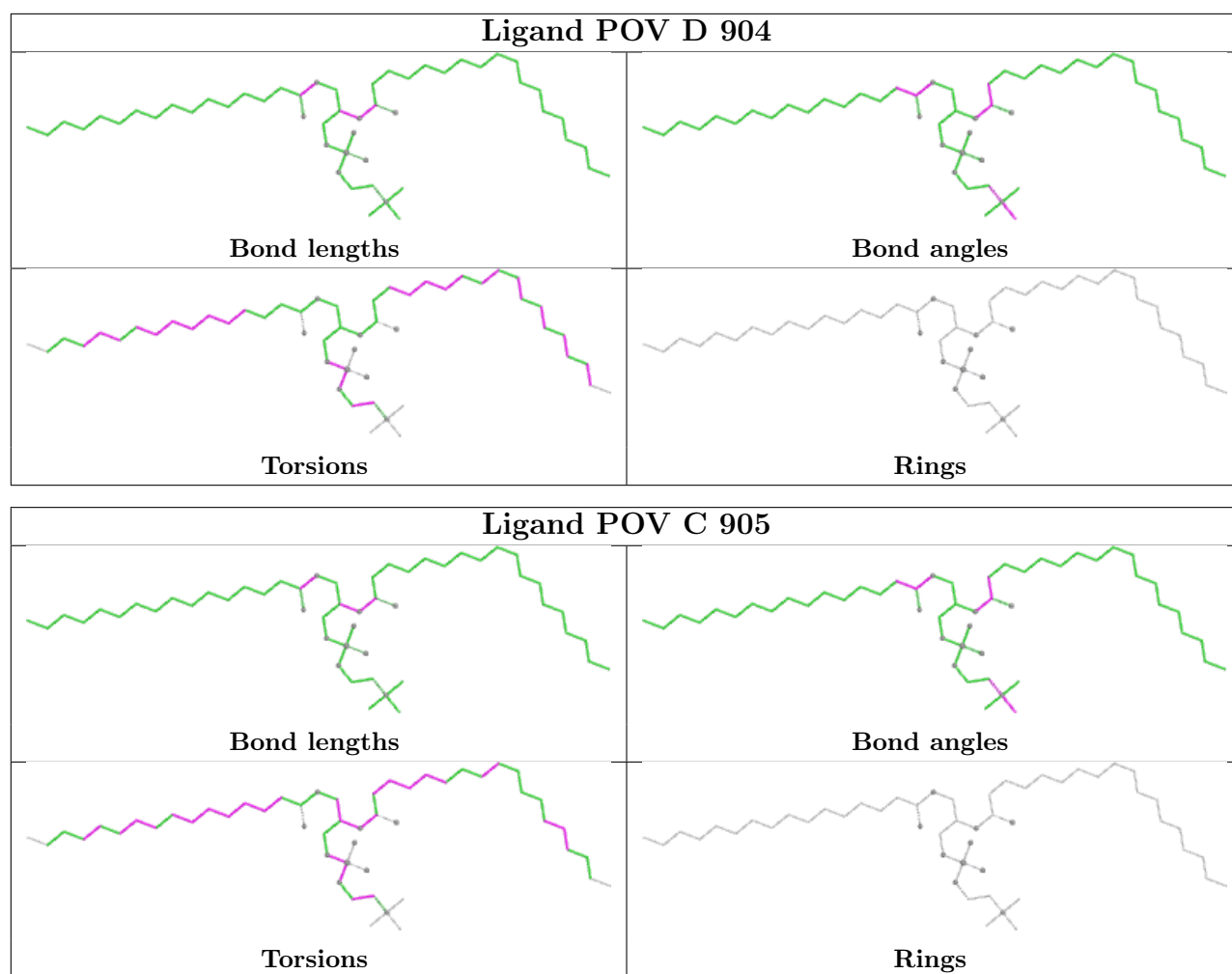












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

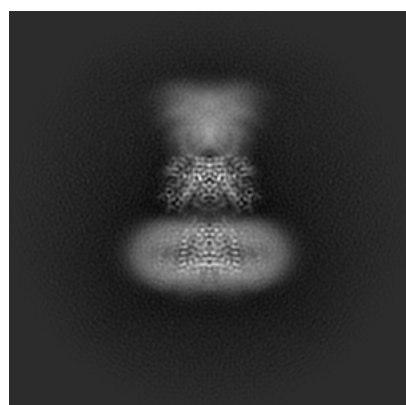
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70920. These allow visual inspection of the internal detail of the map and identification of artifacts.

