



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:48 AM UTC

PDB ID : 7WDB / pdb_00007wdb
EMDB ID : EMD-32436
Title : Human TRPC5 channel in complex with riluzole
Authors : Chen, L.; Wei, M.; Yang, Y.
Deposited on : 2021-12-21
Resolution : 2.40 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

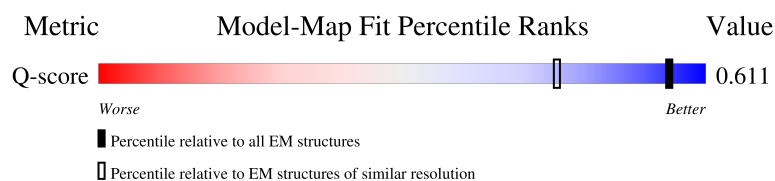
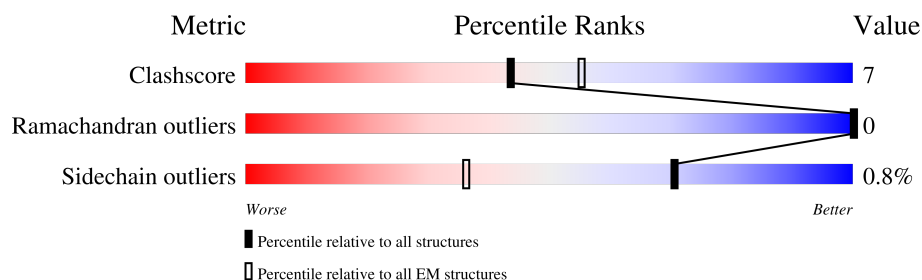
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	764	
1	B	764	
1	C	764	
1	D	764	

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
6	657	A	905	-	X	-	-
6	657	B	905	-	X	-	-
6	657	C	905	-	X	-	-
6	657	D	905	-	X	-	-

2 Entry composition [i](#)

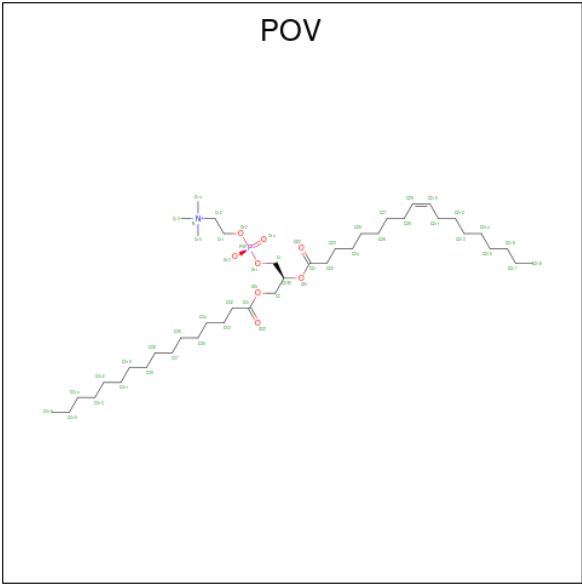
There are 8 unique types of molecules in this entry. The entry contains 22400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Short transient receptor potential channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5420	3534	892	965	29		
1	B	665	Total	C	N	O	S	0	0
			5420	3534	892	965	29		
1	C	665	Total	C	N	O	S	0	0
			5420	3534	892	965	29		
1	D	665	Total	C	N	O	S	0	0
			5420	3534	892	965	29		

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			41	32	8	1	
2	B	1	Total	C	O	P	0
			41	32	8	1	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total 41	C 32	O 8	P 1	0
2	D	1	Total 41	C 32	O 8	P 1	0

- # Y01

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	B	1	Total Zn 1 1	0
4	C	1	Total Zn 1 1	0



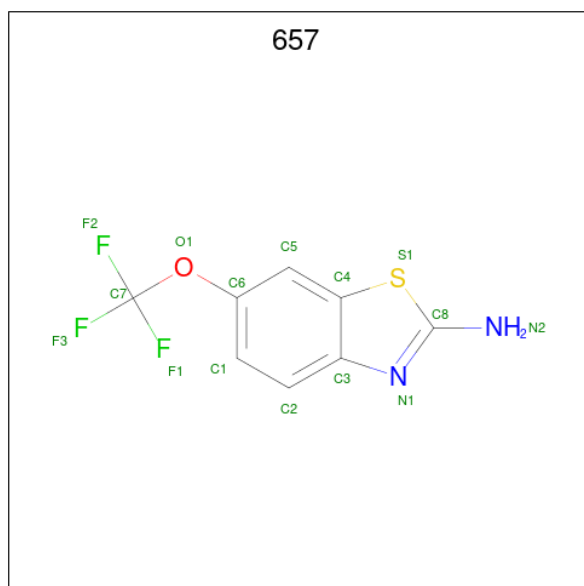
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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

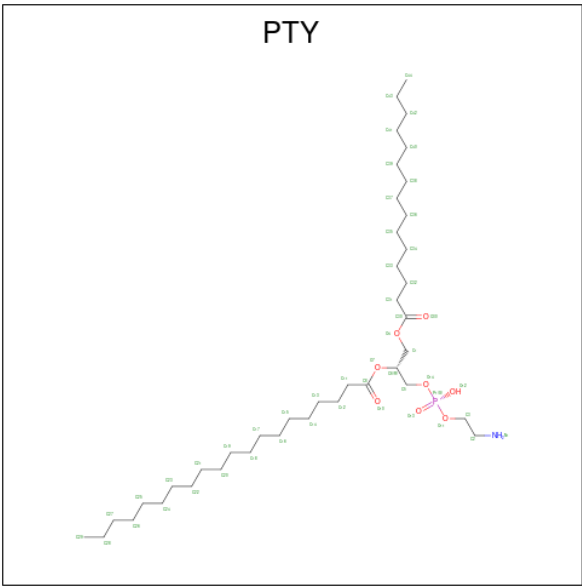
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

- Molecule 6 is 6-(trifluoromethoxy)-1,3-benzothiazol-2-amine (CCD ID: 657) (formula: C₈H₅F₃N₂OS) (labeled as "Ligand of Interest" by depositor).



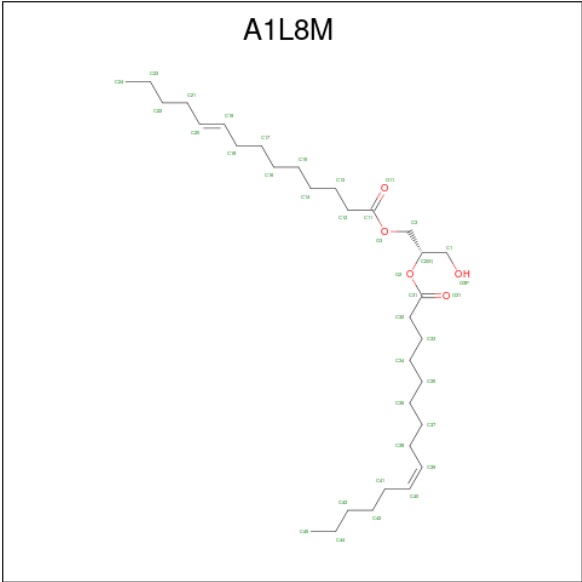
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	F	N	O	S	0
			15	8	3	2	1	1	
6	B	1	Total	C	F	N	O	S	0
			15	8	3	2	1	1	
6	C	1	Total	C	F	N	O	S	0
			15	8	3	2	1	1	
6	D	1	Total	C	F	N	O	S	0
			15	8	3	2	1	1	

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
7	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
7	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
7	D	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 8 is [(2S)-1-oxidanyl-3-[(E)-tetradec-9-enoyl]oxy-propan-2-yl] (Z)-pentadec-9-enoate (CCD ID: A1L8M) (formula: C₃₂H₅₈O₅).

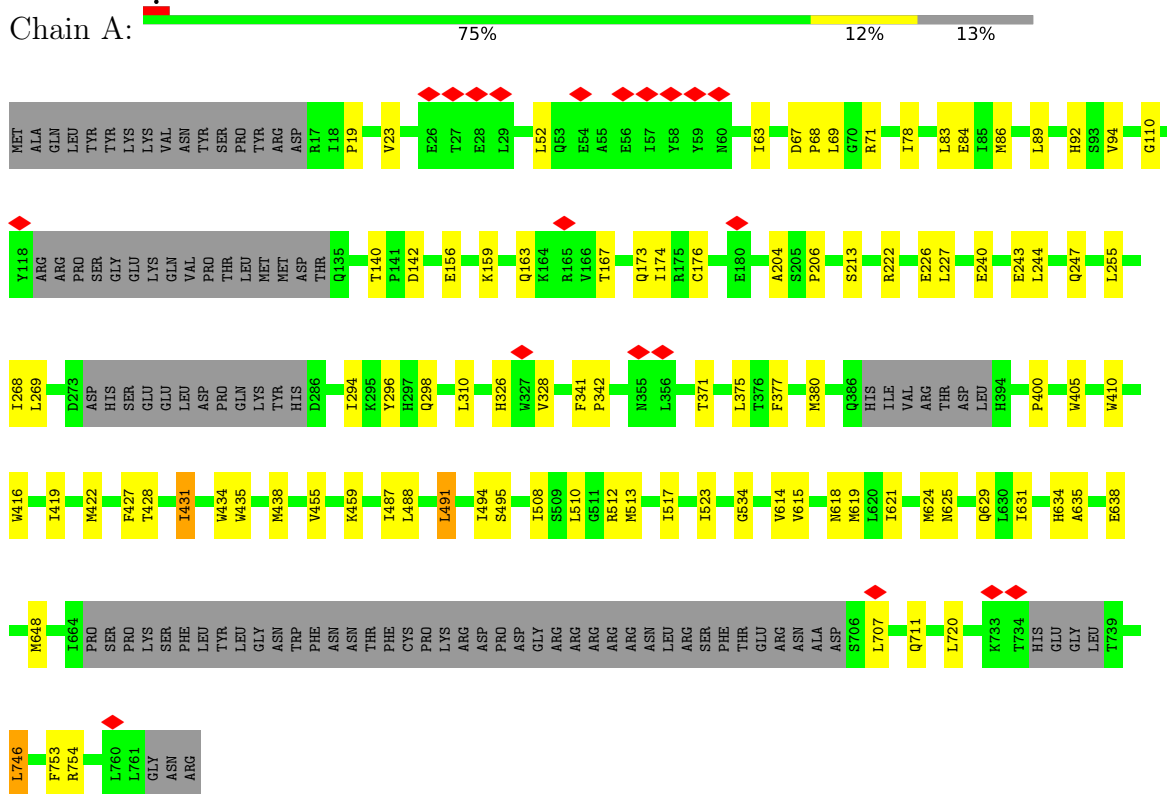


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			37	32	5	
8	B	1	Total	C	O	0
			37	32	5	
8	C	1	Total	C	O	0
			37	32	5	
8	D	1	Total	C	O	0
			37	32	5	

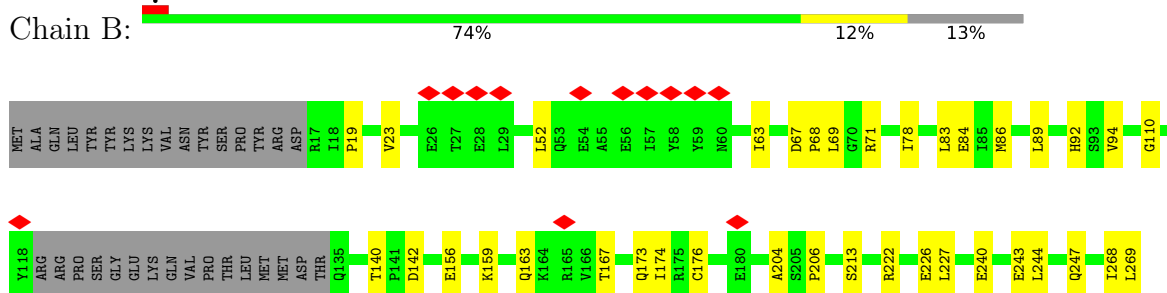
3 Residue-property plots

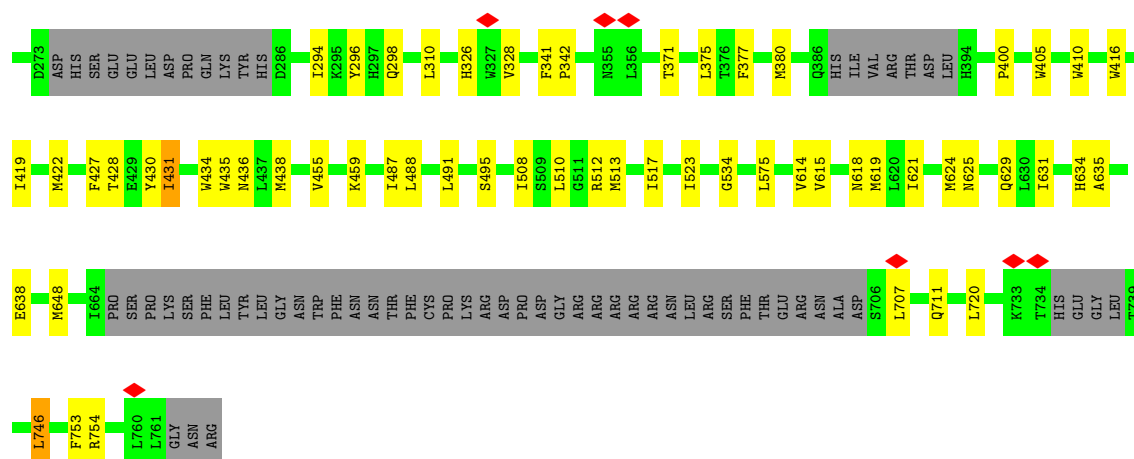
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Short transient receptor potential channel 5



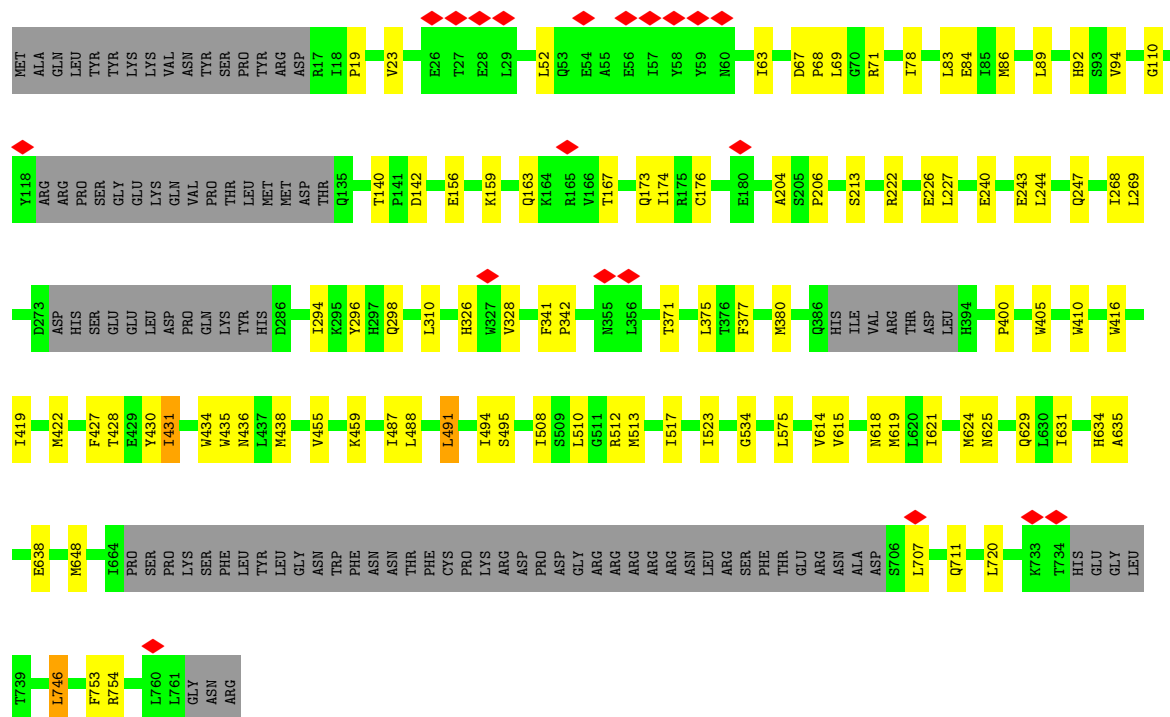
- Molecule 1: Short transient receptor potential channel 5





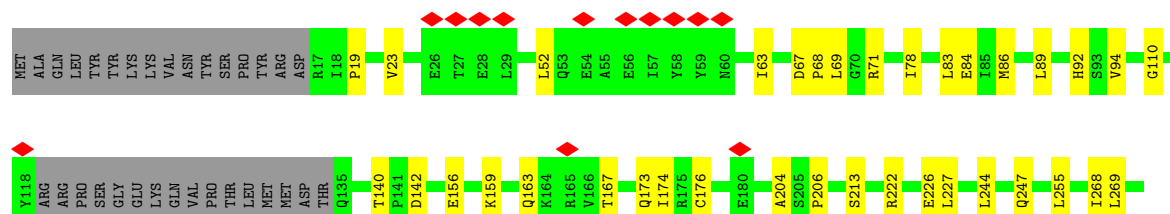
- Molecule 1: Short transient receptor potential channel 5

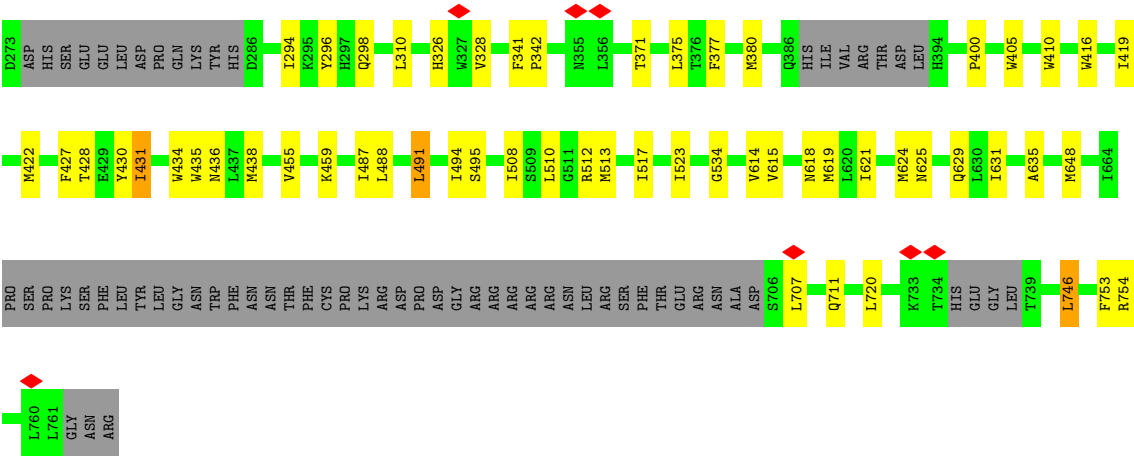
Chain C: 74% 12% 13%



- Molecule 1: Short transient receptor potential channel 5

Chain D: 75% 12% 13%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	295.56, 295.56, 295.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.821, 0.821, 0.821	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, ZN, A1L8M, PTY, 657, CA, Y01

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	0.26	0/5547	0.35	2/7520 (0.0%)
1	B	0.26	0/5547	0.35	2/7520 (0.0%)
1	C	0.26	0/5547	0.35	2/7520 (0.0%)
1	D	0.26	0/5547	0.35	2/7520 (0.0%)
All	All	0.26	0/22188	0.35	8/30080 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	631	ILE	N-CA-C	6.33	117.07	110.62
1	B	631	ILE	N-CA-C	6.30	117.05	110.62
1	A	631	ILE	N-CA-C	6.29	117.04	110.62
1	C	631	ILE	N-CA-C	6.27	117.02	110.62
1	A	635	ALA	N-CA-C	5.55	118.05	111.33
1	C	635	ALA	N-CA-C	5.55	118.05	111.33
1	B	635	ALA	N-CA-C	5.54	118.03	111.33
1	D	635	ALA	N-CA-C	5.54	118.03	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5420	0	5462	78	0
1	B	5420	0	5462	77	0
1	C	5420	0	5462	79	0
1	D	5420	0	5462	75	0
2	A	41	0	56	6	0
2	B	41	0	56	6	0
2	C	41	0	56	5	0
2	D	41	0	56	5	0
3	A	35	0	49	2	0
3	B	35	0	49	3	0
3	C	35	0	49	2	0
3	D	35	0	49	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	50	0	79	8	0
7	B	50	0	79	8	0
7	C	50	0	79	9	0
7	D	50	0	79	8	0
8	A	37	0	0	0	0
8	B	37	0	0	0	0
8	C	37	0	0	0	0
8	D	37	0	0	0	0
All	All	22400	0	22584	294	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 7.

