



## Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 11:41 AM EST

PDB ID : 6O6R  
EMDB ID : EMD-0636  
Title : Structure of the TRPM8 cold receptor by single particle electron cryo-microscopy, AMTB-bound state  
Authors : Diver, M.M.; Cheng, Y.; Julius, D.  
Deposited on : 2019-03-07  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

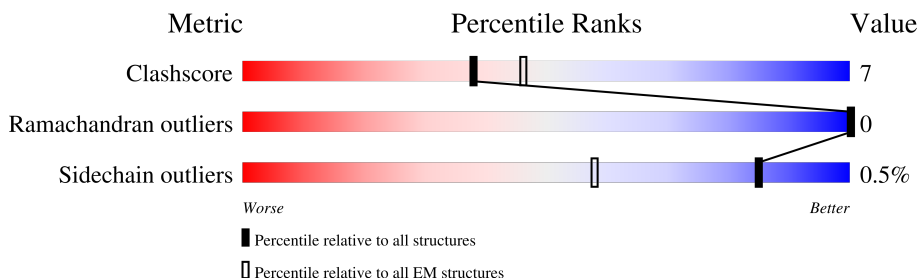
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1098	
1	B	1098	
1	C	1098	
1	D	1098	

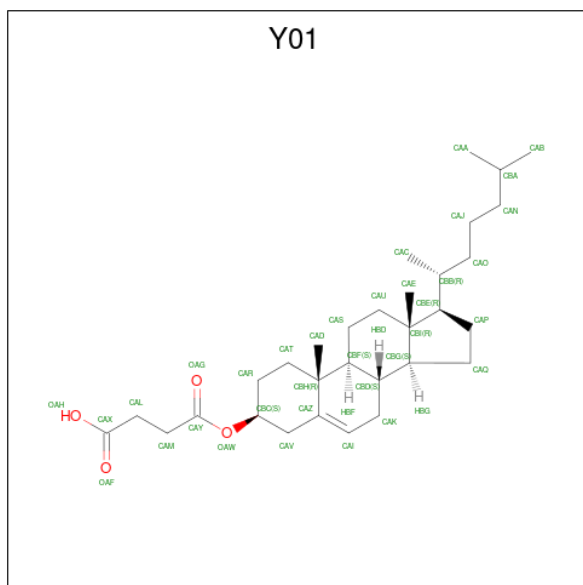


In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily M member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	833	Total 6812	C 4459	N 1118	O 1202	S 33	0	0
1	B	833	Total 6812	C 4459	N 1118	O 1202	S 33	0	0
1	C	833	Total 6812	C 4459	N 1118	O 1202	S 33	0	0
1	D	833	Total 6812	C 4459	N 1118	O 1202	S 33	0	0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



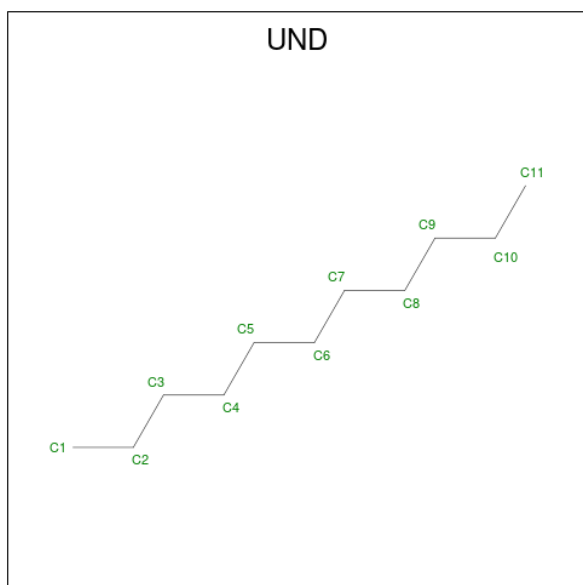
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 35	C 31	O 4	0
2	B	1	Total 35	C 31	O 4	0

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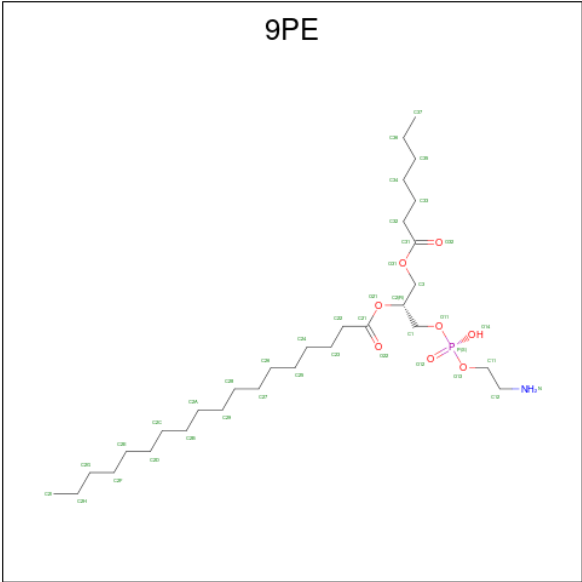
Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	

- Molecule 3 is UNDECANE (three-letter code: UND) (formula: C<sub>11</sub>H<sub>24</sub>).



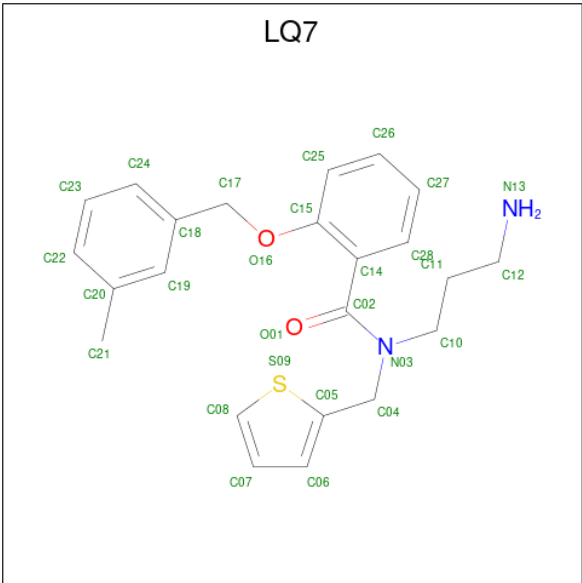
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			11	11	
3	A	1	Total	C	0
			11	11	
3	B	1	Total	C	0
			11	11	
3	B	1	Total	C	0
			11	11	
3	C	1	Total	C	0
			11	11	
3	C	1	Total	C	0
			11	11	
3	D	1	Total	C	0
			11	11	
3	D	1	Total	C	0
			11	11	