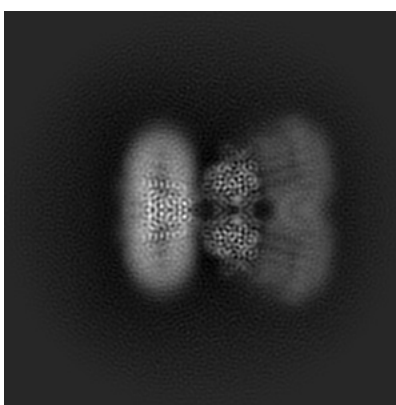
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

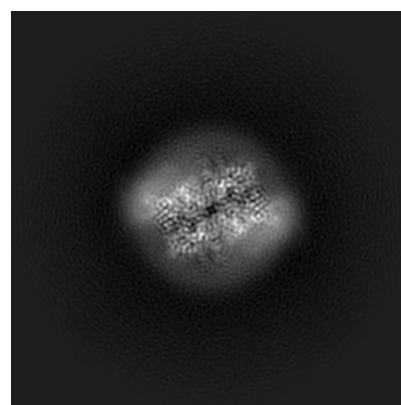
6.1.1 Primary map



X



Y

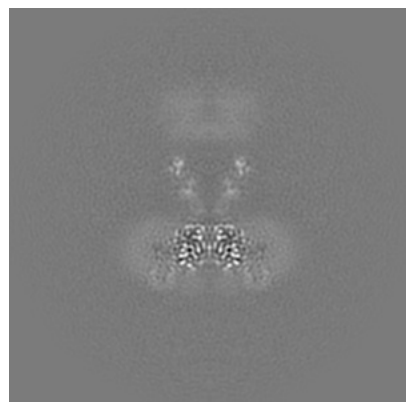


Z

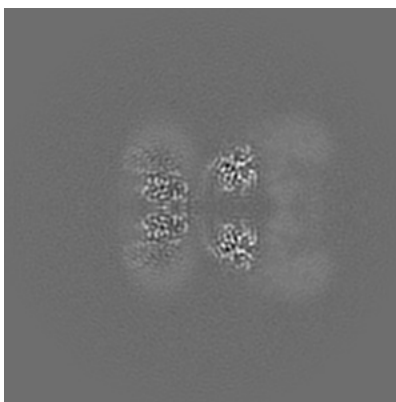
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

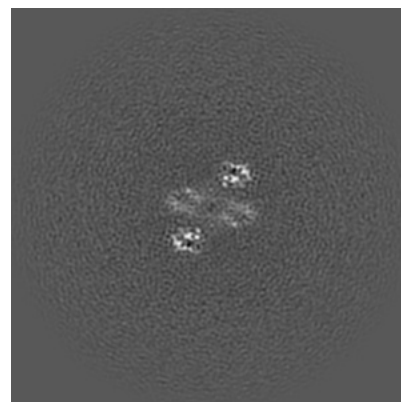
6.2.1 Primary map



X Index: 208



Y Index: 208

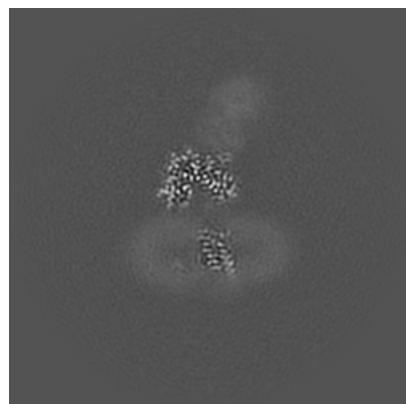


Z Index: 208

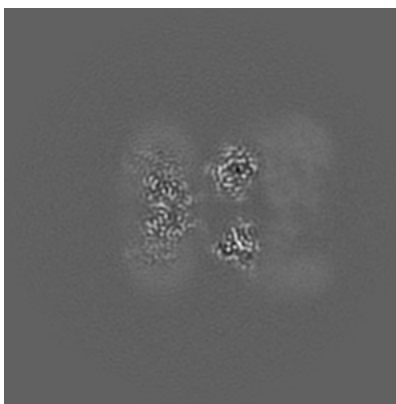
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