All (294) 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)
2:B:901:POV:H32A	2:B:901:POV:C27	1.90	1.02
2:A:901:POV:C27	2:A:901:POV:H32A	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:POV:C27	2:C:901:POV:H32A	1.90	1.01
2:D:901:POV:H32A	2:D:901:POV:C27	1.90	1.00
2:C:901:POV:H32A	2:C:901:POV:H27	1.64	0.79
2:A:901:POV:H32A	2:A:901:POV:H27	1.64	0.78
2:B:901:POV:H32A	2:B:901:POV:H27	1.64	0.78
1:D:427:PHE:O	1:D:431:ILE:HG12	1.84	0.78
1:B:427:PHE:O	1:B:431:ILE:HG12	1.84	0.77
1:C:427:PHE:O	1:C:431:ILE:HG12	1.84	0.77
2:D:901:POV:H32A	2:D:901:POV:H27	1.64	0.77
1:A:427:PHE:O	1:A:431:ILE:HG12	1.84	0.76
1:A:434:TRP:HE3	7:A:906:PTY:O30	1.72	0.72
1:C:434:TRP:HE3	7:C:906:PTY:O30	1.72	0.71
7:A:906:PTY:HC12	7:A:906:PTY:H122	1.72	0.71
1:B:434:TRP:HE3	7:B:906:PTY:O30	1.72	0.71
1:D:434:TRP:HE3	7:D:906:PTY:O30	1.72	0.71
7:B:906:PTY:H122	7:B:906:PTY:HC12	1.72	0.71
7:D:906:PTY:H122	7:D:906:PTY:HC12	1.72	0.70
7:C:906:PTY:HC12	7:C:906:PTY:H122	1.72	0.69
1:B:619:MET:HG3	1:D:624:MET:HE1	1.75	0.69
1:B:624:MET:HE1	1:C:619:MET:HG3	1.75	0.68
1:A:619:MET:HG3	1:C:624:MET:HE1	1.75	0.67
1:A:624:MET:HE1	1:D:619:MET:HG3	1.75	0.67
2:B:901:POV:H32A	2:B:901:POV:C26	2.25	0.66
2:A:901:POV:H32A	2:A:901:POV:C26	2.25	0.66
2:D:901:POV:H32A	2:D:901:POV:C26	2.25	0.66
2:C:901:POV:H32A	2:C:901:POV:C26	2.25	0.65
1:A:69:LEU:HD21	1:C:156:GLU:HG3	1.82	0.62
1:A:156:GLU:HG3	1:D:69:LEU:HD21	1.82	0.62
1:B:156:GLU:HG3	1:C:69:LEU:HD21	1.82	0.62
1:A:375:LEU:HD21	3:A:902:Y01:HAE2	1.81	0.62
1:B:69:LEU:HD21	1:D:156:GLU:HG3	1.82	0.61
1:A:19:PRO:HA	1:C:167:THR:HG22	1.83	0.61
1:A:167:THR:HG22	1:D:19:PRO:HA	1.82	0.61
1:D:375:LEU:HD21	3:D:902:Y01:HAE2	1.81	0.61
1:C:375:LEU:HD21	3:C:902:Y01:HAE2	1.81	0.60
1:B:167:THR:HG22	1:C:19:PRO:HA	1.82	0.60
1:B:375:LEU:HD21	3:B:902:Y01:HAE2	1.81	0.60
1:A:619:MET:HG3	1:C:624:MET:CE	2.32	0.59
1:B:19:PRO:HA	1:D:167:THR:HG22	1.83	0.59
2:C:901:POV:H32A	2:C:901:POV:H26A	1.84	0.59
2:A:901:POV:H32A	2:A:901:POV:H27A	1.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TRP:CE3	7:A:906:PTY:O30	2.56	0.59
1:A:624:MET:CE	1:D:619:MET:HG3	2.32	0.59
1:B:624:MET:CE	1:C:619:MET:HG3	2.32	0.59
2:B:901:POV:H32A	2:B:901:POV:H26A	1.84	0.59
2:D:901:POV:H32A	2:D:901:POV:H26A	1.84	0.59
2:D:901:POV:H32A	2:D:901:POV:H27A	1.79	0.58
1:B:619:MET:HG3	1:D:624:MET:CE	2.32	0.58
1:D:434:TRP:CE3	7:D:906:PTY:O30	2.56	0.58
1:B:434:TRP:CE3	7:B:906:PTY:O30	2.55	0.58
1:C:428:THR:HA	1:C:431:ILE:HD11	1.85	0.58
1:D:428:THR:HA	1:D:431:ILE:HD11	1.85	0.58
2:A:901:POV:H32A	2:A:901:POV:H26A	1.84	0.58
2:C:901:POV:H32A	2:C:901:POV:H27A	1.80	0.58
2:B:901:POV:H32A	2:B:901:POV:H27A	1.80	0.58
1:A:619:MET:HE2	1:C:513:MET:HB2	1.85	0.57
1:B:707:LEU:HG	1:B:711:GLN:NE2	2.20	0.57
1:A:513:MET:HB2	1:D:619:MET:HE2	1.85	0.57
1:B:428:THR:HA	1:B:431:ILE:HD11	1.85	0.57
1:B:619:MET:HE2	1:D:513:MET:HB2	1.85	0.57
1:A:428:THR:HA	1:A:431:ILE:HD11	1.85	0.57
1:B:513:MET:HB2	1:C:619:MET:HE2	1.85	0.57
1:D:707:LEU:HG	1:D:711:GLN:NE2	2.20	0.57
1:C:707:LEU:HG	1:C:711:GLN:NE2	2.20	0.56
1:C:434:TRP:CE3	7:C:906:PTY:O30	2.56	0.56
1:A:707:LEU:HG	1:A:711:GLN:NE2	2.20	0.55
1:A:434:TRP:HB3	7:A:906:PTY:O30	2.07	0.55
1:D:434:TRP:HB3	7:D:906:PTY:O30	2.07	0.55
1:A:67:ASP:OD1	1:A:71:ARG:N	2.40	0.54
1:C:174:ILE:HD11	1:C:226:GLU:HG3	1.90	0.54
1:B:174:ILE:HD11	1:B:226:GLU:HG3	1.89	0.54
1:C:434:TRP:HB3	7:C:906:PTY:O30	2.07	0.54
1:D:67:ASP:OD1	1:D:71:ARG:N	2.40	0.54
1:C:67:ASP:OD1	1:C:71:ARG:N	2.40	0.54
1:A:615:VAL:HG22	1:C:517:ILE:HD13	1.90	0.54
1:B:67:ASP:OD1	1:B:71:ARG:N	2.40	0.54
1:A:174:ILE:HD11	1:A:226:GLU:HG3	1.90	0.53
1:B:434:TRP:HB3	7:B:906:PTY:O30	2.07	0.53
1:D:174:ILE:HD11	1:D:226:GLU:HG3	1.90	0.53
1:B:615:VAL:HG22	1:D:517:ILE:HD13	1.90	0.53
1:A:517:ILE:HD13	1:D:615:VAL:HG22	1.90	0.53
1:C:508:ILE:O	1:C:512:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:O	1:A:247:GLN:NE2	2.43	0.52
1:B:517:ILE:HD13	1:C:615:VAL:HG22	1.89	0.52
1:D:508:ILE:O	1:D:512:ARG:HG2	2.09	0.52
1:A:508:ILE:O	1:A:512:ARG:HG2	2.09	0.52
1:C:204:ALA:O	1:C:247:GLN:NE2	2.43	0.52
1:D:204:ALA:O	1:D:247:GLN:NE2	2.43	0.52
1:D:430:TYR:O	1:D:436:ASN:ND2	2.35	0.52
1:B:508:ILE:O	1:B:512:ARG:HG2	2.09	0.52
1:C:269:LEU:HD12	1:C:310:LEU:HD23	1.93	0.52
1:B:269:LEU:HD12	1:B:310:LEU:HD23	1.93	0.51
1:C:206:PRO:HD3	1:C:247:GLN:NE2	2.25	0.51
1:D:434:TRP:CB	7:D:906:PTY:O30	2.59	0.51
1:A:434:TRP:CB	7:A:906:PTY:O30	2.59	0.51
1:C:434:TRP:CB	7:C:906:PTY:O30	2.59	0.51
1:A:269:LEU:HD12	1:A:310:LEU:HD23	1.93	0.51
1:B:206:PRO:HD3	1:B:247:GLN:NE2	2.25	0.51
1:B:204:ALA:O	1:B:247:GLN:NE2	2.43	0.51
1:A:206:PRO:HD3	1:A:247:GLN:NE2	2.25	0.50
1:B:434:TRP:CB	7:B:906:PTY:O30	2.59	0.50
1:A:746:LEU:HD11	1:D:746:LEU:HB3	1.94	0.50
1:B:746:LEU:HD11	1:C:746:LEU:HB3	1.94	0.50
1:D:206:PRO:HD3	1:D:247:GLN:NE2	2.25	0.50
1:D:269:LEU:HD12	1:D:310:LEU:HD23	1.93	0.50
1:A:140:THR:OG1	1:A:142:ASP:OD1	2.28	0.50
1:A:746:LEU:HB3	1:C:746:LEU:HD11	1.94	0.50
1:A:67:ASP:HB2	1:A:68:PRO:HD2	1.94	0.50
1:B:746:LEU:HB3	1:D:746:LEU:HD11	1.94	0.50
1:C:67:ASP:HB2	1:C:68:PRO:HD2	1.94	0.50
1:B:67:ASP:HB2	1:B:68:PRO:HD2	1.94	0.50
1:D:67:ASP:HB2	1:D:68:PRO:HD2	1.94	0.50
1:C:140:THR:OG1	1:C:142:ASP:OD1	2.28	0.49
1:D:140:THR:OG1	1:D:142:ASP:OD1	2.28	0.49
1:C:341:PHE:CD2	1:C:342:PRO:HD3	2.48	0.49
1:B:83:LEU:HD21	1:B:110:GLY:HA3	1.95	0.49
1:A:341:PHE:CD2	1:A:342:PRO:HD3	2.48	0.49
1:C:435:TRP:CE2	1:C:495:SER:HB3	2.48	0.49
1:A:435:TRP:CE2	1:A:495:SER:HB3	2.48	0.48
1:D:83:LEU:HD21	1:D:110:GLY:HA3	1.95	0.48
1:B:435:TRP:CE2	1:B:495:SER:HB3	2.48	0.48
1:D:341:PHE:CD2	1:D:342:PRO:HD3	2.48	0.48
1:B:140:THR:OG1	1:B:142:ASP:OD1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:CD2	1:B:342:PRO:HD3	2.48	0.48
1:C:83:LEU:HD21	1:C:110:GLY:HA3	1.95	0.48
1:A:380:MET:HE1	1:A:410:TRP:CE3	2.49	0.48
1:B:63:ILE:HD12	1:B:94:VAL:HG12	1.96	0.48
1:D:52:LEU:HD11	1:D:89:LEU:HD23	1.96	0.48
1:D:380:MET:HE1	1:D:410:TRP:CE3	2.49	0.48
1:C:380:MET:HE1	1:C:410:TRP:CE3	2.49	0.48
1:A:63:ILE:HD12	1:A:94:VAL:HG12	1.96	0.47
1:A:83:LEU:HD21	1:A:110:GLY:HA3	1.95	0.47
3:B:902:Y01:HAE2	3:B:902:Y01:HBB	1.76	0.47
1:D:435:TRP:CE2	1:D:495:SER:HB3	2.48	0.47
1:C:326:HIS:ND1	1:C:328:VAL:HG22	2.29	0.47
1:A:52:LEU:HD11	1:A:89:LEU:HD23	1.96	0.47
1:A:326:HIS:ND1	1:A:328:VAL:HG22	2.29	0.47
1:C:296:TYR:HB3	1:C:298:GLN:HE21	1.80	0.47
1:B:52:LEU:HD11	1:B:89:LEU:HD23	1.96	0.47
1:D:326:HIS:ND1	1:D:328:VAL:HG22	2.29	0.47
1:B:326:HIS:ND1	1:B:328:VAL:HG22	2.29	0.47
1:D:63:ILE:HD12	1:D:94:VAL:HG12	1.96	0.47
1:D:296:TYR:HB3	1:D:298:GLN:HE21	1.80	0.47
7:D:906:PTY:HC12	7:D:906:PTY:C12	2.44	0.47
1:A:296:TYR:HB3	1:A:298:GLN:HE21	1.80	0.47
1:A:619:MET:CG	1:C:624:MET:CE	2.93	0.47
1:C:52:LEU:HD11	1:C:89:LEU:HD23	1.96	0.47
1:C:294:ILE:HD12	1:C:648:MET:HE2	1.96	0.47
1:A:294:ILE:HD12	1:A:648:MET:HE2	1.97	0.47
1:A:624:MET:CE	1:D:619:MET:CG	2.93	0.47
1:B:380:MET:HE1	1:B:410:TRP:CE3	2.49	0.47
1:C:63:ILE:HD12	1:C:94:VAL:HG12	1.96	0.46
1:D:294:ILE:HD12	1:D:648:MET:HE2	1.96	0.46
1:A:84:GLU:N	1:A:84:GLU:OE1	2.49	0.46
7:B:906:PTY:HC12	7:B:906:PTY:C12	2.44	0.46
1:C:438:MET:HE3	7:C:906:PTY:H371	1.97	0.46
1:B:294:ILE:HD12	1:B:648:MET:HE2	1.96	0.46
1:A:438:MET:HE3	7:A:906:PTY:H371	1.98	0.46
1:D:438:MET:HE3	7:D:906:PTY:H371	1.98	0.46
1:B:296:TYR:HB3	1:B:298:GLN:HE21	1.80	0.46
1:B:438:MET:HE3	7:B:906:PTY:H371	1.98	0.46
1:D:84:GLU:N	1:D:84:GLU:OE1	2.49	0.46
1:A:753:PHE:CE1	1:D:754:ARG:HA	2.51	0.46
1:A:754:ARG:HA	1:C:753:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:OE1	1:B:84:GLU:N	2.49	0.46
1:C:222:ARG:HG2	1:C:296:TYR:OH	2.16	0.46
1:B:753:PHE:CE1	1:C:754:ARG:HA	2.51	0.46
1:B:624:MET:CE	1:C:619:MET:CG	2.93	0.46
1:B:754:ARG:HA	1:D:753:PHE:CE1	2.51	0.46
1:A:222:ARG:HG2	1:A:296:TYR:CZ	2.52	0.45
1:D:222:ARG:HG2	1:D:296:TYR:CZ	2.52	0.45
1:B:206:PRO:HD3	1:B:247:GLN:HE21	1.82	0.45
1:B:619:MET:CG	1:D:624:MET:CE	2.93	0.45
1:A:222:ARG:HG2	1:A:296:TYR:OH	2.16	0.45
1:B:222:ARG:HG2	1:B:296:TYR:CZ	2.52	0.45
1:C:84:GLU:N	1:C:84:GLU:OE1	2.49	0.45
1:C:86:MET:HE2	1:C:86:MET:HB3	1.90	0.45
1:D:222:ARG:HG2	1:D:296:TYR:OH	2.16	0.45
1:A:159:LYS:O	1:A:163:GLN:HG2	2.17	0.45
1:B:159:LYS:O	1:B:163:GLN:HG2	2.17	0.45
1:C:159:LYS:O	1:C:163:GLN:HG2	2.17	0.45
1:C:422:MET:HE1	1:C:427:PHE:HD1	1.82	0.45
1:A:422:MET:HE1	1:A:427:PHE:HD1	1.82	0.45
1:C:206:PRO:HD3	1:C:247:GLN:HE21	1.82	0.45
1:C:430:TYR:O	1:C:436:ASN:ND2	2.35	0.44
1:D:206:PRO:HD3	1:D:247:GLN:HE21	1.82	0.44
7:A:906:PTY:HC12	7:A:906:PTY:C12	2.44	0.44
1:B:222:ARG:HG2	1:B:296:TYR:OH	2.16	0.44
1:C:222:ARG:HG2	1:C:296:TYR:CZ	2.52	0.44
1:C:268:ILE:HD11	1:C:720:LEU:HD11	1.99	0.44
1:B:455:VAL:O	1:B:459:LYS:HB2	2.18	0.44
1:D:268:ILE:HD11	1:D:720:LEU:HD11	1.99	0.44
1:A:268:ILE:HD11	1:A:720:LEU:HD11	1.99	0.44
1:A:455:VAL:O	1:A:459:LYS:HB2	2.18	0.44
1:A:206:PRO:HD3	1:A:247:GLN:HE21	1.82	0.44
1:B:227:LEU:HD13	1:B:244:LEU:HB3	2.00	0.44
1:B:534:GLY:HA3	1:D:487:ILE:HG13	2.00	0.44
1:B:621:ILE:O	1:B:625:ASN:HB2	2.18	0.44
1:A:487:ILE:HG13	1:D:534:GLY:HA3	2.00	0.44
1:D:455:VAL:O	1:D:459:LYS:HB2	2.18	0.44
1:C:371:THR:HG21	3:C:902:Y01:HAD2	2.00	0.43
1:D:159:LYS:O	1:D:163:GLN:HG2	2.17	0.43
1:A:86:MET:HE2	1:A:86:MET:HB3	1.90	0.43
1:A:227:LEU:HD13	1:A:244:LEU:HB3	2.00	0.43
1:B:371:THR:HG21	3:B:902:Y01:HAD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:MET:HE1	1:B:427:PHE:HD1	1.82	0.43
1:C:78:ILE:HG12	1:C:86:MET:SD	2.59	0.43
1:A:78:ILE:HG12	1:A:86:MET:SD	2.59	0.43
1:A:534:GLY:HA3	1:C:487:ILE:HG13	2.00	0.43
1:B:625:ASN:ND2	1:D:625:ASN:HD21	2.17	0.43
7:C:906:PTY:HC12	7:C:906:PTY:C12	2.44	0.43
1:B:268:ILE:HD11	1:B:720:LEU:HD11	1.99	0.43
1:B:487:ILE:HG13	1:C:534:GLY:HA3	2.00	0.43
1:C:227:LEU:HD13	1:C:244:LEU:HB3	2.00	0.43
1:A:621:ILE:O	1:A:625:ASN:HB2	2.18	0.43
1:C:455:VAL:O	1:C:459:LYS:HB2	2.18	0.43
1:D:371:THR:HG21	3:D:902:Y01:HAD2	2.00	0.43
1:D:78:ILE:HG12	1:D:86:MET:SD	2.59	0.43
1:D:422:MET:HE1	1:D:427:PHE:HD1	1.82	0.43
1:A:371:THR:HG21	3:A:902:Y01:HAD2	2.00	0.43
1:B:78:ILE:HG12	1:B:86:MET:SD	2.59	0.43
1:C:427:PHE:CE2	1:C:431:ILE:HD13	2.54	0.43
1:C:621:ILE:O	1:C:625:ASN:HB2	2.18	0.43
1:D:427:PHE:CE2	1:D:431:ILE:HD13	2.54	0.43
1:D:621:ILE:O	1:D:625:ASN:HB2	2.18	0.43
1:A:416:TRP:HE3	1:A:419:ILE:HD11	1.84	0.43
1:A:625:ASN:HD21	1:D:625:ASN:ND2	2.17	0.43
1:B:416:TRP:HE3	1:B:419:ILE:HD11	1.84	0.43
1:B:619:MET:SD	1:D:510:LEU:HD22	2.59	0.43
1:D:227:LEU:HD13	1:D:244:LEU:HB3	2.00	0.43
1:A:173:GLN:HB3	1:A:176:CYS:HB2	2.01	0.42
1:A:427:PHE:CE2	1:A:431:ILE:HD13	2.54	0.42
7:B:906:PTY:H392	7:B:906:PTY:H361	1.93	0.42
1:A:510:LEU:HD22	1:D:619:MET:SD	2.59	0.42
1:A:614:VAL:O	1:A:618:ASN:ND2	2.52	0.42
1:B:23:VAL:HG21	1:D:213:SER:H	1.84	0.42
1:B:173:GLN:HB3	1:B:176:CYS:HB2	2.01	0.42
1:B:510:LEU:HD22	1:C:619:MET:SD	2.59	0.42
1:D:173:GLN:HB3	1:D:176:CYS:HB2	2.01	0.42
1:C:416:TRP:HE3	1:C:419:ILE:HD11	1.84	0.42
1:B:213:SER:H	1:C:23:VAL:HG21	1.84	0.42
1:B:625:ASN:HD21	1:C:625:ASN:ND2	2.17	0.42
7:A:906:PTY:H411	7:A:906:PTY:H382	1.77	0.42
1:B:431:ILE:HG12	1:B:431:ILE:H	1.66	0.42
1:D:614:VAL:O	1:D:618:ASN:ND2	2.52	0.42
3:D:902:Y01:HAE2	3:D:902:Y01:HBB	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:MET:HE2	1:B:488:LEU:HD22	2.02	0.42
1:D:416:TRP:HE3	1:D:419:ILE:HD11	1.84	0.42
1:A:619:MET:SD	1:C:510:LEU:HD22	2.59	0.42
1:A:625:ASN:ND2	1:C:625:ASN:HD21	2.17	0.42
1:B:427:PHE:CE2	1:B:431:ILE:HD13	2.54	0.42
1:A:23:VAL:HG21	1:C:213:SER:H	1.84	0.42
1:A:52:LEU:HB3	1:A:92:HIS:CD2	2.55	0.42
1:B:614:VAL:O	1:B:618:ASN:ND2	2.52	0.42
1:D:255:LEU:HD23	1:D:255:LEU:HA	1.92	0.42
1:A:213:SER:H	1:D:23:VAL:HG21	1.84	0.42
1:B:634:HIS:O	1:B:638:GLU:HG2	2.20	0.42
1:C:614:VAL:O	1:C:618:ASN:ND2	2.52	0.41
1:D:52:LEU:HB3	1:D:92:HIS:CD2	2.55	0.41
1:A:438:MET:HE2	1:A:488:LEU:HD22	2.01	0.41
1:C:173:GLN:HB3	1:C:176:CYS:HB2	2.01	0.41
1:C:52:LEU:HB3	1:C:92:HIS:CD2	2.55	0.41
1:C:377:PHE:HB2	1:C:410:TRP:CD1	2.56	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.92	0.41
1:A:431:ILE:HG12	1:A:431:ILE:H	1.66	0.41
1:B:240:GLU:O	1:B:243:GLU:HG2	2.21	0.41
1:C:491:LEU:O	1:C:494:ILE:HG12	2.21	0.41
1:A:491:LEU:O	1:A:494:ILE:HG12	2.21	0.41
1:D:377:PHE:HB2	1:D:410:TRP:CD1	2.56	0.41
1:D:438:MET:HE2	1:D:488:LEU:HD22	2.02	0.41
1:D:491:LEU:O	1:D:494:ILE:HG12	2.21	0.41
1:A:377:PHE:HB2	1:A:410:TRP:CD1	2.56	0.41
1:A:634:HIS:O	1:A:638:GLU:HG2	2.20	0.41
1:C:240:GLU:O	1:C:243:GLU:HG2	2.21	0.41
1:C:634:HIS:O	1:C:638:GLU:HG2	2.20	0.41
1:A:240:GLU:O	1:A:243:GLU:HG2	2.21	0.41
2:A:901:POV:H26A	2:A:901:POV:C32	2.50	0.41
1:B:377:PHE:HB2	1:B:410:TRP:CD1	2.56	0.41
1:B:400:PRO:HG2	1:B:405:TRP:CE2	2.56	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.85	0.41
2:B:901:POV:H26A	2:B:901:POV:C32	2.50	0.41
1:C:438:MET:HE2	1:C:488:LEU:HD22	2.02	0.41
7:C:906:PTY:H392	7:C:906:PTY:H361	1.93	0.41
1:D:400:PRO:HG2	1:D:405:TRP:CE2	2.56	0.41
1:B:430:TYR:O	1:B:436:ASN:ND2	2.35	0.41
7:C:906:PTY:H382	7:C:906:PTY:H411	1.77	0.41
1:C:400:PRO:HG2	1:C:405:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HG2	1:A:405:TRP:CE2	2.56	0.40
1:C:575:LEU:HD23	1:C:575:LEU:HA	1.85	0.40
1:C:431:ILE:HG12	1:C:431:ILE:H	1.66	0.40
1:B:52:LEU:HB3	1:B:92:HIS:CD2	2.55	0.40
7:D:906:PTY:H411	7:D:906:PTY:H382	1.77	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	653/764 (86%)	648 (99%)	5 (1%)	0	100	100
1	B	653/764 (86%)	648 (99%)	5 (1%)	0	100	100
1	C	653/764 (86%)	648 (99%)	5 (1%)	0	100	100
1	D	653/764 (86%)	648 (99%)	5 (1%)	0	100	100
All	All	2612/3056 (86%)	2592 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	594/686 (87%)	589 (99%)	5 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	594/686 (87%)	589 (99%)	5 (1%)	73	86
1	C	594/686 (87%)	589 (99%)	5 (1%)	73	86
1	D	594/686 (87%)	589 (99%)	5 (1%)	73	86
All	All	2376/2744 (87%)	2356 (99%)	20 (1%)	70	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	ILE
1	A	491	LEU
1	A	523	ILE
1	A	629	GLN
1	A	746	LEU
1	B	431	ILE
1	B	491	LEU
1	B	523	ILE
1	B	629	GLN
1	B	746	LEU
1	C	431	ILE
1	C	491	LEU
1	C	523	ILE
1	C	629	GLN
1	C	746	LEU
1	D	431	ILE
1	D	491	LEU
1	D	523	ILE
1	D	629	GLN
1	D	746	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	247	GLN
1	A	304	GLN
1	A	386	GLN
1	A	486	ASN
1	A	584	ASN
1	A	711	GLN
1	B	304	GLN