- Molecule 4 is (1R)-2-[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (three-letter code: 9PE) (formula: C<sub>30</sub>H<sub>60</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	D	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 5 is N-(3-aminopropyl)-2-[(3-methylphenyl)methoxy]-N-[(thiophen-2-yl)methyl]benzamide (three-letter code: LQ7) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			28	23	2	2	1	
5	B	1	Total	C	N	O	S	0
			28	23	2	2	1	
5	C	1	Total	C	N	O	S	0
			28	23	2	2	1	
5	D	1	Total	C	N	O	S	0
			28	23	2	2	1	

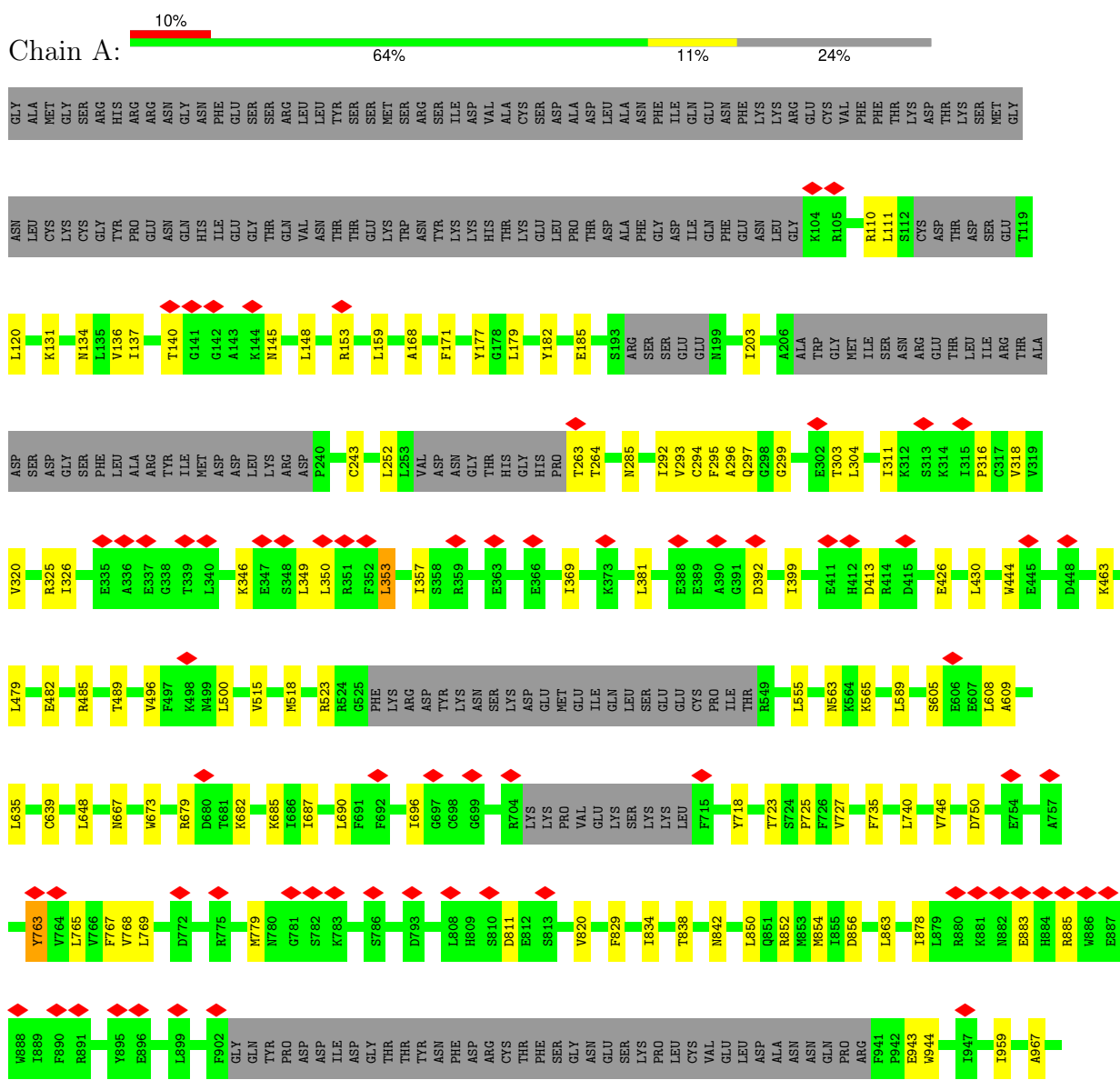
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

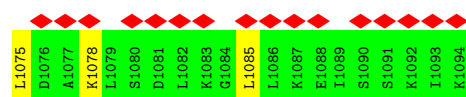
Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Na	0
			2	2	
6	B	2	Total	Na	0
			2	2	
6	C	2	Total	Na	0
			2	2	
6	D	2	Total	Na	0
			2	2	