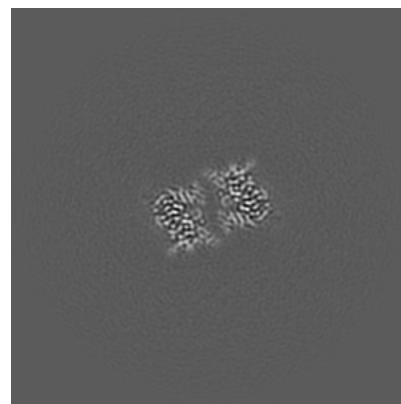
6.3.1 Primary map



X Index: 179



Y Index: 203

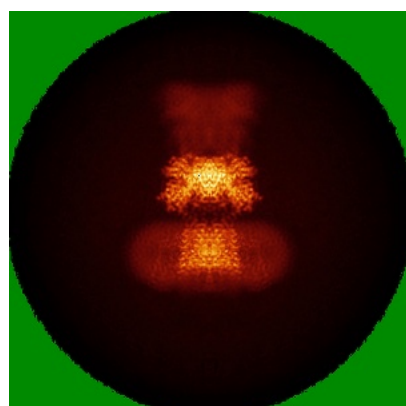


Z Index: 245

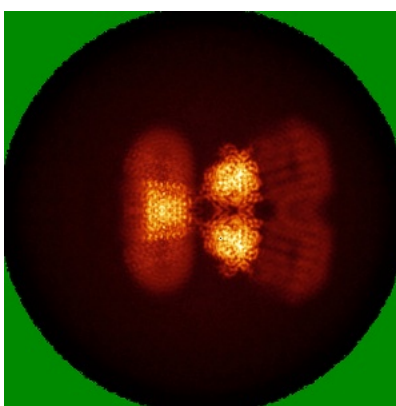
The images above show the largest variance slices of the map in three orthogonal directions.

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

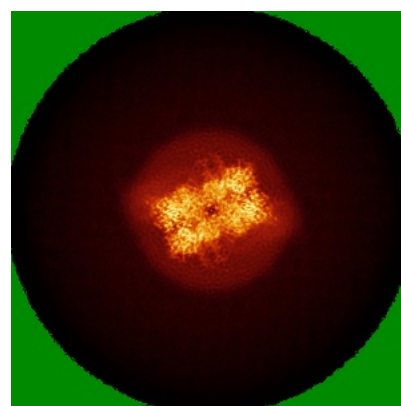
6.4.1 Primary map



X



Y

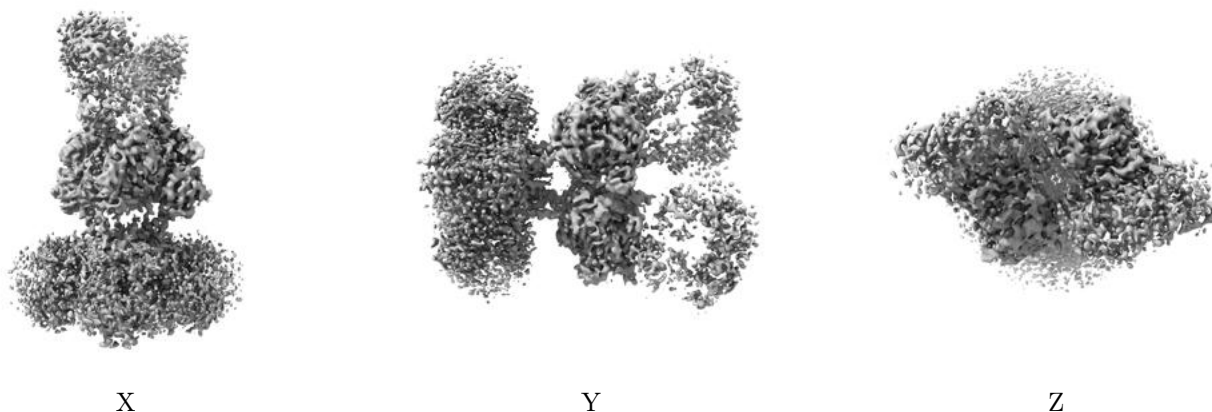


Z

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 4.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