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Mol	Chain	Res	Type
1	B	486	ASN
1	B	584	ASN
1	B	618	ASN
1	B	711	GLN
1	C	247	GLN
1	C	304	GLN
1	C	386	GLN
1	C	486	ASN
1	C	584	ASN
1	C	625	ASN
1	C	711	GLN
1	D	304	GLN
1	D	386	GLN
1	D	486	ASN
1	D	584	ASN
1	D	625	ASN
1	D	711	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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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
2	POV	A	901	-	40,40,51	1.04	2 (5%)	43,45,59	1.13	4 (9%)
6	657	A	905	-	16,16,16	8.35	12 (75%)	24,24,24	8.45	8 (33%)
6	657	B	905	-	16,16,16	8.34	12 (75%)	24,24,24	8.45	8 (33%)
3	Y01	D	902	-	38,38,38	1.01	2 (5%)	57,57,57	1.43	7 (12%)
7	PTY	A	906	-	49,49,49	1.00	3 (6%)	52,54,54	1.44	7 (13%)
8	A1L8M	B	907	-	36,36,36	0.98	3 (8%)	38,38,38	1.23	3 (7%)
8	A1L8M	A	907	-	36,36,36	0.98	3 (8%)	38,38,38	1.23	3 (7%)
2	POV	B	901	-	40,40,51	1.04	2 (5%)	43,45,59	1.13	4 (9%)
3	Y01	C	902	-	38,38,38	1.01	2 (5%)	57,57,57	1.44	7 (12%)
6	657	C	905	-	16,16,16	8.34	12 (75%)	24,24,24	8.44	8 (33%)
2	POV	D	901	-	40,40,51	1.04	2 (5%)	43,45,59	1.12	4 (9%)
8	A1L8M	C	907	-	36,36,36	0.98	3 (8%)	38,38,38	1.23	3 (7%)
7	PTY	B	906	-	49,49,49	1.00	3 (6%)	52,54,54	1.44	7 (13%)
7	PTY	C	906	-	49,49,49	1.00	3 (6%)	52,54,54	1.44	7 (13%)
6	657	D	905	-	16,16,16	8.34	12 (75%)	24,24,24	8.45	8 (33%)
3	Y01	B	902	-	38,38,38	1.01	2 (5%)	57,57,57	1.43	7 (12%)
7	PTY	D	906	-	49,49,49	1.00	3 (6%)	52,54,54	1.44	7 (13%)
2	POV	C	901	-	40,40,51	1.04	2 (5%)	43,45,59	1.12	4 (9%)
8	A1L8M	D	907	-	36,36,36	0.98	3 (8%)	38,38,38	1.23	3 (7%)
3	Y01	A	902	-	38,38,38	1.01	2 (5%)	57,57,57	1.44	7 (12%)

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
2	POV	A	901	-	-	14/42/42/55	-
6	657	A	905	-	-	0/5/5/5	0/2/2/2
6	657	B	905	-	-	0/5/5/5	0/2/2/2
3	Y01	D	902	-	-	11/19/77/77	0/4/4/4
7	PTY	A	906	-	-	25/53/53/53	-
8	A1L8M	B	907	-	-	7/38/38/38	-
8	A1L8M	A	907	-	-	7/38/38/38	-
2	POV	B	901	-	-	14/42/42/55	-
3	Y01	C	902	-	-	11/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	657	C	905	-	-	0/5/5/5	0/2/2/2
2	POV	D	901	-	-	14/42/42/55	-
8	A1L8M	C	907	-	-	7/38/38/38	-
7	PTY	B	906	-	-	25/53/53/53	-
7	PTY	C	906	-	-	25/53/53/53	-
6	657	D	905	-	-	0/5/5/5	0/2/2/2
3	Y01	B	902	-	-	11/19/77/77	0/4/4/4
7	PTY	D	906	-	-	25/53/53/53	-
2	POV	C	901	-	-	14/42/42/55	-
8	A1L8M	D	907	-	-	7/38/38/38	-
3	Y01	A	902	-	-	11/19/77/77	0/4/4/4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	905	657	C8-S1	-18.72	1.55	1.76
6	C	905	657	C8-S1	-18.72	1.55	1.76
6	D	905	657	C8-S1	-18.72	1.55	1.76
6	B	905	657	C8-S1	-18.67	1.55	1.76
6	A	905	657	C8-N1	10.96	1.44	1.31
6	B	905	657	C8-N1	10.96	1.44	1.31
6	C	905	657	C8-N1	10.96	1.44	1.31
6	D	905	657	C8-N1	10.96	1.44	1.31
6	A	905	657	C2-C3	10.67	1.56	1.40
6	B	905	657	C2-C3	10.67	1.56	1.40
6	C	905	657	C2-C3	10.67	1.56	1.40
6	D	905	657	C2-C3	10.67	1.56	1.40
6	C	905	657	C4-S1	-10.37	1.53	1.74
6	A	905	657	C4-S1	-10.35	1.53	1.74
6	B	905	657	C4-S1	-10.35	1.53	1.74
6	D	905	657	C4-S1	-10.35	1.53	1.74
6	A	905	657	C5-C4	9.49	1.54	1.39
6	B	905	657	C5-C4	9.49	1.54	1.39
6	C	905	657	C5-C4	9.49	1.54	1.39
6	D	905	657	C5-C4	9.49	1.54	1.39
6	A	905	657	C3-N1	9.11	1.58	1.39
6	B	905	657	C3-N1	9.11	1.58	1.39
6	C	905	657	C3-N1	9.11	1.58	1.39
6	D	905	657	C3-N1	9.11	1.58	1.39
6	A	905	657	C2-C1	8.70	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	905	657	C2-C1	8.70	1.52	1.38
6	C	905	657	C2-C1	8.61	1.52	1.38
6	D	905	657	C2-C1	8.61	1.52	1.38
6	A	905	657	C5-C6	8.18	1.52	1.39
6	B	905	657	C5-C6	8.15	1.52	1.39
6	C	905	657	C5-C6	8.15	1.52	1.39
6	D	905	657	C5-C6	8.14	1.52	1.39
6	A	905	657	C1-C6	7.24	1.52	1.38
6	B	905	657	C1-C6	7.24	1.52	1.38
6	C	905	657	C1-C6	7.24	1.52	1.38
6	D	905	657	C1-C6	7.24	1.52	1.38
6	D	905	657	C8-N2	5.82	1.45	1.34
6	A	905	657	C8-N2	5.78	1.45	1.34
6	C	905	657	C8-N2	5.78	1.45	1.34
6	B	905	657	C8-N2	5.78	1.45	1.34
7	A	906	PTY	O4-C30	4.56	1.46	1.33
7	B	906	PTY	O4-C30	4.54	1.46	1.33
7	C	906	PTY	O4-C30	4.54	1.46	1.33
7	D	906	PTY	O4-C30	4.54	1.46	1.33
2	B	901	POV	O31-C31	4.29	1.45	1.33
2	C	901	POV	O31-C31	4.29	1.45	1.33
2	D	901	POV	O31-C31	4.29	1.45	1.33
2	A	901	POV	O31-C31	4.28	1.45	1.33
3	A	902	Y01	OAW-CAY	4.13	1.45	1.34
3	B	902	Y01	OAW-CAY	4.12	1.45	1.34
3	C	902	Y01	OAW-CAY	4.12	1.45	1.34
3	D	902	Y01	OAW-CAY	4.12	1.45	1.34
7	A	906	PTY	O7-C8	3.98	1.45	1.34
7	B	906	PTY	O7-C8	3.96	1.45	1.34
7	C	906	PTY	O7-C8	3.96	1.45	1.34
7	D	906	PTY	O7-C8	3.96	1.45	1.34
2	A	901	POV	O21-C21	3.82	1.45	1.34
2	B	901	POV	O21-C21	3.82	1.45	1.34
2	C	901	POV	O21-C21	3.82	1.45	1.34
2	D	901	POV	O21-C21	3.82	1.45	1.34
8	A	907	A1L8M	O3-C11	3.56	1.43	1.33
8	B	907	A1L8M	O3-C11	3.56	1.43	1.33
8	C	907	A1L8M	O3-C11	3.56	1.43	1.33
8	D	907	A1L8M	O3-C11	3.53	1.43	1.33
8	D	907	A1L8M	O2-C31	3.52	1.44	1.34
8	A	907	A1L8M	O2-C31	3.51	1.44	1.34
8	C	907	A1L8M	O2-C31	3.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	907	A1L8M	O2-C31	3.49	1.44	1.34
6	B	905	657	C3-C4	3.37	1.45	1.40
6	A	905	657	C3-C4	3.35	1.45	1.40
6	D	905	657	C3-C4	3.35	1.45	1.40
6	C	905	657	C3-C4	3.32	1.45	1.40
8	D	907	A1L8M	O2-C2	-2.30	1.41	1.46
8	C	907	A1L8M	O2-C2	-2.30	1.41	1.46
8	A	907	A1L8M	O2-C2	-2.29	1.41	1.46
8	B	907	A1L8M	O2-C2	-2.29	1.41	1.46
6	A	905	657	O1-C7	2.20	1.43	1.31
6	B	905	657	O1-C7	2.20	1.43	1.31
6	C	905	657	O1-C7	2.20	1.43	1.31
6	D	905	657	O1-C7	2.19	1.43	1.31
3	B	902	Y01	CBH-CBF	-2.12	1.52	1.56
3	C	902	Y01	CBH-CBF	-2.12	1.52	1.56
7	D	906	PTY	O7-C6	-2.09	1.41	1.46
3	D	902	Y01	CBH-CBF	-2.09	1.52	1.56
7	A	906	PTY	O7-C6	-2.08	1.41	1.46
7	B	906	PTY	O7-C6	-2.08	1.41	1.46
7	C	906	PTY	O7-C6	-2.08	1.41	1.46
3	A	902	Y01	CBH-CBF	-2.07	1.52	1.56