### 3 Residue-property plots

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

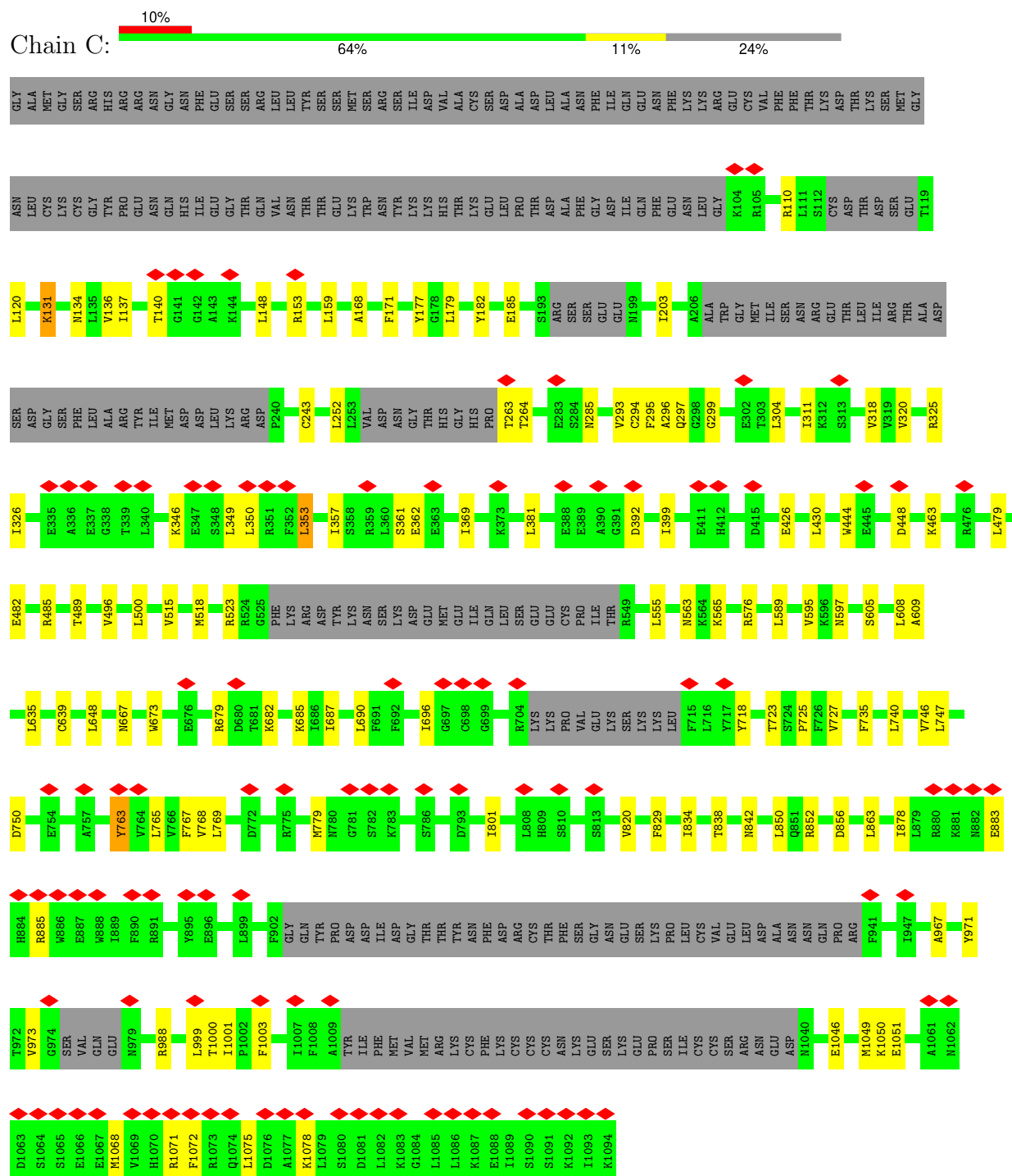
- Molecule 1: Transient receptor potential cation channel subfamily M member 8



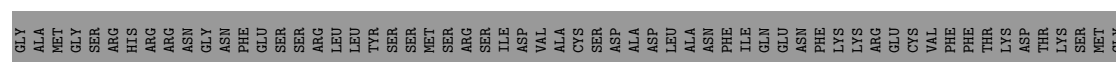




• Molecule 1: Transient receptor potential cation channel subfamily M member 8



• Molecule 1: Transient receptor potential cation channel subfamily M member 8





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	92836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.290	Depositor
Minimum map value	-0.175	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	338.88, 338.88, 338.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LQ7, UND, Y01, 9PE, NA

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	0.34	0/6970	0.55	4/9426 (0.0%)
1	B	0.35	0/6970	0.55	4/9426 (0.0%)
1	C	0.34	0/6970	0.55	4/9426 (0.0%)
1	D	0.34	0/6970	0.55	4/9426 (0.0%)
All	All	0.34	0/27880	0.55	16/37704 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	353	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	353	LEU	CA-CB-CG	5.86	128.78	115.30
1	C	353	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	148	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	148	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	148	LEU	CA-CB-CG	5.45	127.84	115.30
1	C	148	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	349	LEU	CA-CB-CG	5.39	127.71	115.30
1	C	349	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	349	LEU	CA-CB-CG	5.38	127.66	115.30
1	D	349	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	639	CYS	CA-CB-SG	5.14	123.25	114.00
1	A	639	CYS	CA-CB-SG	5.12	123.22	114.00
1	B	639	CYS	CA-CB-SG	5.12	123.21	114.00
1	D	639	CYS	CA-CB-SG	5.08	123.15	114.00