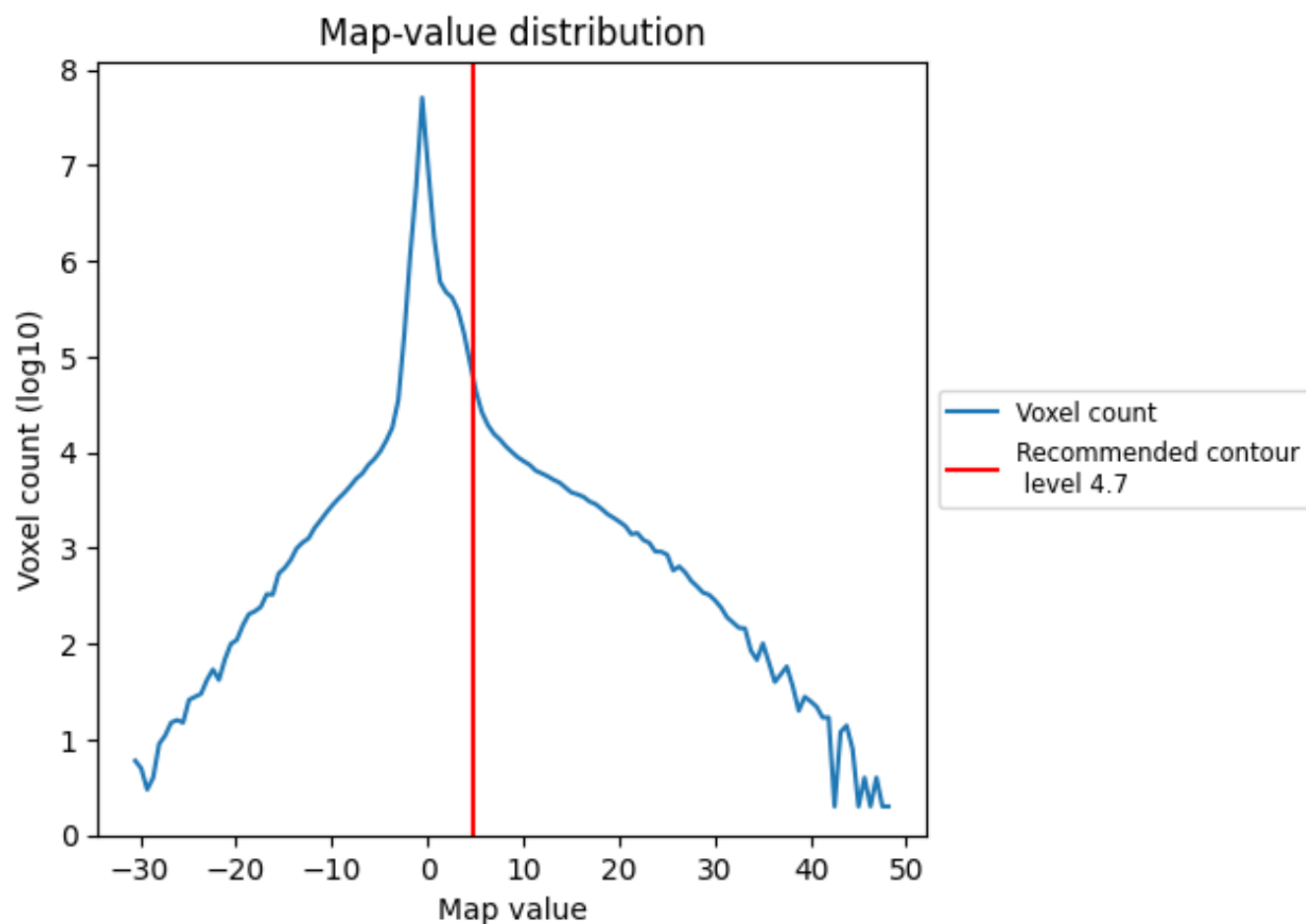
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