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	905	657	C4-S1-C8	38.22	106.96	88.89
6	A	905	657	C4-S1-C8	38.19	106.94	88.89
6	D	905	657	C4-S1-C8	38.19	106.94	88.89
6	C	905	657	C4-S1-C8	38.13	106.92	88.89
6	B	905	657	S1-C8-N1	-12.52	107.95	115.72
6	A	905	657	S1-C8-N1	-12.49	107.97	115.72
6	C	905	657	S1-C8-N1	-12.49	107.97	115.72
6	D	905	657	S1-C8-N1	-12.49	107.97	115.72
6	D	905	657	S1-C8-N2	5.85	126.49	120.13
6	A	905	657	S1-C8-N2	5.84	126.48	120.13
6	C	905	657	S1-C8-N2	5.84	126.48	120.13
6	B	905	657	S1-C8-N2	5.81	126.44	120.13
7	A	906	PTY	O7-C8-C11	5.39	123.15	111.48
7	D	906	PTY	O7-C8-C11	5.39	123.13	111.48
7	B	906	PTY	O7-C8-C11	5.38	123.12	111.48
7	C	906	PTY	O7-C8-C11	5.38	123.12	111.48
6	C	905	657	C4-C3-N1	-4.54	107.28	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	905	657	C4-C3-N1	-4.53	107.30	115.20
6	D	905	657	C4-C3-N1	-4.53	107.30	115.20
6	B	905	657	C4-C3-N1	-4.51	107.33	115.20
3	B	902	Y01	OAW-CAY-CAM	4.00	120.12	111.48
3	C	902	Y01	OAW-CAY-CAM	4.00	120.12	111.48
3	D	902	Y01	OAW-CAY-CAM	4.00	120.12	111.48
3	A	902	Y01	OAW-CAY-CAM	3.99	120.12	111.48
3	B	902	Y01	CAV-CAZ-CBH	3.81	121.30	116.42
3	C	902	Y01	CAV-CAZ-CBH	3.81	121.30	116.42
3	A	902	Y01	CAV-CAZ-CBH	3.80	121.28	116.42
3	D	902	Y01	CAV-CAZ-CBH	3.79	121.27	116.42
8	D	907	A1L8M	O2-C31-C32	3.75	119.60	111.48
8	A	907	A1L8M	O2-C31-C32	3.74	119.56	111.48
8	C	907	A1L8M	O2-C31-C32	3.74	119.56	111.48
8	B	907	A1L8M	O2-C31-C32	3.73	119.56	111.48
7	A	906	PTY	O7-C8-O10	-3.66	115.14	123.70
7	B	906	PTY	O7-C8-O10	-3.65	115.16	123.70
7	C	906	PTY	O7-C8-O10	-3.65	115.16	123.70
7	D	906	PTY	O7-C8-O10	-3.65	115.16	123.70
6	C	905	657	C5-C4-C3	-3.59	119.32	121.99
6	A	905	657	C5-C4-C3	-3.56	119.34	121.99
6	D	905	657	C5-C4-C3	-3.56	119.34	121.99
6	B	905	657	C5-C4-C3	-3.53	119.37	121.99
8	A	907	A1L8M	O3-C11-C12	3.44	122.33	111.83
8	B	907	A1L8M	O3-C11-C12	3.44	122.33	111.83
8	C	907	A1L8M	O3-C11-C12	3.44	122.33	111.83
8	D	907	A1L8M	O3-C11-C12	3.43	122.31	111.83
2	A	901	POV	O21-C21-C22	3.08	118.14	111.48
2	B	901	POV	O21-C21-C22	3.08	118.14	111.48
2	C	901	POV	O21-C21-C22	3.07	118.13	111.48
2	D	901	POV	O21-C21-C22	3.06	118.10	111.48
2	A	901	POV	O31-C31-C32	3.01	121.00	111.83
2	C	901	POV	O31-C31-C32	2.99	120.96	111.83
2	B	901	POV	O31-C31-C32	2.99	120.96	111.83
2	D	901	POV	O31-C31-C32	2.99	120.94	111.83
7	C	906	PTY	O4-C1-C6	2.90	116.75	108.40
7	D	906	PTY	O4-C1-C6	2.90	116.75	108.40
7	A	906	PTY	O4-C1-C6	2.89	116.72	108.40
7	B	906	PTY	O4-C1-C6	2.88	116.70	108.40
3	C	902	Y01	CBI-CBE-CBB	-2.84	115.10	119.50
3	D	902	Y01	CBI-CBE-CBB	-2.83	115.13	119.50
3	A	902	Y01	CBD-CAK-CAI	-2.81	108.87	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	Y01	CBI-CBE-CBB	-2.81	115.16	119.50
3	B	902	Y01	CBI-CBE-CBB	-2.81	115.16	119.50
3	B	902	Y01	CBD-CAK-CAI	-2.79	108.89	112.76
3	C	902	Y01	CBD-CAK-CAI	-2.79	108.89	112.76
3	D	902	Y01	CBD-CAK-CAI	-2.78	108.92	112.76
6	A	905	657	C3-N1-C8	-2.71	108.96	110.57
6	B	905	657	C3-N1-C8	-2.71	108.96	110.57
6	C	905	657	C3-N1-C8	-2.71	108.96	110.57
6	D	905	657	C3-N1-C8	-2.71	108.96	110.57
7	B	906	PTY	O7-C6-C1	-2.69	98.69	108.34
7	A	906	PTY	O7-C6-C1	-2.69	98.71	108.34
7	C	906	PTY	O7-C6-C1	-2.69	98.71	108.34
7	D	906	PTY	O7-C6-C1	-2.68	98.73	108.34
8	A	907	A1L8M	O3-C11-O11	-2.61	117.10	123.63
8	B	907	A1L8M	O3-C11-O11	-2.61	117.10	123.63
8	C	907	A1L8M	O3-C11-O11	-2.60	117.12	123.63
8	D	907	A1L8M	O3-C11-O11	-2.60	117.13	123.63
7	B	906	PTY	O4-C30-C31	2.51	119.50	111.83
7	C	906	PTY	O4-C30-C31	2.51	119.50	111.83
7	D	906	PTY	O4-C30-C31	2.51	119.50	111.83
7	A	906	PTY	O4-C30-C31	2.51	119.47	111.83
3	B	902	Y01	CBC-OAW-CAY	-2.46	111.90	117.80
3	C	902	Y01	CBC-OAW-CAY	-2.46	111.90	117.80
3	D	902	Y01	CBC-OAW-CAY	-2.46	111.90	117.80
3	A	902	Y01	CBC-OAW-CAY	-2.45	111.94	117.80
2	D	901	POV	O13-P-O14	2.41	120.22	110.83
2	A	901	POV	O13-P-O14	2.40	120.19	110.83
2	B	901	POV	O13-P-O14	2.40	120.17	110.83
2	C	901	POV	O13-P-O14	2.40	120.17	110.83
7	D	906	PTY	O12-P1-O11	-2.38	96.78	107.57
7	A	906	PTY	O12-P1-O11	-2.37	96.81	107.57
7	B	906	PTY	O12-P1-O11	-2.37	96.81	107.57
7	C	906	PTY	O12-P1-O11	-2.37	96.84	107.57
7	B	906	PTY	O4-C30-O30	-2.33	117.79	123.63
7	C	906	PTY	O4-C30-O30	-2.33	117.79	123.63
7	D	906	PTY	O4-C30-O30	-2.33	117.79	123.63
7	A	906	PTY	O4-C30-O30	-2.32	117.81	123.63
6	A	905	657	C5-C4-S1	2.31	131.83	126.07
6	B	905	657	C5-C4-S1	2.31	131.83	126.07
6	D	905	657	C5-C4-S1	2.31	131.83	126.07
6	A	905	657	C6-C5-C4	2.31	121.33	117.87
6	C	905	657	C5-C4-S1	2.30	131.81	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	905	657	C6-C5-C4	2.29	121.31	117.87
6	C	905	657	C6-C5-C4	2.29	121.31	117.87
6	D	905	657	C6-C5-C4	2.28	121.28	117.87
2	A	901	POV	O31-C31-O32	-2.13	118.30	123.63
2	B	901	POV	O31-C31-O32	-2.11	118.34	123.63
2	C	901	POV	O31-C31-O32	-2.11	118.34	123.63
2	D	901	POV	O31-C31-O32	-2.10	118.38	123.63
3	D	902	Y01	CAV-CAZ-CAI	-2.08	117.76	120.57
3	A	902	Y01	CAS-CAU-CBI	-2.06	109.27	112.74
3	A	902	Y01	CAV-CAZ-CAI	-2.05	117.78	120.57
3	B	902	Y01	CAV-CAZ-CAI	-2.05	117.78	120.57
3	C	902	Y01	CAV-CAZ-CAI	-2.05	117.78	120.57
3	C	902	Y01	CAS-CAU-CBI	-2.05	109.28	112.74
3	D	902	Y01	CAS-CAU-CBI	-2.04	109.29	112.74
3	B	902	Y01	CAS-CAU-CBI	-2.04	109.30	112.74

There are no chirality outliers.

All (228) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C1-O11-P-O12
2	A	901	POV	C1-O11-P-O13
2	A	901	POV	C1-O11-P-O14
2	B	901	POV	C1-O11-P-O12
2	B	901	POV	C1-O11-P-O13
2	B	901	POV	C1-O11-P-O14
2	C	901	POV	C1-O11-P-O12
2	C	901	POV	C1-O11-P-O13
2	C	901	POV	C1-O11-P-O14
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C1-O11-P-O14
7	A	906	PTY	N1-C2-C3-O11
7	A	906	PTY	O10-C8-O7-C6
7	A	906	PTY	C3-O11-P1-O12
7	A	906	PTY	C3-O11-P1-O13
7	A	906	PTY	C3-O11-P1-O14
7	A	906	PTY	C5-O14-P1-O11
7	A	906	PTY	C5-O14-P1-O12
7	A	906	PTY	C5-O14-P1-O13
7	B	906	PTY	N1-C2-C3-O11
7	B	906	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
7	B	906	PTY	C3-O11-P1-O12
7	B	906	PTY	C3-O11-P1-O13
7	B	906	PTY	C3-O11-P1-O14
7	B	906	PTY	C5-O14-P1-O11
7	B	906	PTY	C5-O14-P1-O12
7	B	906	PTY	C5-O14-P1-O13
7	C	906	PTY	N1-C2-C3-O11
7	C	906	PTY	O10-C8-O7-C6
7	C	906	PTY	C3-O11-P1-O12
7	C	906	PTY	C3-O11-P1-O13
7	C	906	PTY	C3-O11-P1-O14
7	C	906	PTY	C5-O14-P1-O11
7	C	906	PTY	C5-O14-P1-O12
7	C	906	PTY	C5-O14-P1-O13
7	D	906	PTY	N1-C2-C3-O11
7	D	906	PTY	O10-C8-O7-C6
7	D	906	PTY	C3-O11-P1-O12
7	D	906	PTY	C3-O11-P1-O13
7	D	906	PTY	C3-O11-P1-O14
7	D	906	PTY	C5-O14-P1-O11
7	D	906	PTY	C5-O14-P1-O12
7	D	906	PTY	C5-O14-P1-O13
7	A	906	PTY	C31-C30-O4-C1
7	B	906	PTY	C31-C30-O4-C1
7	C	906	PTY	C31-C30-O4-C1
7	D	906	PTY	C31-C30-O4-C1
7	A	906	PTY	C11-C8-O7-C6
7	B	906	PTY	C11-C8-O7-C6
7	C	906	PTY	C11-C8-O7-C6
7	D	906	PTY	C11-C8-O7-C6
7	A	906	PTY	O30-C30-O4-C1
7	B	906	PTY	O30-C30-O4-C1
7	C	906	PTY	O30-C30-O4-C1
7	D	906	PTY	O30-C30-O4-C1
2	A	901	POV	C21-C22-C23-C24
2	B	901	POV	C21-C22-C23-C24
2	C	901	POV	C21-C22-C23-C24
2	D	901	POV	C21-C22-C23-C24
3	A	902	Y01	OAG-CAY-OAW-CBC
3	B	902	Y01	OAG-CAY-OAW-CBC
3	C	902	Y01	OAG-CAY-OAW-CBC
3	A	902	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	B	902	Y01	CAM-CAY-OAW-CBC
3	C	902	Y01	CAM-CAY-OAW-CBC
3	D	902	Y01	CAM-CAY-OAW-CBC
3	D	902	Y01	OAG-CAY-OAW-CBC
7	A	906	PTY	O14-C5-C6-C1
7	B	906	PTY	O14-C5-C6-C1
7	C	906	PTY	O14-C5-C6-C1
7	D	906	PTY	O14-C5-C6-C1
7	A	906	PTY	C20-C21-C22-C23
7	B	906	PTY	C20-C21-C22-C23
7	C	906	PTY	C20-C21-C22-C23
7	D	906	PTY	C20-C21-C22-C23
7	A	906	PTY	C30-C31-C32-C33
7	B	906	PTY	C30-C31-C32-C33
7	C	906	PTY	C30-C31-C32-C33
7	D	906	PTY	C30-C31-C32-C33
7	A	906	PTY	C34-C35-C36-C37
7	B	906	PTY	C34-C35-C36-C37
7	C	906	PTY	C34-C35-C36-C37
7	D	906	PTY	C34-C35-C36-C37
8	A	907	A1L8M	C33-C34-C35-C36
8	C	907	A1L8M	C33-C34-C35-C36
8	D	907	A1L8M	C33-C34-C35-C36
8	B	907	A1L8M	C33-C34-C35-C36
2	A	901	POV	O11-C1-C2-O21
2	B	901	POV	O11-C1-C2-O21
2	C	901	POV	O11-C1-C2-O21
2	D	901	POV	O11-C1-C2-O21
2	A	901	POV	C311-C310-C39-C38
2	B	901	POV	C311-C310-C39-C38
2	C	901	POV	C311-C310-C39-C38
2	D	901	POV	C311-C310-C39-C38
2	A	901	POV	C36-C37-C38-C39
2	C	901	POV	C36-C37-C38-C39
2	D	901	POV	C36-C37-C38-C39
2	B	901	POV	C36-C37-C38-C39
8	B	907	A1L8M	C36-C37-C38-C39
8	A	907	A1L8M	C36-C37-C38-C39
8	C	907	A1L8M	C36-C37-C38-C39
8	D	907	A1L8M	C36-C37-C38-C39
3	A	902	Y01	CAC-CBB-CBE-CBI
3	B	902	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	C	902	Y01	CAC-CBB-CBE-CBI
3	D	902	Y01	CAC-CBB-CBE-CBI
2	A	901	POV	C213-C214-C215-C216
2	B	901	POV	C213-C214-C215-C216
2	C	901	POV	C213-C214-C215-C216
2	D	901	POV	C213-C214-C215-C216
3	A	902	Y01	CAO-CBB-CBE-CBI
3	B	902	Y01	CAO-CBB-CBE-CBI
3	C	902	Y01	CAO-CBB-CBE-CBI
3	D	902	Y01	CAO-CBB-CBE-CBI
2	A	901	POV	O11-C1-C2-C3
2	B	901	POV	O11-C1-C2-C3
2	C	901	POV	O11-C1-C2-C3
2	D	901	POV	O11-C1-C2-C3
7	A	906	PTY	O14-C5-C6-O7
7	B	906	PTY	O14-C5-C6-O7
7	C	906	PTY	O14-C5-C6-O7
7	D	906	PTY	O14-C5-C6-O7
7	A	906	PTY	C18-C19-C20-C21
7	B	906	PTY	C18-C19-C20-C21
7	C	906	PTY	C18-C19-C20-C21
7	D	906	PTY	C18-C19-C20-C21
2	C	901	POV	C23-C24-C25-C26
2	B	901	POV	C23-C24-C25-C26
2	D	901	POV	C23-C24-C25-C26
2	A	901	POV	C23-C24-C25-C26
7	A	906	PTY	C35-C36-C37-C38
7	C	906	PTY	C35-C36-C37-C38
7	B	906	PTY	C35-C36-C37-C38
7	D	906	PTY	C35-C36-C37-C38
7	A	906	PTY	C41-C42-C43-C44
7	D	906	PTY	C41-C42-C43-C44
7	B	906	PTY	C41-C42-C43-C44
7	C	906	PTY	C41-C42-C43-C44
8	B	907	A1L8M	C35-C36-C37-C38
8	A	907	A1L8M	C35-C36-C37-C38
8	C	907	A1L8M	C35-C36-C37-C38
8	D	907	A1L8M	C35-C36-C37-C38
7	C	906	PTY	C31-C32-C33-C34
7	B	906	PTY	C31-C32-C33-C34
7	A	906	PTY	C31-C32-C33-C34
7	D	906	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	A	906	PTY	C14-C15-C16-C17
7	B	906	PTY	C14-C15-C16-C17
7	D	906	PTY	C14-C15-C16-C17
7	C	906	PTY	C14-C15-C16-C17
7	A	906	PTY	C38-C39-C40-C41
7	B	906	PTY	C38-C39-C40-C41
7	C	906	PTY	C38-C39-C40-C41
7	D	906	PTY	C38-C39-C40-C41
3	D	902	Y01	CAO-CBB-CBE-CAP
3	A	902	Y01	CAO-CBB-CBE-CAP
3	B	902	Y01	CAO-CBB-CBE-CAP
3	C	902	Y01	CAO-CBB-CBE-CAP
7	A	906	PTY	C32-C33-C34-C35
7	C	906	PTY	C32-C33-C34-C35
7	D	906	PTY	C32-C33-C34-C35
7	B	906	PTY	C32-C33-C34-C35
3	A	902	Y01	CAC-CBB-CBE-CAP
3	B	902	Y01	CAC-CBB-CBE-CAP
3	C	902	Y01	CAC-CBB-CBE-CAP
3	D	902	Y01	CAC-CBB-CBE-CAP
2	A	901	POV	C37-C38-C39-C310
2	D	901	POV	C37-C38-C39-C310
2	B	901	POV	C37-C38-C39-C310
2	C	901	POV	C37-C38-C39-C310
8	A	907	A1L8M	C42-C43-C44-C45
8	B	907	A1L8M	C42-C43-C44-C45
8	C	907	A1L8M	C42-C43-C44-C45
8	D	907	A1L8M	C42-C43-C44-C45
2	D	901	POV	C212-C213-C214-C215
2	A	901	POV	C212-C213-C214-C215
2	B	901	POV	C212-C213-C214-C215
2	C	901	POV	C212-C213-C214-C215
8	A	907	A1L8M	C37-C38-C39-C40
8	B	907	A1L8M	C37-C38-C39-C40
8	C	907	A1L8M	C37-C38-C39-C40
8	D	907	A1L8M	C37-C38-C39-C40
2	A	901	POV	O21-C2-C3-O31
2	B	901	POV	O21-C2-C3-O31
2	C	901	POV	O21-C2-C3-O31
2	D	901	POV	O21-C2-C3-O31
7	A	906	PTY	C15-C16-C17-C18
7	B	906	PTY	C15-C16-C17-C18