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	6812	0	6863	104	0
1	B	6812	0	6863	102	0
1	C	6812	0	6863	101	0
1	D	6812	0	6863	100	0
2	A	35	0	46	5	0
2	B	35	0	46	5	0
2	C	35	0	46	4	0
2	D	35	0	46	4	0
3	A	22	0	46	0	0
3	B	22	0	46	0	0
3	C	22	0	46	0	0
3	D	22	0	46	0	0
4	A	37	0	50	2	0
4	B	37	0	50	2	0
4	C	37	0	50	2	0
4	D	37	0	50	2	0
5	A	28	0	0	0	0
5	B	28	0	0	0	0
5	C	28	0	0	0	0
5	D	28	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	27744	0	28020	401	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 (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:VAL:HG23	1:A:1003:PHE:CZ	1.40	1.56
1:B:768:VAL:HG23	1:B:1003:PHE:CZ	1.41	1.55
1:C:768:VAL:HG23	1:C:1003:PHE:CZ	1.40	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:768:VAL:HG23	1:D:1003:PHE:CZ	1.40	1.52
1:C:769:LEU:HD12	1:C:1003:PHE:CE1	1.47	1.48
1:D:769:LEU:HD12	1:D:1003:PHE:CE1	1.47	1.47
1:A:769:LEU:HD12	1:A:1003:PHE:CE1	1.47	1.46
1:B:769:LEU:HD12	1:B:1003:PHE:CE1	1.47	1.46
1:A:768:VAL:HG23	1:A:1003:PHE:CE1	1.62	1.34
1:C:768:VAL:HG23	1:C:1003:PHE:CE1	1.62	1.34
1:D:768:VAL:HG23	1:D:1003:PHE:CE1	1.62	1.34
1:C:768:VAL:CG2	1:C:1003:PHE:CZ	2.11	1.33
1:B:768:VAL:HG23	1:B:1003:PHE:CE1	1.63	1.32
1:D:768:VAL:CG2	1:D:1003:PHE:CZ	2.12	1.31
1:A:768:VAL:CG2	1:A:1003:PHE:CZ	2.11	1.31
1:B:768:VAL:CG2	1:B:1003:PHE:CZ	2.11	1.29
1:A:735:PHE:CE2	1:A:1003:PHE:CD2	2.23	1.27
1:B:769:LEU:CD1	1:B:1003:PHE:CZ	2.18	1.27
1:D:769:LEU:CD1	1:D:1003:PHE:CZ	2.18	1.26
1:A:769:LEU:CD1	1:A:1003:PHE:CZ	2.18	1.26
1:B:769:LEU:HD12	1:B:1003:PHE:CZ	1.70	1.26
1:C:735:PHE:CE2	1:C:1003:PHE:CD2	2.23	1.26
1:D:735:PHE:CE2	1:D:1003:PHE:CD2	2.23	1.26
1:B:735:PHE:CE2	1:B:1003:PHE:CD2	2.23	1.26
1:A:769:LEU:HD12	1:A:1003:PHE:CZ	1.70	1.25
1:C:769:LEU:CD1	1:C:1003:PHE:CZ	2.18	1.25
1:D:769:LEU:HD12	1:D:1003:PHE:CZ	1.70	1.25
1:C:769:LEU:HD12	1:C:1003:PHE:CZ	1.70	1.24
1:B:735:PHE:CE2	1:B:1003:PHE:HD2	1.69	1.05
1:A:768:VAL:CG2	1:A:1003:PHE:CE2	2.39	1.05
1:B:768:VAL:CG2	1:B:1003:PHE:CE2	2.39	1.04
1:A:735:PHE:CE2	1:A:1003:PHE:HD2	1.69	1.04
1:C:768:VAL:CG2	1:C:1003:PHE:CE2	2.39	1.04
1:D:769:LEU:CD1	1:D:1003:PHE:CE1	2.39	1.04
1:D:768:VAL:CG2	1:D:1003:PHE:CE2	2.39	1.03
1:C:769:LEU:HD13	1:C:1003:PHE:CZ	1.92	1.02
1:C:769:LEU:CD1	1:C:1003:PHE:CE1	2.39	1.02
1:A:769:LEU:HD13	1:A:1003:PHE:CZ	1.92	1.02
1:D:769:LEU:HD13	1:D:1003:PHE:CZ	1.92	1.02
1:B:769:LEU:HD13	1:B:1003:PHE:CZ	1.92	1.01
1:D:735:PHE:CE2	1:D:1003:PHE:HD2	1.69	1.01
1:B:769:LEU:CD1	1:B:1003:PHE:CE1	2.39	0.96
1:A:769:LEU:CD1	1:A:1003:PHE:CE1	2.39	0.96
1:C:735:PHE:CE2	1:C:1003:PHE:HD2	1.69	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:735:PHE:HE2	1:C:1003:PHE:CD2	1.89	0.90
1:A:768:VAL:HG23	1:A:1003:PHE:CE2	2.06	0.89
1:B:768:VAL:HG23	1:B:1003:PHE:CE2	2.06	0.89
1:C:768:VAL:HG23	1:C:1003:PHE:CE2	2.06	0.87
1:A:735:PHE:HE2	1:A:1003:PHE:CD2	1.89	0.86
1:A:735:PHE:HE2	1:A:1003:PHE:CE2	1.95	0.85
1:D:735:PHE:HE2	1:D:1003:PHE:CD2	1.89	0.85
1:D:735:PHE:HE2	1:D:1003:PHE:CE2	1.95	0.85
1:B:735:PHE:HE2	1:B:1003:PHE:CE2	1.95	0.84
1:B:735:PHE:CE2	1:B:1003:PHE:CE2	2.66	0.83
1:B:735:PHE:HE2	1:B:1003:PHE:CD2	1.89	0.83
1:D:735:PHE:CE2	1:D:1003:PHE:CE2	2.66	0.83
1:C:735:PHE:HE2	1:C:1003:PHE:CE2	1.95	0.83
1:A:735:PHE:CE2	1:A:1003:PHE:CE2	2.66	0.83
1:C:735:PHE:CE2	1:C:1003:PHE:CE2	2.66	0.83
1:C:768:VAL:HG22	1:C:1003:PHE:CZ	2.16	0.81
1:D:768:VAL:HG22	1:D:1003:PHE:CZ	2.16	0.80
1:A:768:VAL:HG22	1:A:1003:PHE:CZ	2.16	0.79
1:D:768:VAL:HG23	1:D:1003:PHE:CE2	2.06	0.78
1:B:768:VAL:HG22	1:B:1003:PHE:CZ	2.16	0.77
1:D:299:GLY:HA2	1:D:326:ILE:HG12	1.76	0.68