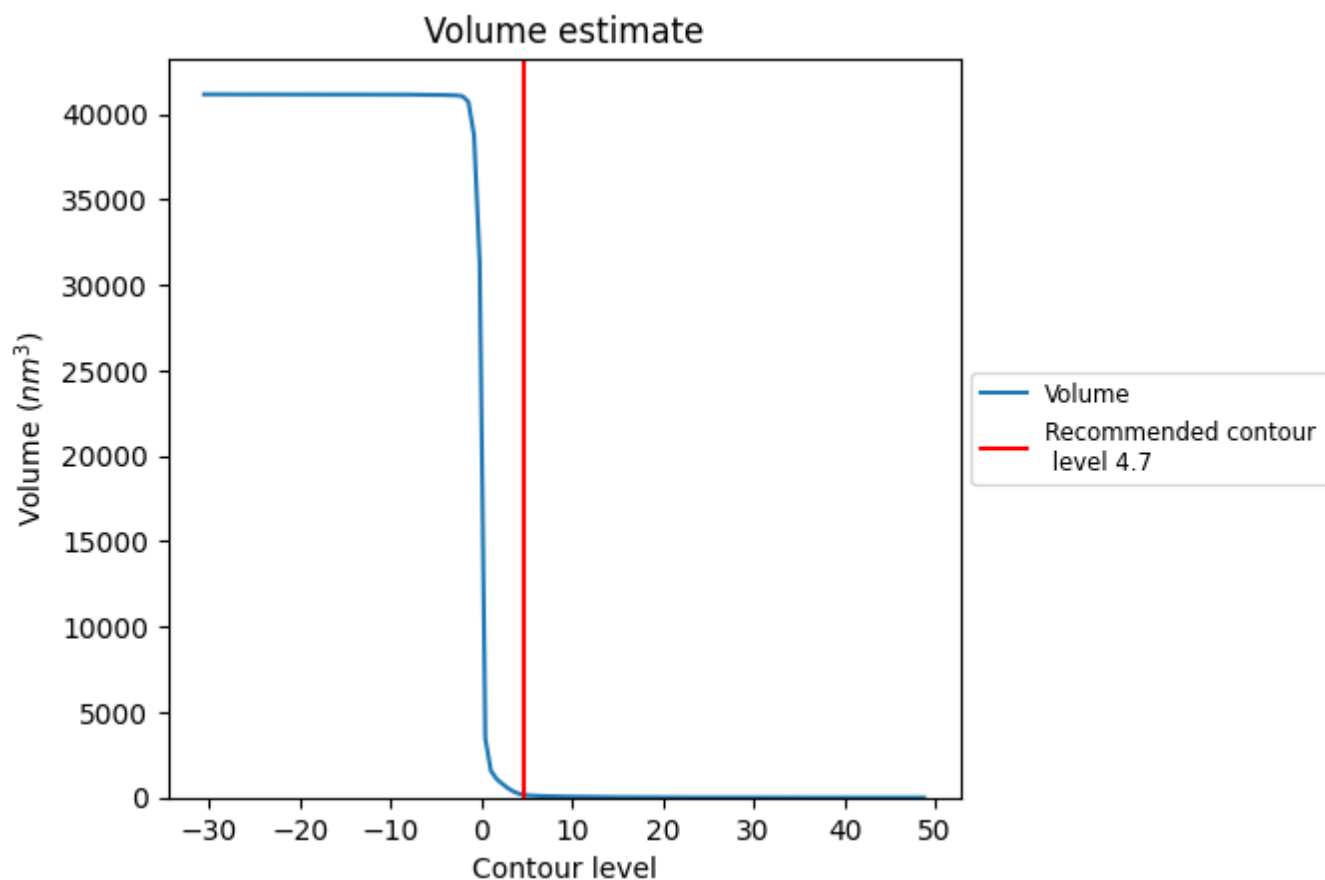
This section contains the results of statistical analysis of the map.

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.