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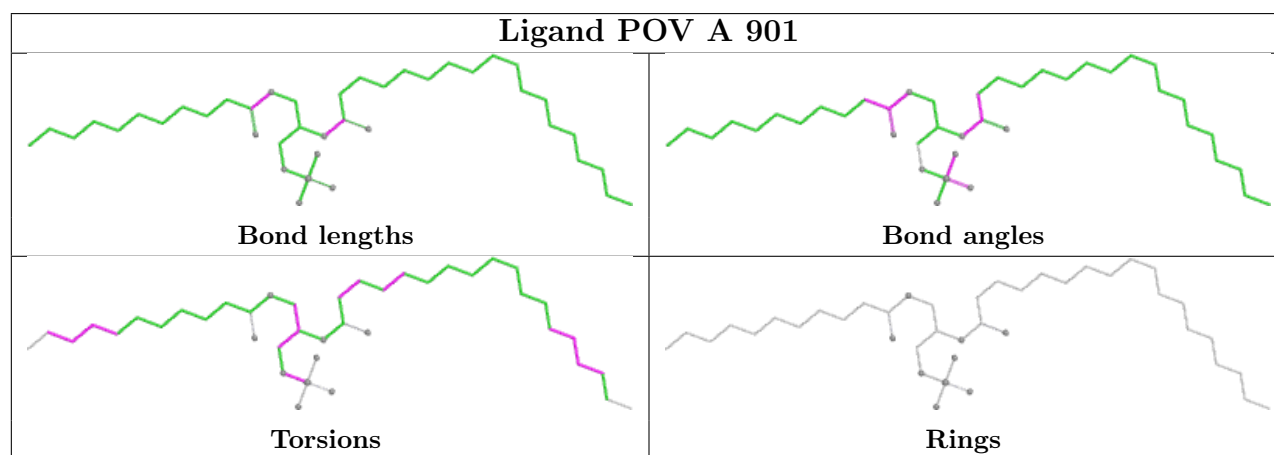
Mol	Chain	Res	Type	Atoms
7	C	906	PTY	C15-C16-C17-C18
7	D	906	PTY	C15-C16-C17-C18
2	D	901	POV	C214-C215-C216-C217
2	A	901	POV	C214-C215-C216-C217
2	B	901	POV	C214-C215-C216-C217
2	C	901	POV	C214-C215-C216-C217
7	B	906	PTY	C16-C17-C18-C19
7	D	906	PTY	C16-C17-C18-C19
7	A	906	PTY	C16-C17-C18-C19
7	C	906	PTY	C16-C17-C18-C19
3	A	902	Y01	CAM-CAL-CAX-OAH
3	B	902	Y01	CAM-CAL-CAX-OAH
3	C	902	Y01	CAM-CAL-CAX-OAH
3	D	902	Y01	CAM-CAL-CAX-OAH
8	A	907	A1L8M	C39-C40-C41-C42
8	B	907	A1L8M	C39-C40-C41-C42
8	C	907	A1L8M	C39-C40-C41-C42
8	D	907	A1L8M	C39-C40-C41-C42
3	D	902	Y01	CAM-CAL-CAX-OAF
3	A	902	Y01	CAM-CAL-CAX-OAF
3	B	902	Y01	CAM-CAL-CAX-OAF
3	C	902	Y01	CAM-CAL-CAX-OAF
3	A	902	Y01	CAL-CAM-CAY-OAW
3	B	902	Y01	CAL-CAM-CAY-OAW
3	C	902	Y01	CAL-CAM-CAY-OAW
3	D	902	Y01	CAL-CAM-CAY-OAW
3	B	902	Y01	CAN-CAJ-CAO-CBB
3	A	902	Y01	CAN-CAJ-CAO-CBB
3	C	902	Y01	CAN-CAJ-CAO-CBB
3	D	902	Y01	CAN-CAJ-CAO-CBB
3	B	902	Y01	CAL-CAM-CAY-OAG
3	C	902	Y01	CAL-CAM-CAY-OAG
3	D	902	Y01	CAL-CAM-CAY-OAG
3	A	902	Y01	CAL-CAM-CAY-OAG
8	A	907	A1L8M	O2-C31-C32-C33
8	B	907	A1L8M	O2-C31-C32-C33
8	C	907	A1L8M	O2-C31-C32-C33
8	D	907	A1L8M	O2-C31-C32-C33

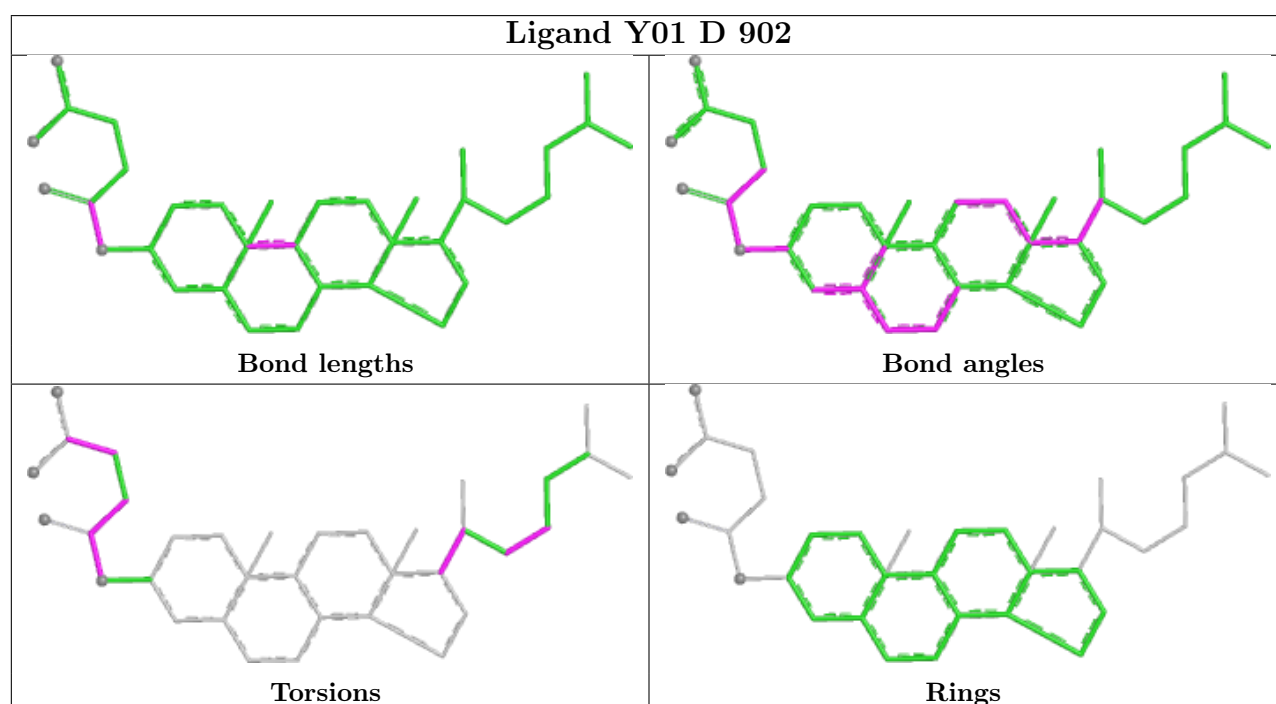
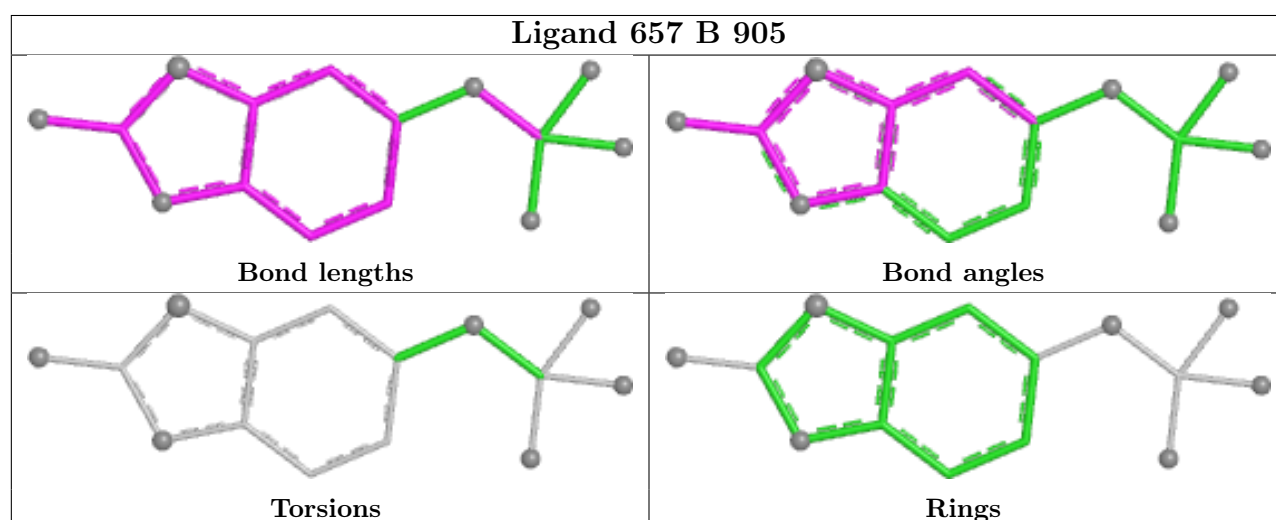
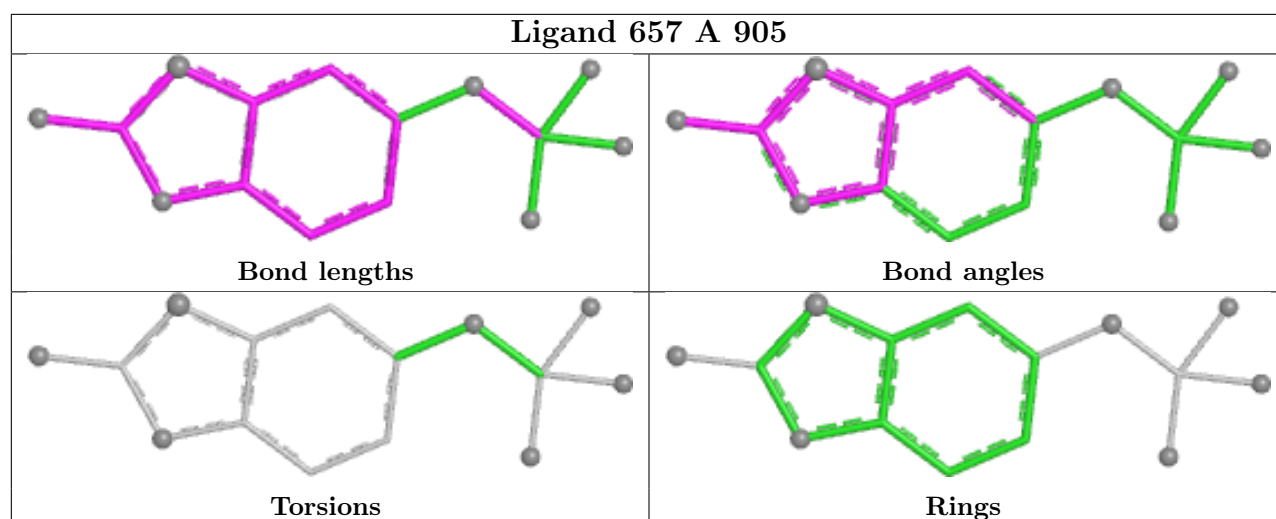
There are no ring outliers.

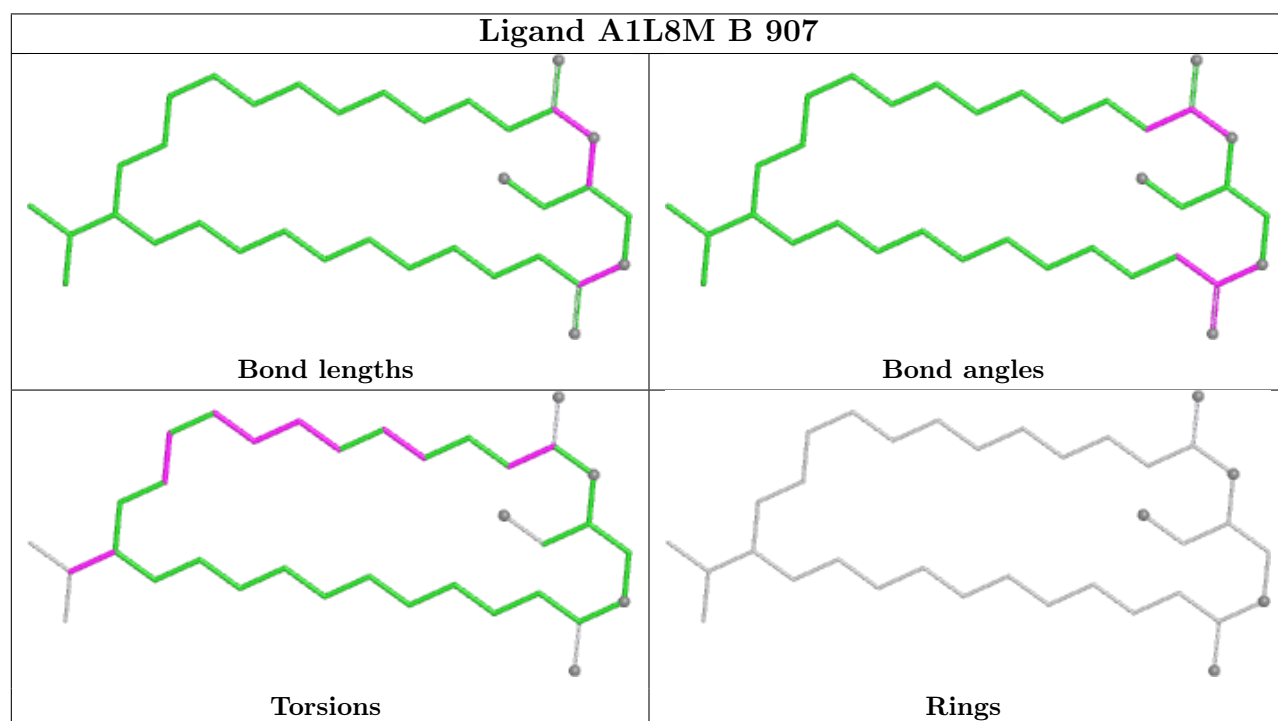
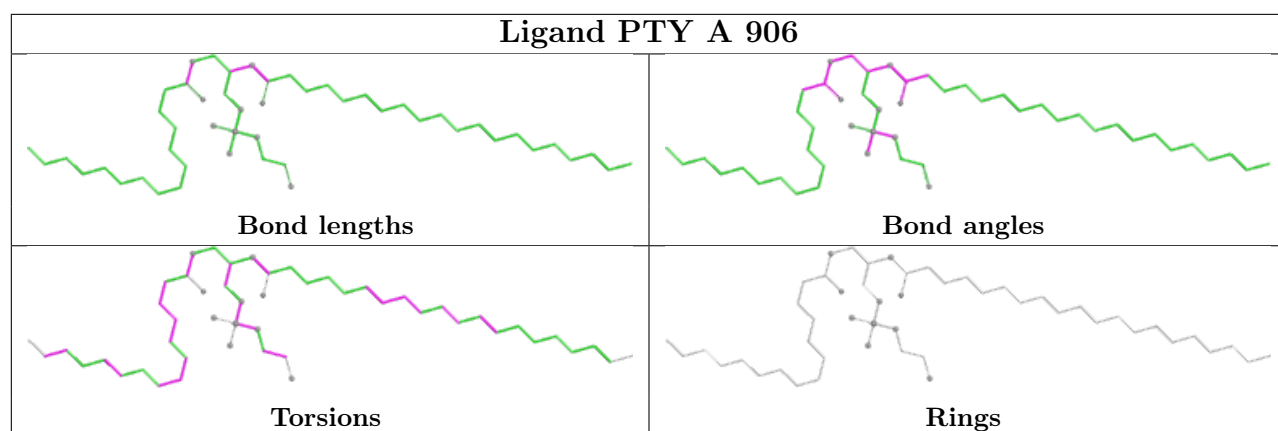
12 monomers are involved in 65 short contacts:

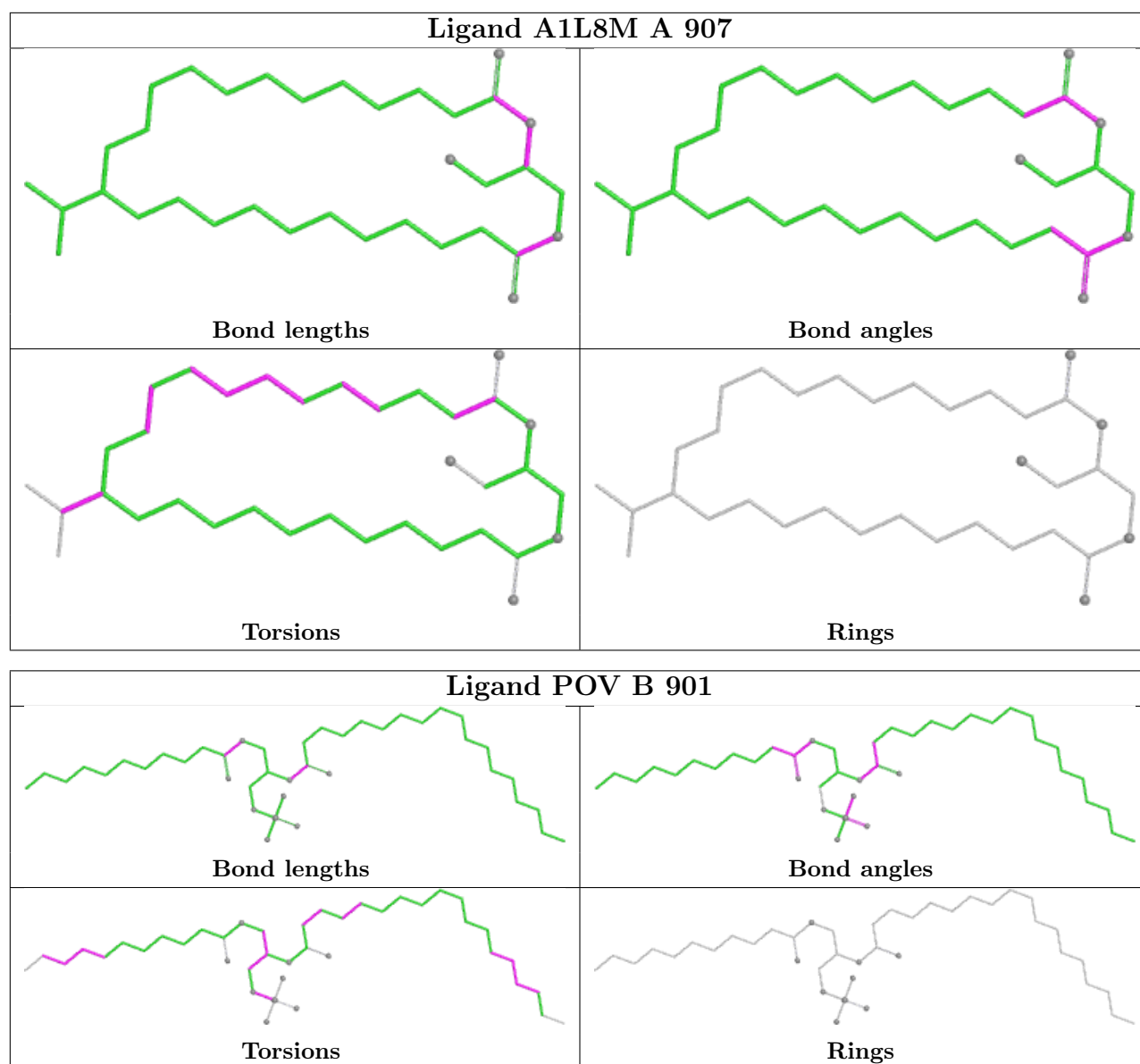
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	POV	6	0
3	D	902	Y01	3	0
7	A	906	PTY	8	0
2	B	901	POV	6	0
3	C	902	Y01	2	0
2	D	901	POV	5	0
7	B	906	PTY	8	0
7	C	906	PTY	9	0
3	B	902	Y01	3	0
7	D	906	PTY	8	0
2	C	901	POV	5	0
3	A	902	Y01	2	0

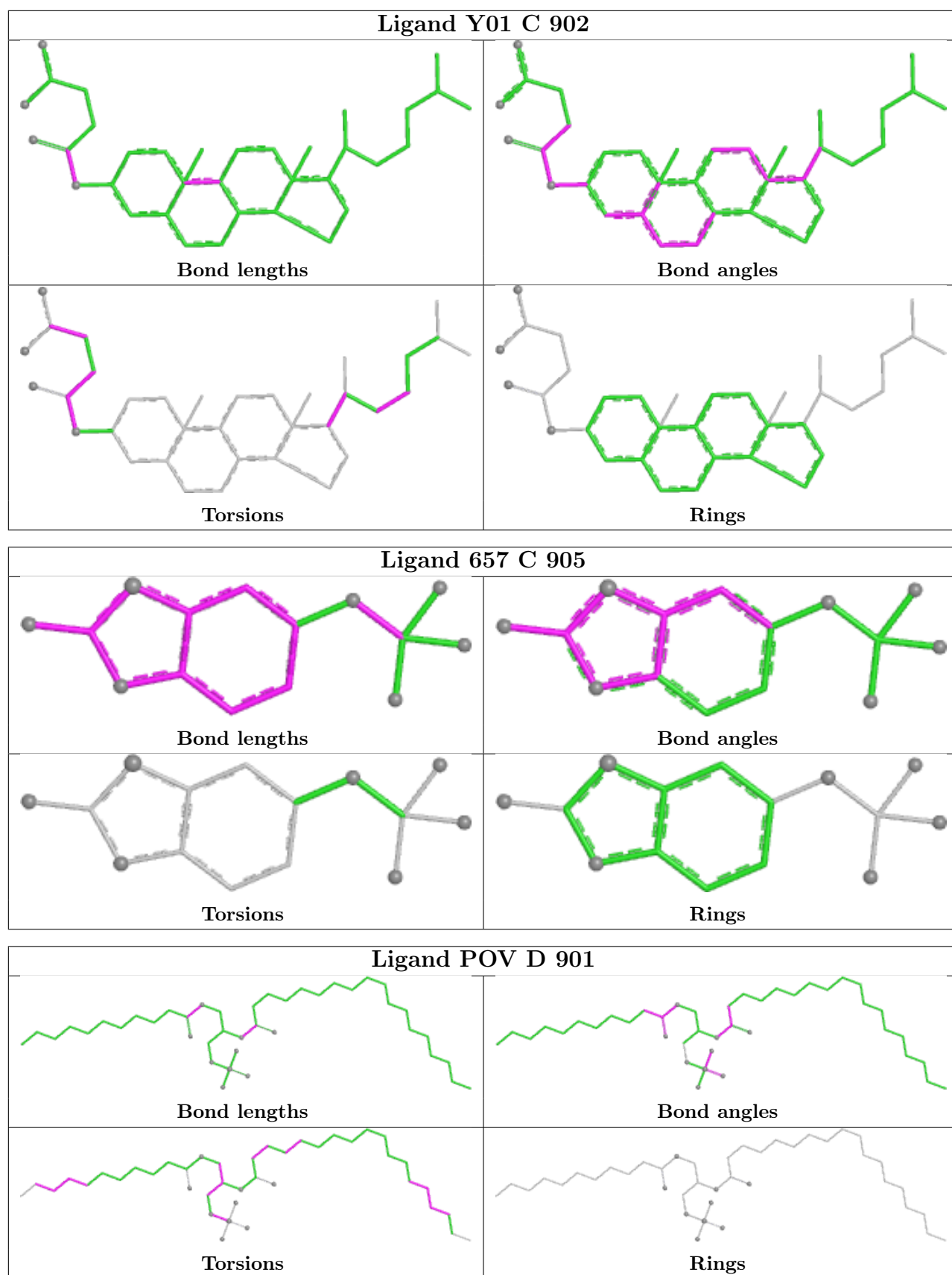
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

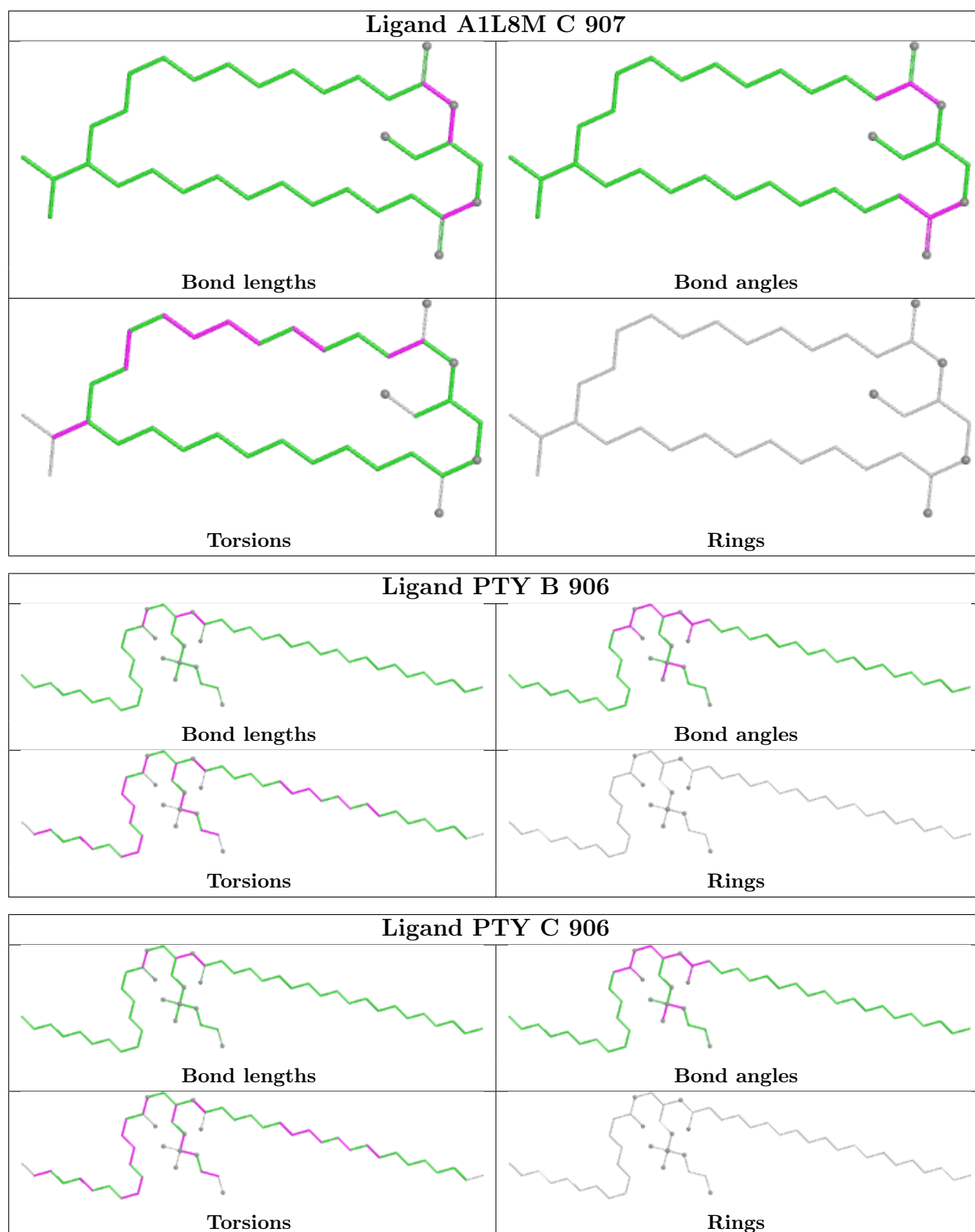


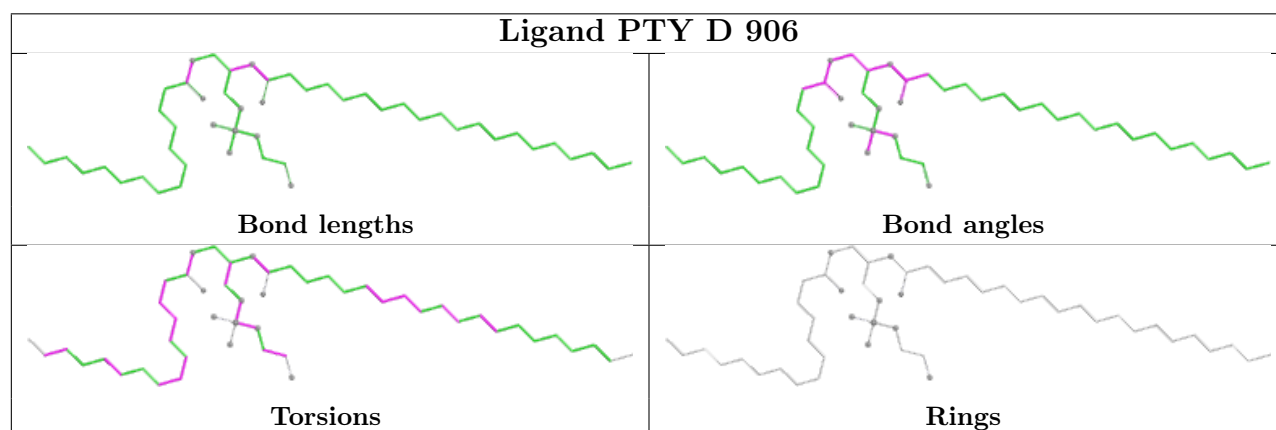
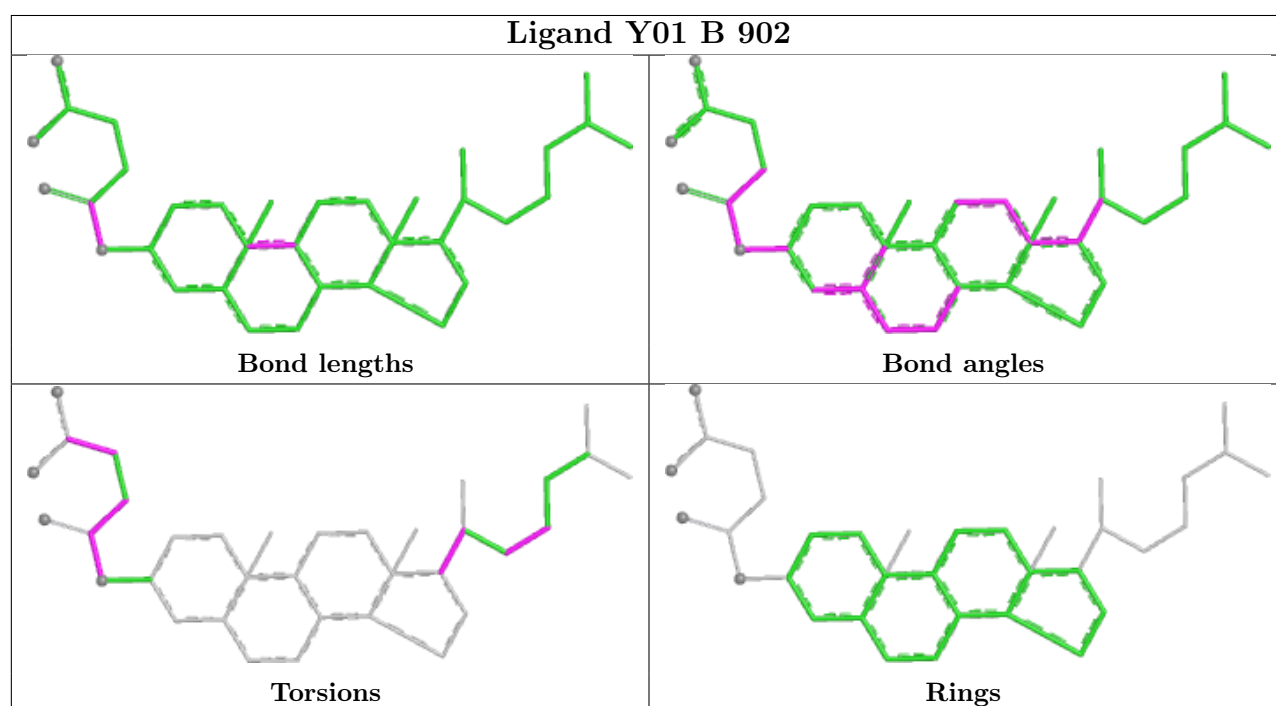
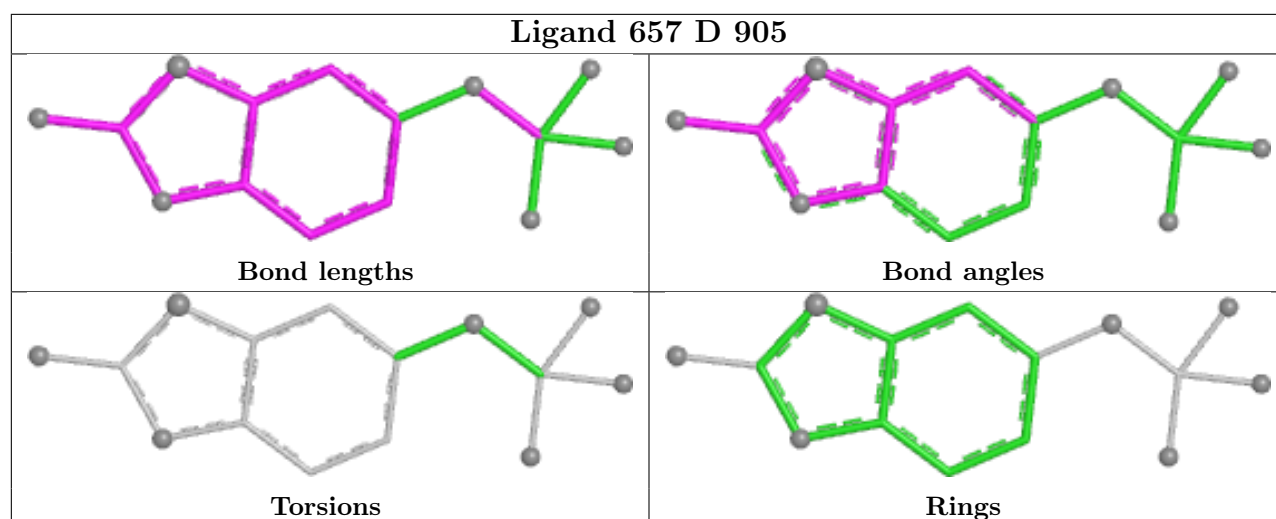