1:B:765:LEU:O	1:B:1003:PHE:HZ	1.78	0.67
1:A:765:LEU:O	1:A:1003:PHE:HZ	1.78	0.67
1:A:299:GLY:HA2	1:A:326:ILE:HG12	1.76	0.66
1:C:299:GLY:HA2	1:C:326:ILE:HG12	1.76	0.66
1:C:765:LEU:O	1:C:1003:PHE:HZ	1.78	0.66
1:D:765:LEU:O	1:D:1003:PHE:HZ	1.78	0.66
1:B:299:GLY:HA2	1:B:326:ILE:HG12	1.76	0.66
1:D:140:THR:OG1	1:D:297:GLN:NE2	2.31	0.64
1:B:140:THR:OG1	1:B:297:GLN:NE2	2.31	0.63
1:A:140:THR:OG1	1:A:297:GLN:NE2	2.31	0.63
1:C:140:THR:OG1	1:C:297:GLN:NE2	2.31	0.63
1:A:878:ILE:HG12	1:B:820:VAL:HG12	1.80	0.62
1:C:883:GLU:HA	1:C:885:ARG:HE	1.65	0.62
1:A:883:GLU:HA	1:A:885:ARG:HE	1.65	0.61
1:B:883:GLU:HA	1:B:885:ARG:HE	1.65	0.61
1:D:768:VAL:HG21	1:D:1003:PHE:CE2	2.35	0.61
1:D:883:GLU:HA	1:D:885:ARG:HE	1.65	0.61
1:A:735:PHE:CZ	1:A:1003:PHE:HD2	2.18	0.60
1:A:765:LEU:O	1:A:1003:PHE:CZ	2.54	0.60
1:D:735:PHE:CZ	1:D:1003:PHE:HD2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:HB3	1:A:353:LEU:HD13	1.84	0.60
1:A:820:VAL:HG12	1:D:878:ILE:HG12	1.83	0.60
1:C:765:LEU:O	1:C:1003:PHE:CZ	2.54	0.60
1:D:765:LEU:O	1:D:1003:PHE:CZ	2.54	0.59
1:A:768:VAL:HG21	1:A:1003:PHE:CE2	2.35	0.59
1:B:765:LEU:O	1:B:1003:PHE:CZ	2.54	0.59
1:D:325:ARG:HB3	1:D:353:LEU:HD13	1.84	0.59
1:B:325:ARG:HB3	1:B:353:LEU:HD13	1.84	0.58
1:B:489:THR:HB	1:B:523:ARG:HG2	1.85	0.58
1:C:325:ARG:HB3	1:C:353:LEU:HD13	1.84	0.58
1:C:489:THR:HB	1:C:523:ARG:HG2	1.85	0.58
1:B:768:VAL:HG21	1:B:1003:PHE:CE2	2.35	0.58
1:C:735:PHE:CZ	1:C:1003:PHE:HD2	2.18	0.57
1:A:489:THR:HB	1:A:523:ARG:HG2	1.85	0.57
1:D:489:THR:HB	1:D:523:ARG:HG2	1.85	0.57
1:C:153:ARG:NH1	1:D:1051:GLU:OE1	2.38	0.56
1:A:299:GLY:HA3	1:A:325:ARG:HB2	1.88	0.56
1:D:299:GLY:HA3	1:D:325:ARG:HB2	1.88	0.56
1:C:878:ILE:HG12	1:D:820:VAL:HG12	1.88	0.56
1:B:299:GLY:HA3	1:B:325:ARG:HB2	1.88	0.55
1:A:768:VAL:C	1:A:1003:PHE:CE1	2.80	0.55
1:C:735:PHE:CD2	1:C:1003:PHE:CD2	2.91	0.55
1:D:768:VAL:C	1:D:1003:PHE:CE1	2.80	0.55
1:C:296:ALA:HB3	1:C:320:VAL:HG12	1.89	0.55
1:C:768:VAL:HG21	1:C:1003:PHE:CE2	2.35	0.55
1:A:296:ALA:HB3	1:A:320:VAL:HG12	1.89	0.54
1:A:735:PHE:CD2	1:A:1003:PHE:CD2	2.91	0.54
1:C:768:VAL:C	1:C:1003:PHE:CE1	2.80	0.54
1:C:299:GLY:HA3	1:C:325:ARG:HB2	1.88	0.54
1:B:296:ALA:HB3	1:B:320:VAL:HG12	1.89	0.54
1:B:768:VAL:C	1:B:1003:PHE:CE1	2.80	0.54
1:B:285:ASN:ND2	1:B:426:GLU:OE1	2.41	0.54
1:B:768:VAL:HG22	1:B:1003:PHE:CE2	2.39	0.54
1:A:838:THR:O	1:A:842:ASN:ND2	2.41	0.54
1:D:285:ASN:ND2	1:D:426:GLU:OE1	2.41	0.54
1:D:296:ALA:HB3	1:D:320:VAL:HG12	1.89	0.54
1:B:838:THR:O	1:B:842:ASN:ND2	2.41	0.53
1:B:735:PHE:CZ	1:B:1003:PHE:HD2	2.18	0.53
1:B:878:ILE:HG12	1:C:820:VAL:HG12	1.91	0.53
1:C:285:ASN:ND2	1:C:426:GLU:OE1	2.41	0.53
1:D:293:VAL:HG21	1:D:399:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASN:ND2	1:C:444:TRP:O	2.37	0.53
1:A:293:VAL:HG21	1:A:399:ILE:HG23	1.91	0.53
1:A:850:LEU:HD12	1:D:966:VAL:HG21	1.90	0.53
1:C:838:THR:O	1:C:842:ASN:ND2	2.41	0.53
1:A:285:ASN:ND2	1:A:426:GLU:OE1	2.41	0.53
1:B:293:VAL:HG21	1:B:399:ILE:HG23	1.91	0.52
1:B:988:ARG:NH2	2:B:1301:Y01:OAF	2.42	0.52
1:C:293:VAL:HG21	1:C:399:ILE:HG23	1.91	0.52
1:A:735:PHE:CZ	1:A:1003:PHE:CD2	2.92	0.52
1:C:735:PHE:CZ	1:C:1003:PHE:CD2	2.92	0.52
1:D:768:VAL:HG23	1:D:1003:PHE:CD1	2.36	0.52
4:B:1303:9PE:H25A	4:B:1303:9PE:H36	1.92	0.52
2:C:1301:Y01:HAC3	4:C:1303:9PE:H27	1.92	0.52
4:C:1303:9PE:H36	4:C:1303:9PE:H25A	1.92	0.52
1:D:735:PHE:CZ	1:D:1003:PHE:CD2	2.92	0.52
1:A:589:LEU:HB2	1:A:609:ALA:HB2	1.92	0.52
2:D:1301:Y01:HAC3	4:D:1303:9PE:H27	1.92	0.52
1:D:735:PHE:CD2	1:D:1003:PHE:CD2	2.91	0.52
1:A:988:ARG:NH2	2:A:1301:Y01:OAF	2.42	0.51
1:D:838:THR:O	1:D:842:ASN:ND2	2.41	0.51