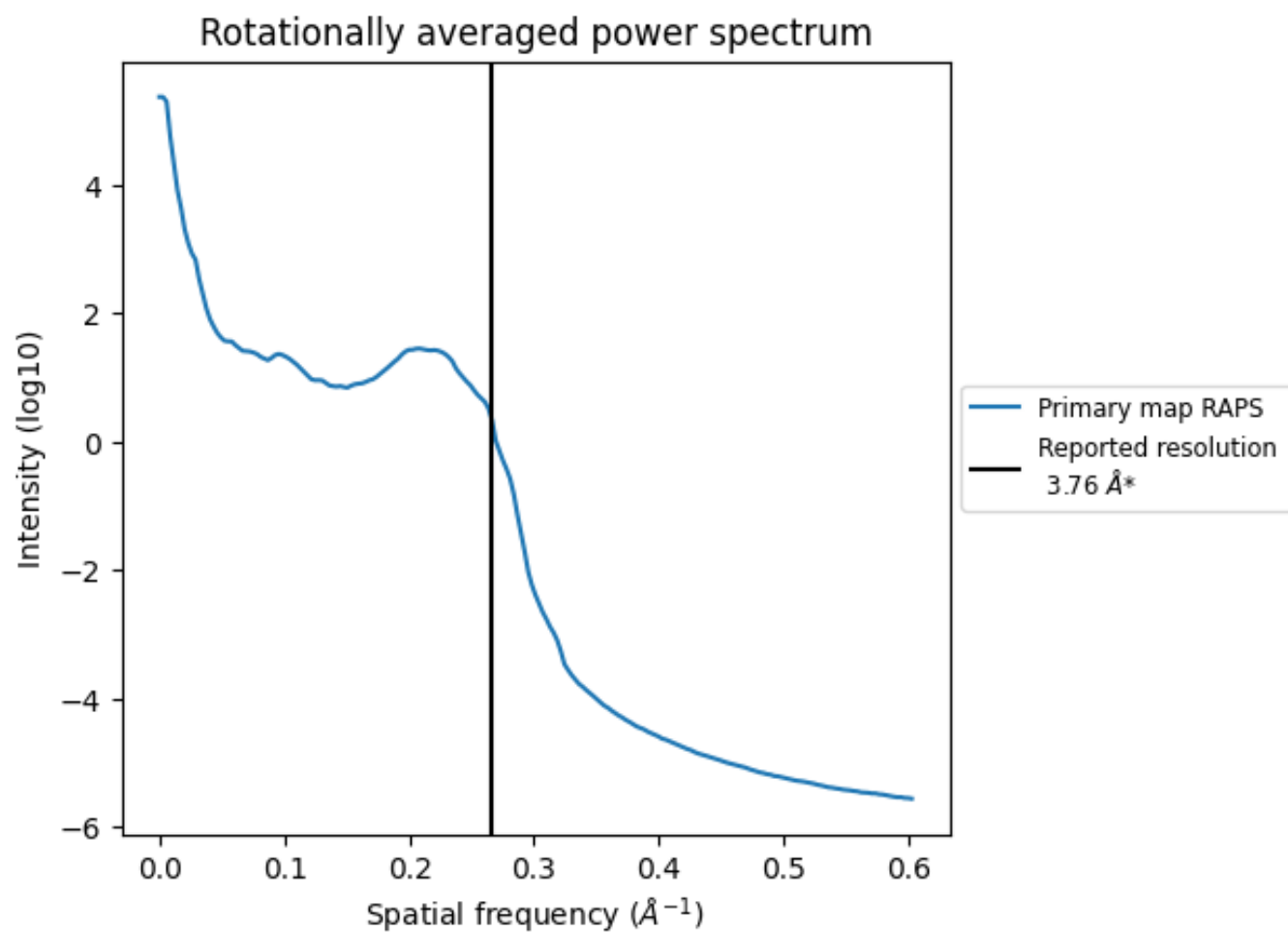
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm^3 ; this corresponds to an approximate mass of 147 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 0.266 Å⁻¹

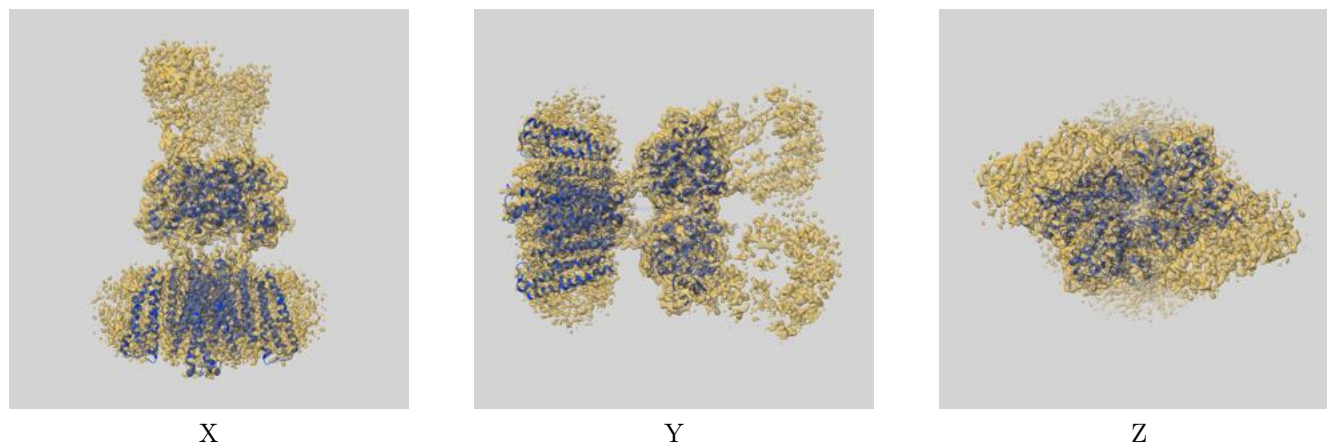
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