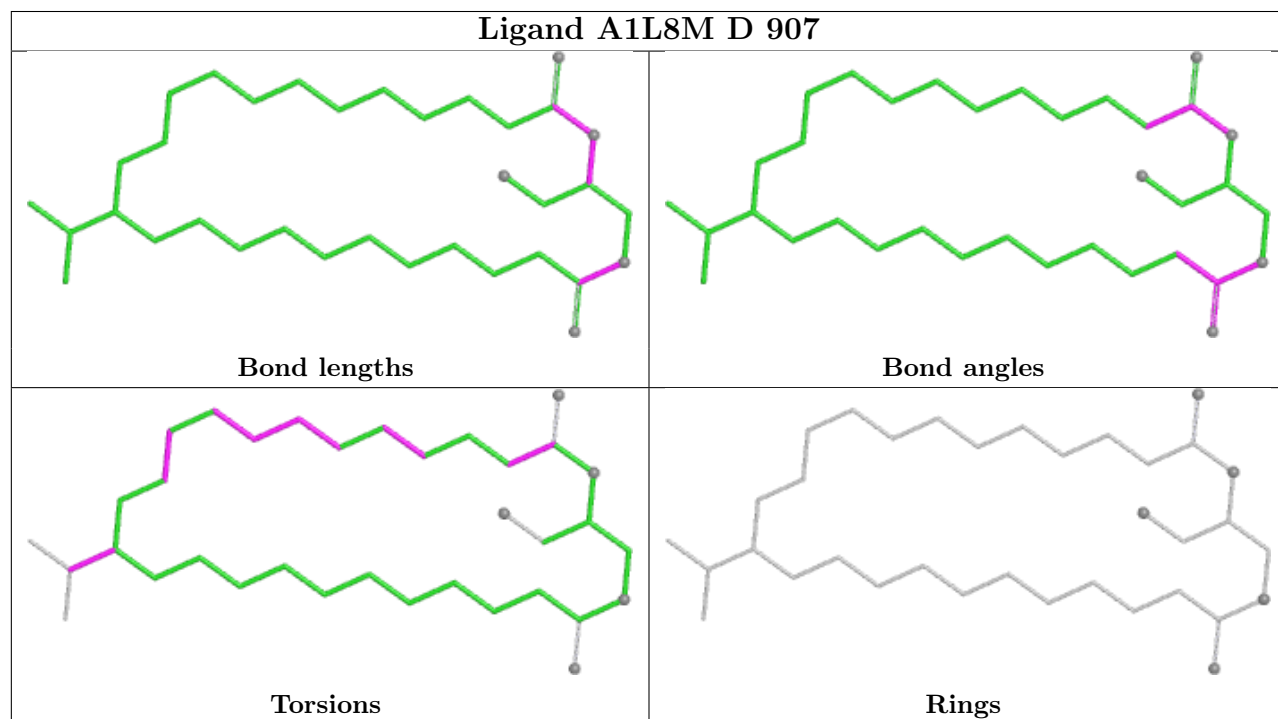
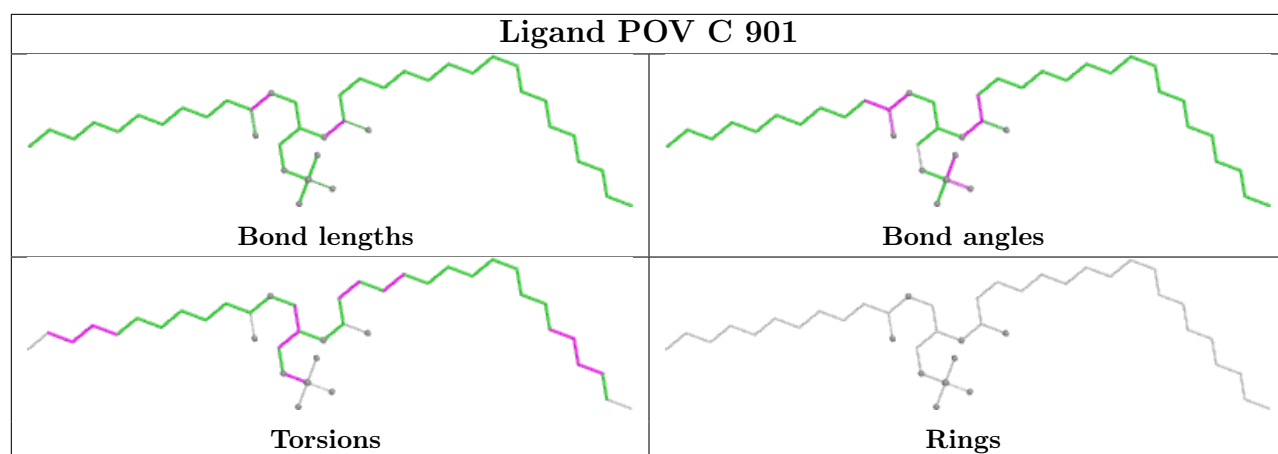


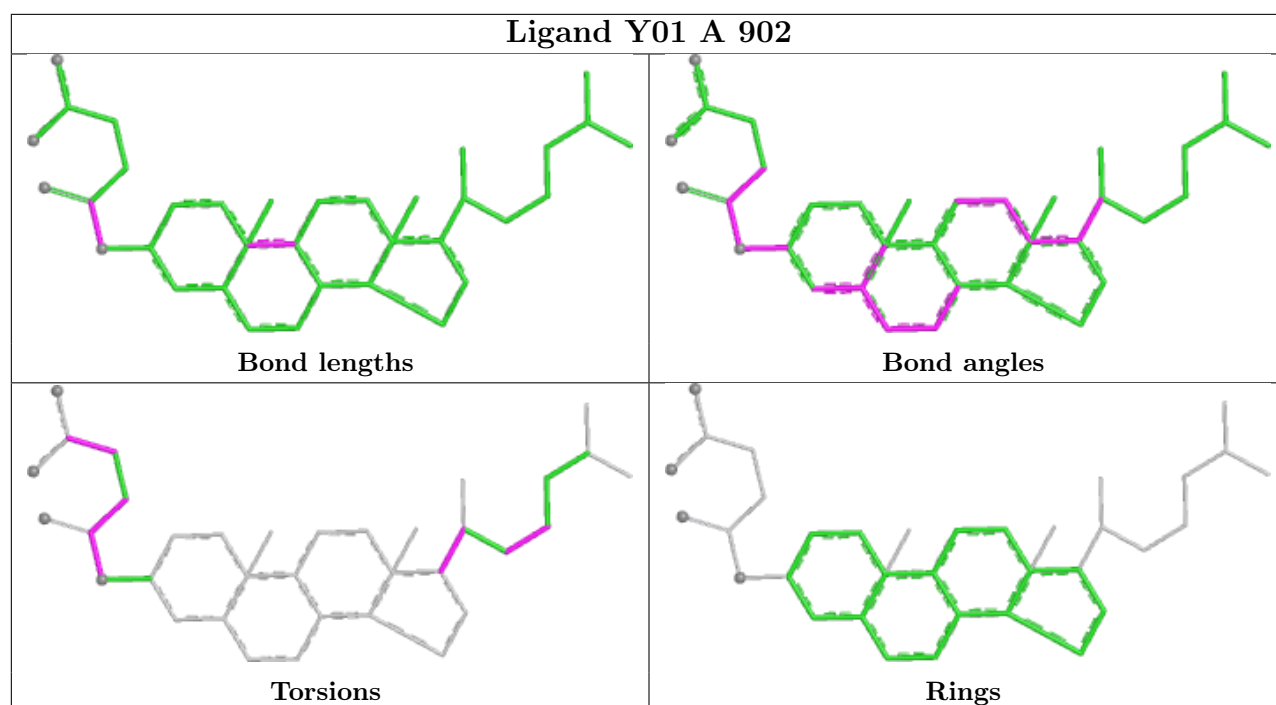












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

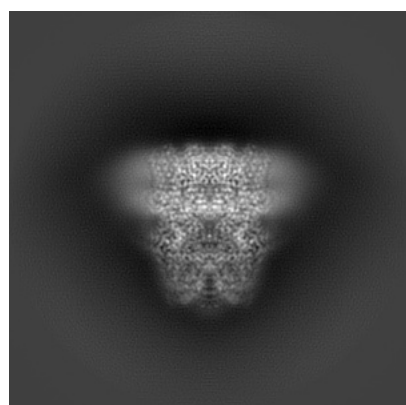
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32436. These allow visual inspection of the internal detail of the map and identification of artifacts.

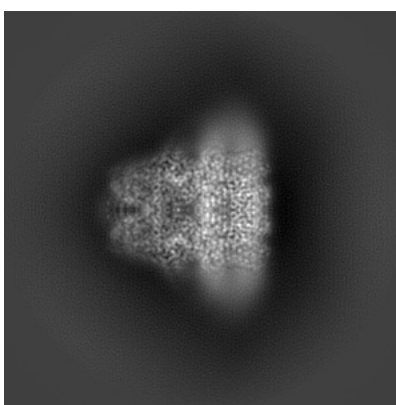
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

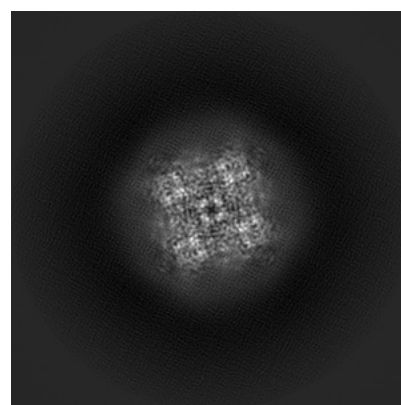
6.1.1 Primary map



X



Y

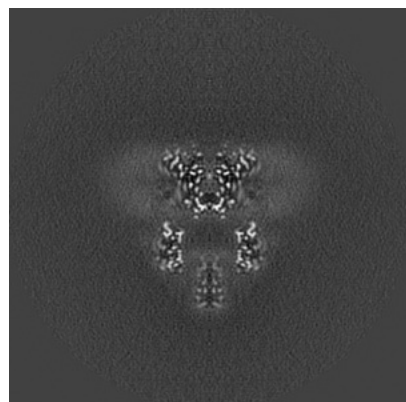


Z

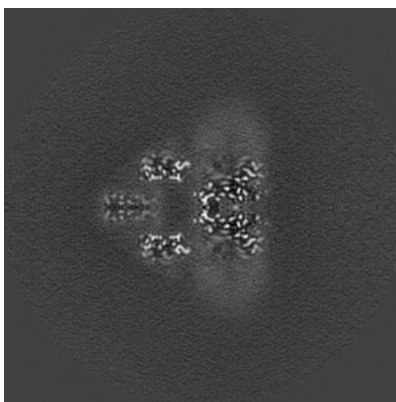
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

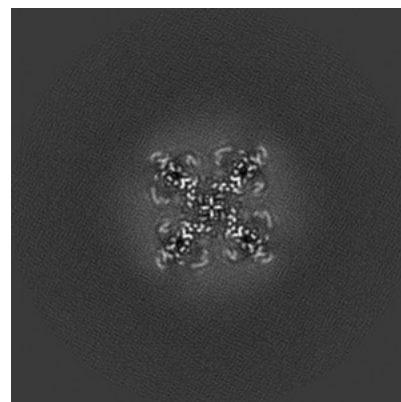
6.2.1 Primary map



X Index: 180



Y Index: 180

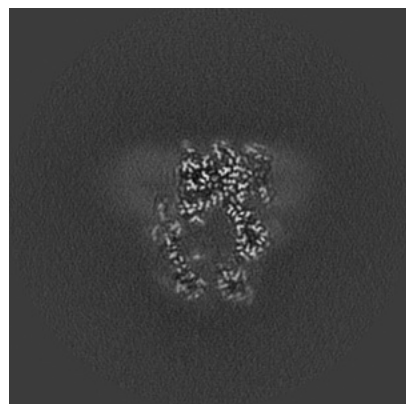


Z Index: 180

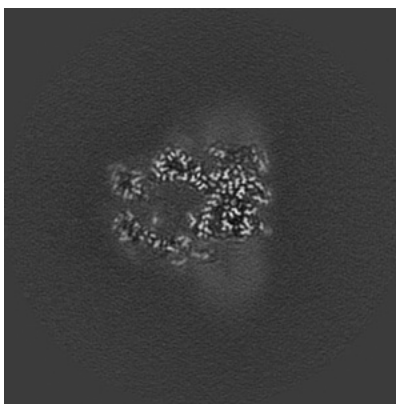
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

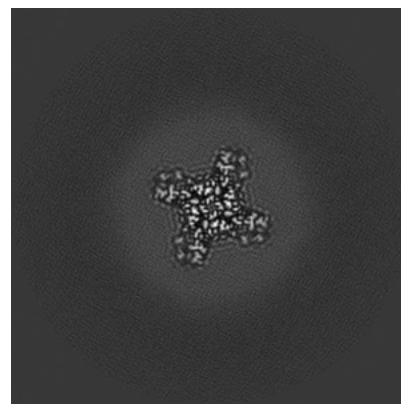
6.3.1 Primary map



X Index: 198



Y Index: 162

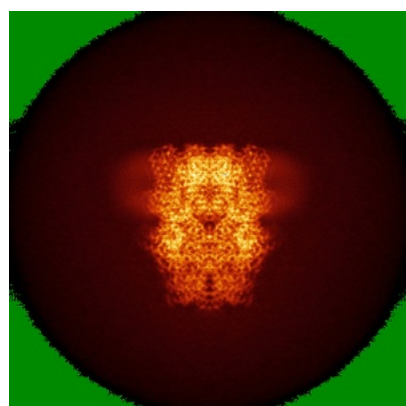


Z Index: 212

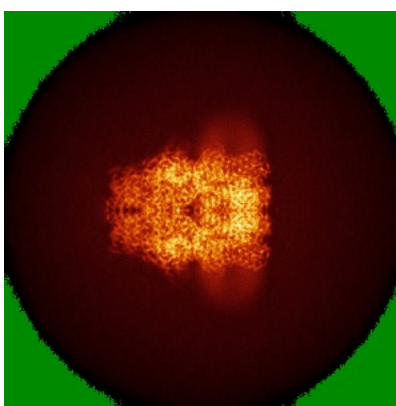
The images above show the largest variance slices of the map in three orthogonal directions.

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

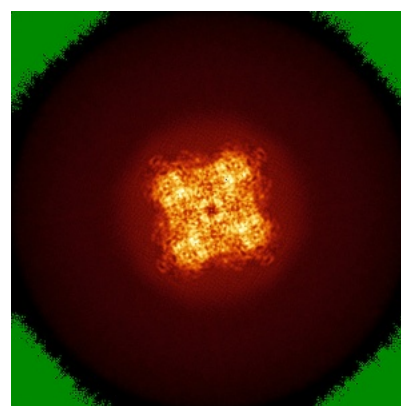
6.4.1 Primary map



X



Y

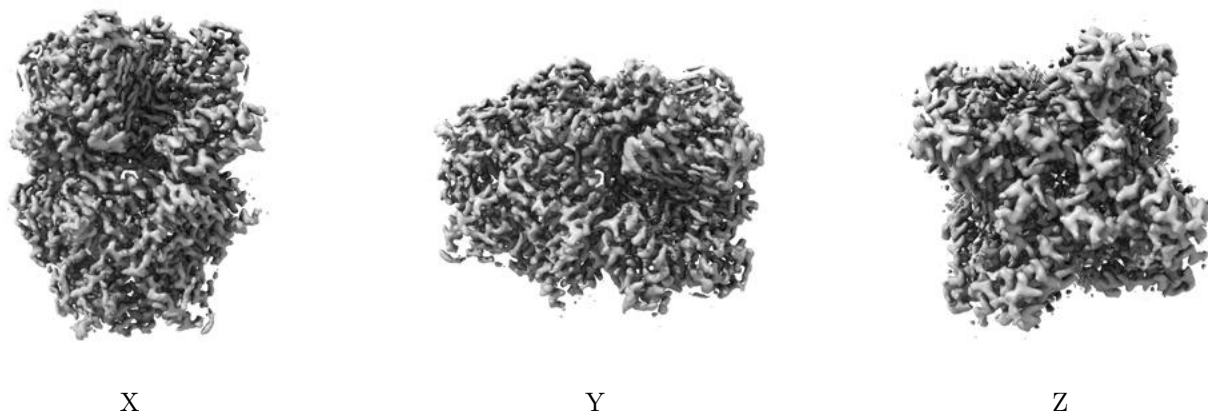


Z

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

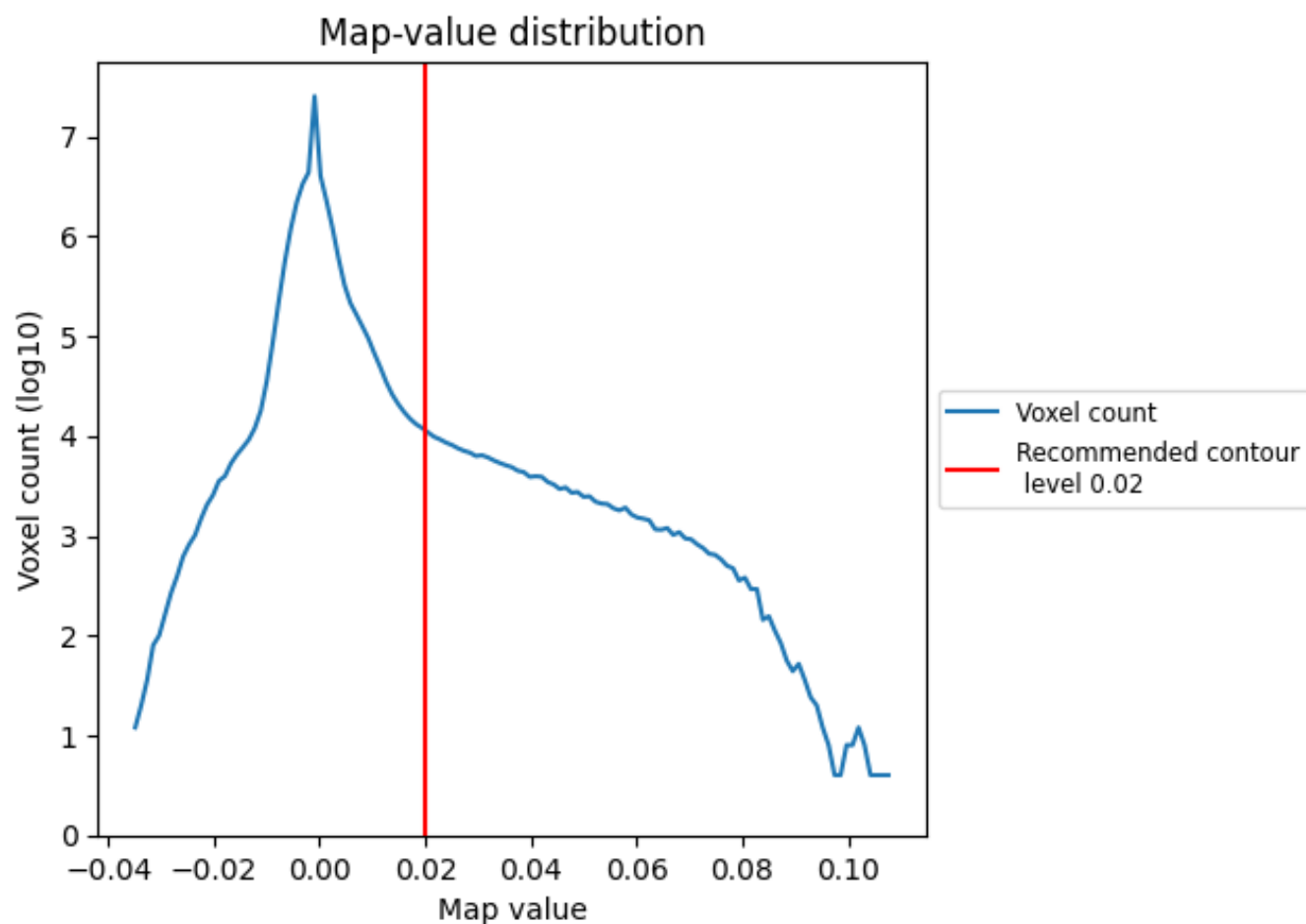
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