1:B:589:LEU:HB2	1:B:609:ALA:HB2	1.92	0.51
1:A:145:ASN:ND2	1:B:444:TRP:O	2.41	0.51
1:B:735:PHE:CD2	1:B:1003:PHE:CD2	2.91	0.51
1:D:589:LEU:HB2	1:D:609:ALA:HB2	1.92	0.51
2:B:1301:Y01:HAC3	4:B:1303:9PE:H27	1.92	0.51
2:A:1301:Y01:HAC3	4:A:1303:9PE:H27	1.92	0.51
1:C:563:ASN:HD21	1:C:605:SER:HB3	1.76	0.51
1:A:834:ILE:HG23	1:D:863:LEU:HD13	1.92	0.51
1:D:137:ILE:HB	1:D:294:CYS:HA	1.93	0.51
1:D:430:LEU:HD22	1:D:463:LYS:HB3	1.93	0.51
1:D:1075:LEU:HA	1:D:1078:LYS:HB2	1.93	0.51
1:C:430:LEU:HD22	1:C:463:LYS:HB3	1.93	0.51
1:C:856:ASP:HB3	1:C:967:ALA:HA	1.93	0.51
1:A:137:ILE:HB	1:A:294:CYS:HA	1.93	0.50
1:B:563:ASN:HD21	1:B:605:SER:HB3	1.76	0.50
1:A:565:LYS:HD2	1:A:608:LEU:HD13	1.94	0.50
4:A:1303:9PE:H25A	4:A:1303:9PE:H36	1.92	0.50
1:B:565:LYS:HD2	1:B:608:LEU:HD13	1.94	0.50
1:B:1075:LEU:HA	1:B:1078:LYS:HB2	1.92	0.50
1:C:1075:LEU:HA	1:C:1078:LYS:HB2	1.93	0.50
1:D:988:ARG:NH2	2:D:1301:Y01:OAF	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:ASN:HD21	1:D:605:SER:HB3	1.76	0.50
1:D:856:ASP:HB3	1:D:967:ALA:HA	1.93	0.50
1:B:999:LEU:HD23	1:B:1001:ILE:HD11	1.93	0.50
4:D:1303:9PE:H25A	4:D:1303:9PE:H36	1.92	0.50
1:B:137:ILE:HB	1:B:294:CYS:HA	1.93	0.50
1:C:137:ILE:HB	1:C:294:CYS:HA	1.93	0.50
1:A:856:ASP:HB3	1:A:967:ALA:HA	1.93	0.50
1:B:153:ARG:NH1	1:C:1051:GLU:OE1	2.44	0.50
1:C:768:VAL:HG22	1:C:1003:PHE:CE2	2.39	0.50
1:C:863:LEU:HD13	1:D:834:ILE:HG23	1.93	0.50
1:D:999:LEU:HD23	1:D:1001:ILE:HD11	1.93	0.50
1:A:563:ASN:HD21	1:A:605:SER:HB3	1.76	0.50
1:B:430:LEU:HD22	1:B:463:LYS:HB3	1.93	0.50
1:C:565:LYS:HD2	1:C:608:LEU:HD13	1.94	0.50
1:C:768:VAL:HG23	1:C:1003:PHE:CD1	2.36	0.50
1:D:565:LYS:HD2	1:D:608:LEU:HD13	1.94	0.50
1:B:311:ILE:HG23	1:B:381:LEU:HD12	1.94	0.50
1:A:430:LEU:HD22	1:A:463:LYS:HB3	1.93	0.49
1:A:768:VAL:HG23	1:A:1003:PHE:CD1	2.36	0.49
1:A:863:LEU:HD13	1:B:834:ILE:HG23	1.94	0.49
1:B:136:VAL:HG11	1:B:159:LEU:HD11	1.95	0.49
1:B:856:ASP:HB3	1:B:967:ALA:HA	1.93	0.49
1:C:182:TYR:HA	1:C:185:GLU:HG2	1.95	0.49
1:C:667:ASN:OD1	1:C:679:ARG:NH2	2.43	0.49
1:A:1075:LEU:HA	1:A:1078:LYS:HB2	1.93	0.49
1:B:768:VAL:HG23	1:B:1003:PHE:CD1	2.36	0.49
1:C:589:LEU:HB2	1:C:609:ALA:HB2	1.92	0.49
1:C:999:LEU:HD23	1:C:1001:ILE:HD11	1.93	0.49
1:B:667:ASN:OD1	1:B:679:ARG:NH2	2.43	0.49
1:A:999:LEU:HD23	1:A:1001:ILE:HD11	1.93	0.49
1:A:311:ILE:HG23	1:A:381:LEU:HD12	1.94	0.49
1:B:182:TYR:HA	1:B:185:GLU:HG2	1.95	0.49
1:D:134:ASN:HB3	1:D:168:ALA:HB2	1.95	0.49
1:A:134:ASN:HB3	1:A:168:ALA:HB2	1.95	0.49
1:B:137:ILE:O	1:B:295:PHE:N	2.42	0.49
1:C:134:ASN:HB3	1:C:168:ALA:HB2	1.95	0.49
1:D:136:VAL:HG11	1:D:159:LEU:HD11	1.95	0.49
1:D:482:GLU:HA	1:D:485:ARG:HG2	1.95	0.49
1:D:1068:MET:HB3	1:D:1071:ARG:HB2	1.95	0.49
1:D:182:TYR:HA	1:D:185:GLU:HG2	1.95	0.49
1:D:311:ILE:HG23	1:D:381:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:735:PHE:HZ	1:C:765:LEU:HD22	1.78	0.49
1:A:350:LEU:HD13	1:A:357:ILE:HD13	1.95	0.48
1:B:482:GLU:HA	1:B:485:ARG:HG2	1.95	0.48
1:B:134:ASN:HB3	1:B:168:ALA:HB2	1.95	0.48
1:A:136:VAL:HG11	1:A:159:LEU:HD11	1.95	0.48
1:A:182:TYR:HA	1:A:185:GLU:HG2	1.95	0.48
1:B:735:PHE:HZ	1:B:765:LEU:HD22	1.78	0.48
1:C:1068:MET:HB3	1:C:1071:ARG:HB2	1.95	0.48
1:C:137:ILE:O	1:C:295:PHE:N	2.42	0.48
1:A:735:PHE:HZ	1:A:765:LEU:HD22	1.78	0.48
1:A:838:THR:HG22	1:A:850:LEU:HD11	1.96	0.48
1:C:136:VAL:HG11	1:C:159:LEU:HD11	1.94	0.48
1:A:263:THR:OG1	1:A:264:THR:N	2.47	0.48
1:B:263:THR:OG1	1:B:264:THR:N	2.47	0.48
1:A:1068:MET:HB3	1:A:1071:ARG:HB2	1.95	0.48
1:C:350:LEU:HD13	1:C:357:ILE:HD13	1.95	0.48
1:A:479:LEU:HD21	1:A:555:LEU:HD22	1.95	0.48