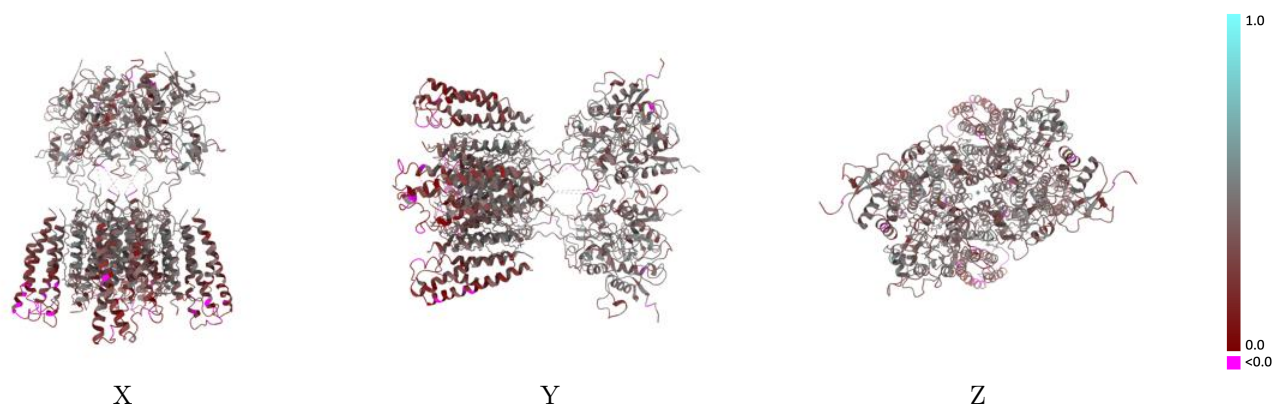
This section contains information regarding the fit between EMDB map EMD-70920 and PDB model 9OVV. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



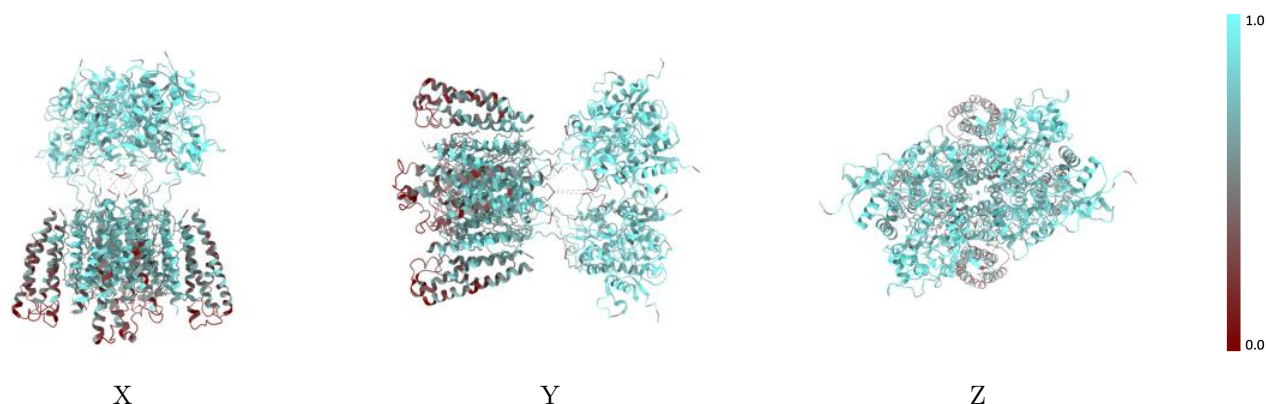
The images above show the 3D surface view of the map at the recommended contour level 4.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