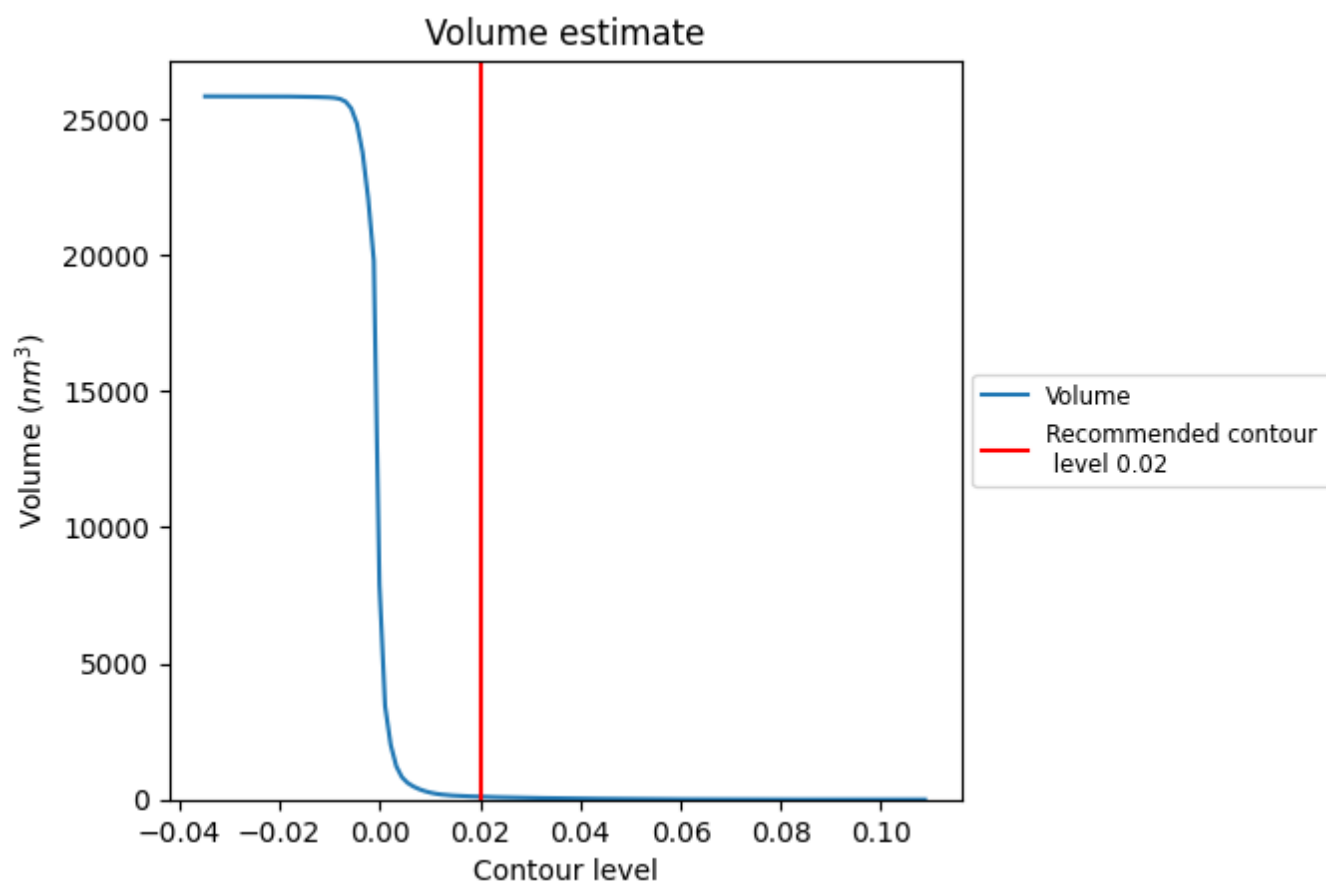
This section contains the results of statistical analysis of the map.

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.

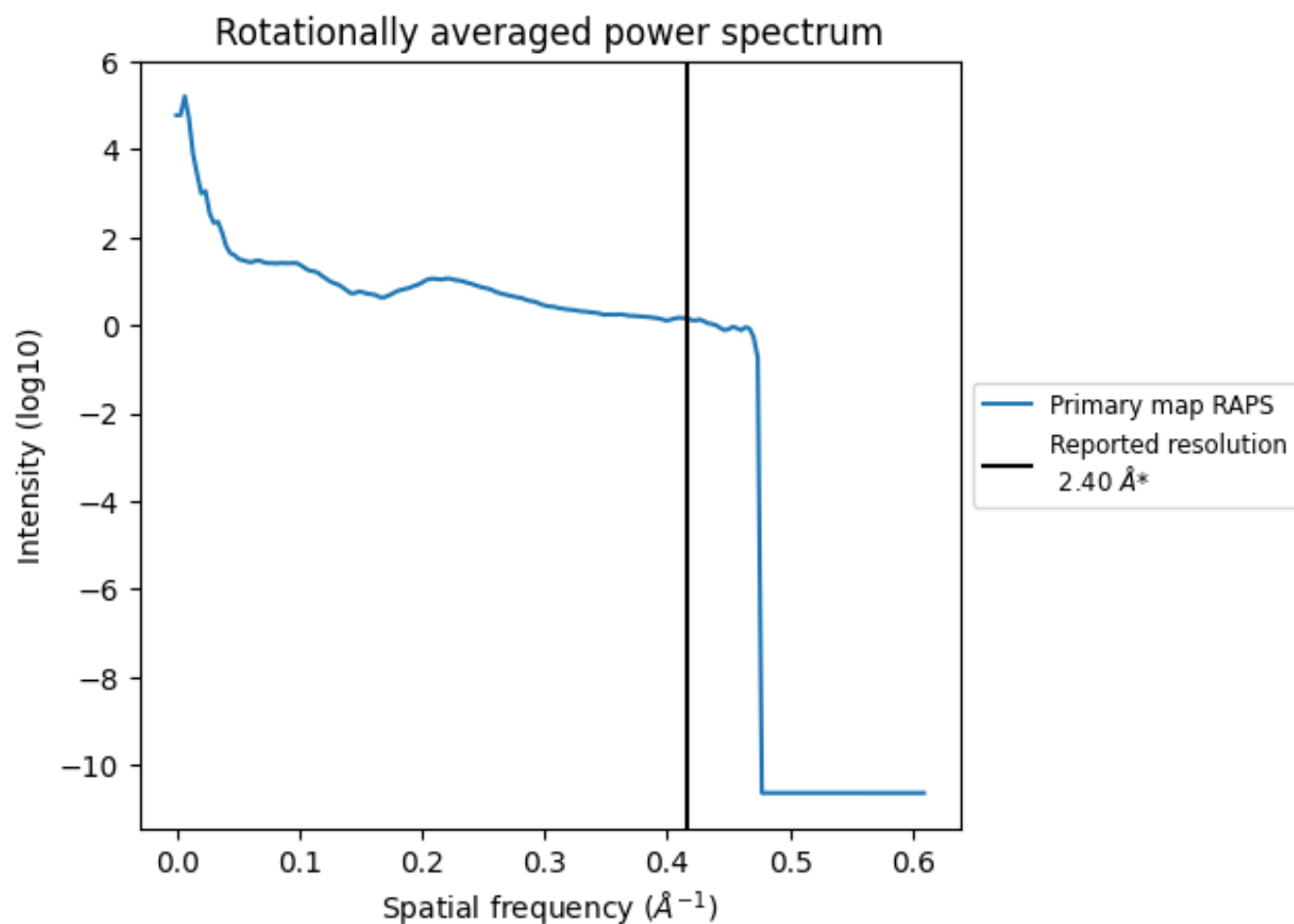
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 94 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 0.417 Å⁻¹

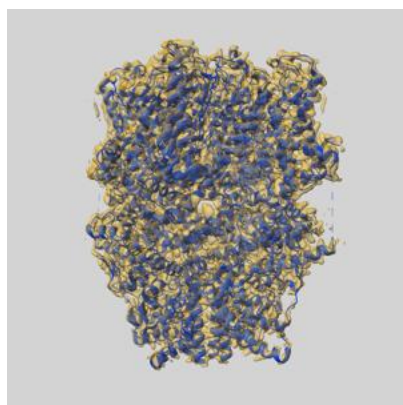
8 Fourier-Shell correlation ⓘ

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

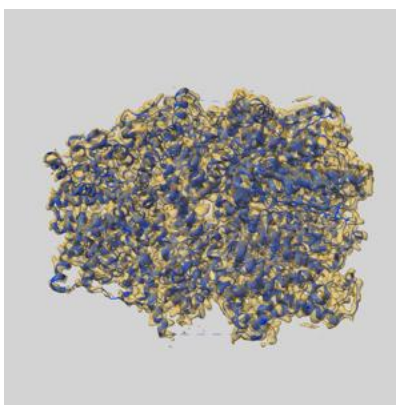
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32436 and PDB model 7WDB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

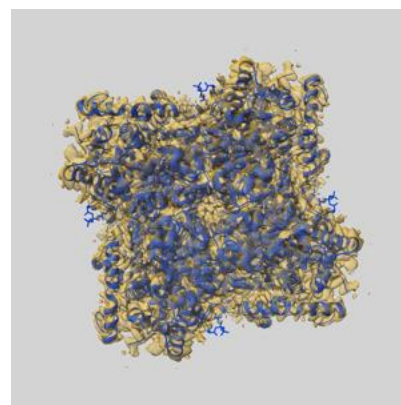
9.1 Map-model overlay [i](#)



X



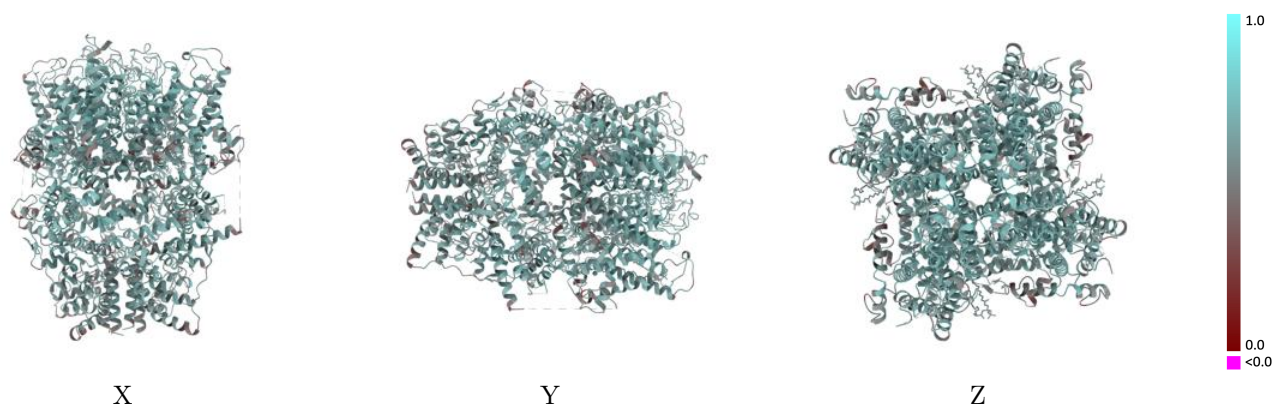
Y



Z

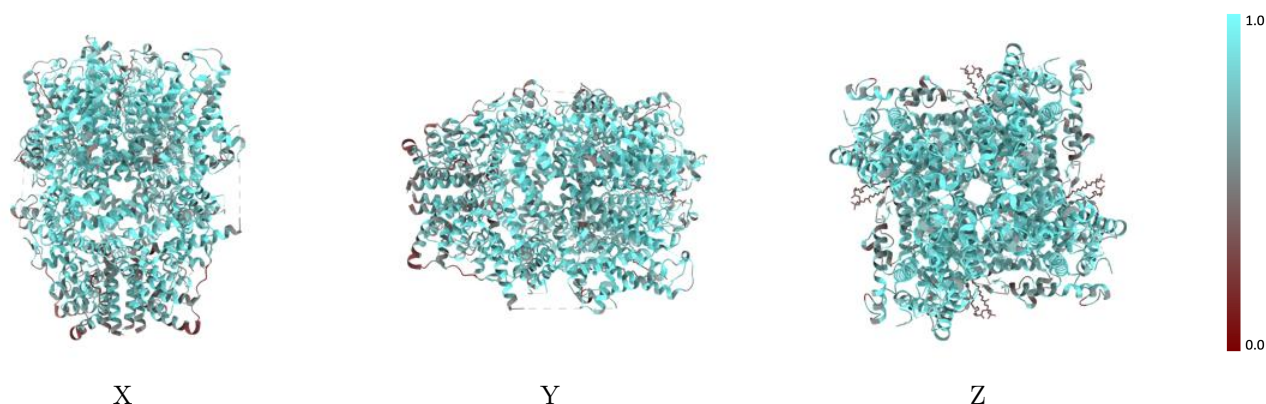
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



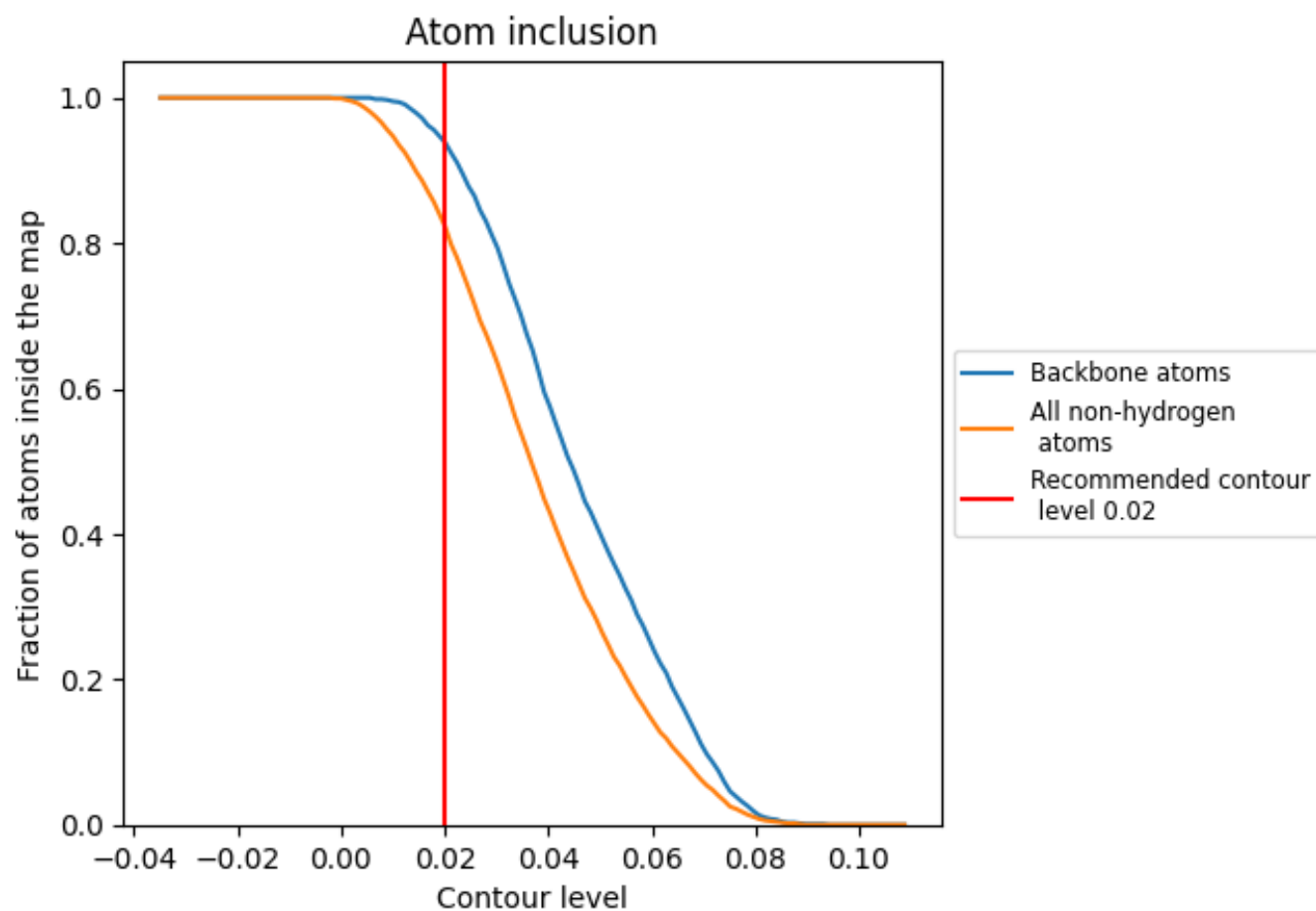
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.6110
A	0.8240	0.6100
B	0.8240	0.6100
C	0.8240	0.6100
D	0.8240	0.6110