1:B:350:LEU:HD13	1:B:357:ILE:HD13	1.95	0.48
1:D:768:VAL:HG22	1:D:1003:PHE:CE2	2.39	0.48
1:C:482:GLU:HA	1:C:485:ARG:HG2	1.95	0.48
1:C:838:THR:HG22	1:C:850:LEU:HD11	1.96	0.48
1:C:988:ARG:NH2	2:C:1301:Y01:OAF	2.42	0.48
1:C:311:ILE:HG23	1:C:381:LEU:HD12	1.94	0.47
1:A:482:GLU:HA	1:A:485:ARG:HG2	1.95	0.47
1:B:479:LEU:HD21	1:B:555:LEU:HD22	1.95	0.47
1:C:263:THR:OG1	1:C:264:THR:N	2.47	0.47
1:D:735:PHE:HZ	1:D:765:LEU:HD22	1.78	0.47
1:B:1068:MET:HB3	1:B:1071:ARG:HB2	1.95	0.47
1:C:479:LEU:HD21	1:C:555:LEU:HD22	1.95	0.47
1:A:1050:LYS:HB3	1:A:1050:LYS:HE2	1.69	0.47
1:D:350:LEU:HD13	1:D:357:ILE:HD13	1.95	0.47
1:A:769:LEU:N	1:A:1003:PHE:CE1	2.83	0.47
1:B:838:THR:HG22	1:B:850:LEU:HD11	1.96	0.47
1:D:479:LEU:HD21	1:D:555:LEU:HD22	1.96	0.47
1:A:1068:MET:O	1:A:1072:PHE:N	2.45	0.47
1:B:120:LEU:HD21	1:B:252:LEU:HD21	1.97	0.47
1:B:735:PHE:CZ	1:B:1003:PHE:CD2	2.92	0.47
1:D:120:LEU:HD21	1:D:252:LEU:HD21	1.97	0.47
1:D:838:THR:HG22	1:D:850:LEU:HD11	1.96	0.47
1:A:1085:LEU:HD22	1:D:1086:LEU:HB3	1.96	0.47
1:A:120:LEU:HD21	1:A:252:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:TRP:HA	1:A:725:PRO:HG2	1.97	0.47
1:B:673:TRP:HA	1:B:725:PRO:HG2	1.97	0.47
1:B:346:LYS:HE2	1:B:369:ILE:HD11	1.97	0.46
1:C:120:LEU:HD21	1:C:252:LEU:HD21	1.97	0.46
1:A:854:MET:HE2	1:D:962:VAL:HG11	1.96	0.46
1:B:769:LEU:N	1:B:1003:PHE:CE1	2.83	0.46
1:B:1068:MET:O	1:B:1072:PHE:N	2.45	0.46
1:C:687:ILE:HG12	2:C:1301:Y01:HAQ2	1.98	0.46
1:D:769:LEU:N	1:D:1003:PHE:CE1	2.83	0.46
1:A:346:LYS:HE2	1:A:369:ILE:HD11	1.97	0.46
1:B:687:ILE:HG12	2:B:1301:Y01:HAQ2	1.97	0.46
1:C:448:ASP:OD1	1:C:448:ASP:N	2.46	0.46
1:D:448:ASP:OD1	1:D:448:ASP:N	2.46	0.46
1:D:687:ILE:HG12	2:D:1301:Y01:HAQ2	1.98	0.46
1:C:769:LEU:N	1:C:1003:PHE:CE1	2.83	0.46
1:D:667:ASN:OD1	1:D:679:ARG:NH2	2.43	0.46
1:C:673:TRP:HA	1:C:725:PRO:HG2	1.97	0.46
1:D:263:THR:OG1	1:D:264:THR:N	2.47	0.46
1:D:673:TRP:HA	1:D:725:PRO:HG2	1.97	0.46
1:D:763:TYR:O	1:D:767:PHE:N	2.48	0.46
1:D:515:VAL:HA	1:D:518:MET:HG2	1.98	0.45
1:A:667:ASN:OD1	1:A:679:ARG:NH2	2.43	0.45
1:B:413:ASP:OD1	1:B:413:ASP:N	2.40	0.45
1:D:346:LYS:HE2	1:D:369:ILE:HD11	1.97	0.45
1:C:515:VAL:HA	1:C:518:MET:HG2	1.98	0.45
1:A:687:ILE:HG12	2:A:1301:Y01:HAQ2	1.97	0.45
1:D:1050:LYS:HE2	1:D:1050:LYS:HB3	1.69	0.45
1:B:1068:MET:HG2	1:B:1071:ARG:HD2	1.99	0.45
1:C:1050:LYS:HE2	1:C:1050:LYS:HB3	1.69	0.45
1:D:1068:MET:O	1:D:1072:PHE:N	2.45	0.45
1:A:1068:MET:HG2	1:A:1071:ARG:HD2	1.99	0.45
1:D:723:THR:O	1:D:1000:THR:OG1	2.35	0.45
1:B:863:LEU:HD13	1:C:834:ILE:HG23	1.99	0.45
1:A:179:LEU:HD22	1:A:297:GLN:HE22	1.82	0.44
1:A:444:TRP:O	1:D:145:ASN:ND2	2.48	0.44
1:A:723:THR:O	1:A:1000:THR:OG1	2.35	0.44
1:C:179:LEU:HD22	1:C:297:GLN:HE22	1.83	0.44
1:C:346:LYS:HE2	1:C:369:ILE:HD11	1.97	0.44
1:B:515:VAL:HA	1:B:518:MET:HG2	1.98	0.44
1:C:763:TYR:O	1:C:767:PHE:N	2.48	0.44
1:B:179:LEU:HD22	1:B:297:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:LEU:HD21	1:C:727:VAL:HG13	1.99	0.44
1:C:723:THR:O	1:C:1000:THR:OG1	2.35	0.44
1:C:1068:MET:HG2	1:C:1071:ARG:HD2	1.99	0.44
1:D:413:ASP:OD1	1:D:413:ASP:N	2.40	0.44
1:A:515:VAL:HA	1:A:518:MET:HG2	1.98	0.44
1:A:690:LEU:HD21	1:A:727:VAL:HG13	1.99	0.44
1:D:1068:MET:HG2	1:D:1071:ARG:HD2	1.99	0.44
2:D:1301:Y01:HAC3	2:D:1301:Y01:HAJ1	1.78	0.44
1:D:179:LEU:HD22	1:D:297:GLN:HE22	1.83	0.43
1:A:696:ILE:HB	1:A:718:TYR:HE1	1.83	0.43
1:A:763:TYR:O	1:A:767:PHE:N	2.48	0.43
1:B:696:ILE:HB	1:B:718:TYR:HE1	1.83	0.43
1:B:723:THR:O	1:B:1000:THR:OG1	2.35	0.43
1:D:690:LEU:HD21	1:D:727:VAL:HG13	1.99	0.43
2:A:1301:Y01:HAC3	2:A:1301:Y01:HAJ1	1.78	0.43