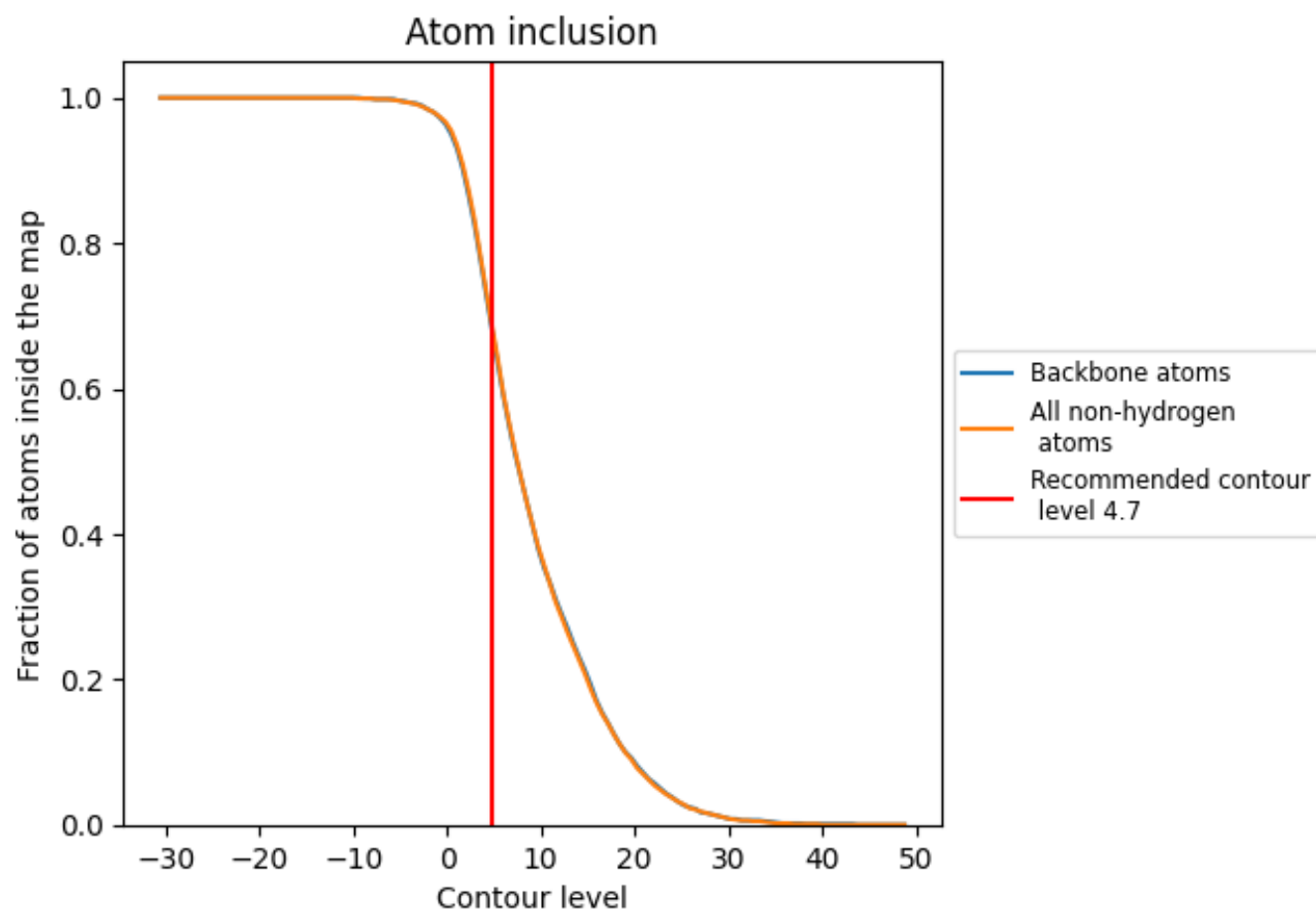
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 69% 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 (4.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6930	<div></div> 0.3470
A	<div></div> 0.7870	<div></div> 0.3840
B	<div></div> 0.7830	<div></div> 0.3880
C	<div></div> 0.7850	<div></div> 0.3850
D	<div></div> 0.7880	<div></div> 0.3970
E	<div></div> 0.4170	<div></div> 0.2040
F	<div></div> 0.4440	<div></div> 0.2080
G	<div></div> 0.4620	<div></div> 0.2480
H	<div></div> 0.4860	<div></div> 0.2440

1.0

0.0

<0.0