1:C:1068:MET:O	1:C:1072:PHE:N	2.45	0.43
1:A:177:TYR:HE2	1:A:243:CYS:H	1.67	0.43
1:C:576:ARG:HD2	1:C:576:ARG:HA	1.78	0.43
1:D:177:TYR:HE2	1:D:243:CYS:H	1.67	0.43
2:B:1301:Y01:HAC3	2:B:1301:Y01:HAJ1	1.78	0.43
1:C:696:ILE:HB	1:C:718:TYR:HE1	1.83	0.43
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.92	0.43
1:A:137:ILE:O	1:A:295:PHE:N	2.42	0.43
1:A:768:VAL:HG22	1:A:1003:PHE:CE2	2.39	0.43
1:A:769:LEU:N	1:A:1003:PHE:CZ	2.87	0.43
1:A:171:PHE:HE1	1:A:203:ILE:HD12	1.84	0.43
1:D:769:LEU:N	1:D:1003:PHE:CZ	2.87	0.43
1:B:177:TYR:HE2	1:B:243:CYS:H	1.67	0.43
1:B:769:LEU:HD13	1:B:1003:PHE:HZ	1.73	0.43
1:A:740:LEU:HD21	1:A:829:PHE:HB3	2.01	0.43
1:B:690:LEU:HD21	1:B:727:VAL:HG13	1.99	0.43
1:B:746:VAL:HA	1:B:750:ASP:HB3	2.01	0.43
1:C:294:CYS:HB3	1:C:318:VAL:HG22	2.01	0.43
2:C:1301:Y01:HAO1	2:C:1301:Y01:HAP1	1.76	0.43
1:A:959:ILE:HD12	1:A:959:ILE:HA	1.91	0.42
1:A:1051:GLU:OE1	1:D:153:ARG:NH1	2.52	0.42
1:B:294:CYS:HB3	1:B:318:VAL:HG22	2.02	0.42
1:C:746:VAL:HA	1:C:750:ASP:HB3	2.01	0.42
1:C:177:TYR:HE2	1:C:243:CYS:H	1.67	0.42
1:B:171:PHE:HE1	1:B:203:ILE:HD12	1.84	0.42
2:B:1301:Y01:HAP1	2:B:1301:Y01:HAO1	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PHE:HE1	1:C:203:ILE:HD12	1.84	0.42
1:D:696:ILE:HB	1:D:718:TYR:HE1	1.83	0.42
1:B:769:LEU:N	1:B:1003:PHE:CZ	2.87	0.42
1:C:740:LEU:HD21	1:C:829:PHE:HB3	2.02	0.42
1:D:740:LEU:HD21	1:D:829:PHE:HB3	2.01	0.42
1:C:304:LEU:HD13	1:C:326:ILE:HD12	2.02	0.42
1:C:747:LEU:HD12	1:C:747:LEU:HA	1.89	0.42
1:D:304:LEU:HD13	1:D:326:ILE:HD12	2.02	0.42
1:D:746:VAL:HA	1:D:750:ASP:HB3	2.01	0.42
1:D:852:ARG:HD2	1:D:971:TYR:HA	2.01	0.42
1:A:496:VAL:O	1:A:500:LEU:N	2.53	0.42
1:B:682:LYS:HB2	1:B:685:LYS:HB2	2.01	0.42
1:B:763:TYR:O	1:B:767:PHE:N	2.48	0.42
1:C:769:LEU:N	1:C:1003:PHE:CZ	2.87	0.42
1:C:852:ARG:HD2	1:C:971:TYR:HA	2.01	0.42
1:D:137:ILE:O	1:D:295:PHE:N	2.42	0.42
1:D:682:LYS:HB2	1:D:685:LYS:HB2	2.01	0.42
1:A:746:VAL:HA	1:A:750:ASP:HB3	2.01	0.42
1:B:740:LEU:HD21	1:B:829:PHE:HB3	2.01	0.42
1:C:769:LEU:CD1	1:C:1003:PHE:CE2	2.94	0.42
1:B:131:LYS:HB2	1:B:131:LYS:HE3	1.93	0.42
1:D:294:CYS:HB3	1:D:318:VAL:HG22	2.01	0.41
1:A:834:ILE:O	1:A:838:THR:OG1	2.31	0.41
1:D:303:THR:HG23	1:D:326:ILE:HD11	2.02	0.41
1:C:682:LYS:HB2	1:C:685:LYS:HB2	2.01	0.41
1:C:769:LEU:HD13	1:C:1003:PHE:HZ	1.73	0.41
1:A:294:CYS:HB3	1:A:318:VAL:HG22	2.01	0.41
1:A:304:LEU:HD13	1:A:326:ILE:HD12	2.02	0.41
1:A:682:LYS:HB2	1:A:685:LYS:HB2	2.02	0.41
1:B:304:LEU:HD13	1:B:326:ILE:HD12	2.02	0.41
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.91	0.41
1:D:576:ARG:HA	1:D:576:ARG:HD2	1.78	0.41
1:A:303:THR:HG23	1:A:326:ILE:HD11	2.02	0.41
1:A:852:ARG:HD2	1:A:971:TYR:HA	2.01	0.41
1:C:801:ILE:HD13	1:C:801:ILE:HA	1.94	0.41
1:D:171:PHE:HE1	1:D:203:ILE:HD12	1.84	0.41
1:D:330:ILE:H	1:D:330:ILE:HG13	1.71	0.41
1:D:959:ILE:HD12	1:D:959:ILE:HA	1.91	0.41
1:B:1001:ILE:HA	1:B:1002:PRO:HD3	1.95	0.41
1:C:973:VAL:HG21	1:D:846:LYS:HG2	2.03	0.41
1:A:811:ASP:OD1	1:A:811:ASP:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:ASP:OD1	1:B:811:ASP:N	2.46	0.41
1:A:392:ASP:OD1	1:A:392:ASP:N	2.54	0.41
1:A:635:LEU:HD22	1:A:648:LEU:HG	2.03	0.41
1:B:183:ILE:HD13	1:B:183:ILE:HA	1.90	0.41
1:B:852:ARG:HD2	1:B:971:TYR:HA	2.01	0.41
1:C:496:VAL:O	1:C:500:LEU:N	2.53	0.41
1:C:595:VAL:HG12	1:C:597:ASN:H	1.86	0.41
1:D:392:ASP:OD1	1:D:392:ASP:N	2.54	0.41
1:A:413:ASP:OD1	1:A:413:ASP:N	2.40	0.41
1:A:153:ARG:NH1	1:B:1051:GLU:OE1	2.55	0.40
2:A:1301:Y01:HAP1	2:A:1301:Y01:HAO1	1.75	0.40
1:B:392:ASP:OD1	1:B:392:ASP:N	2.54	0.40
1:C:635:LEU:HD22	1:C:648:LEU:HG	2.03	0.40
1:A:943:GLU:HG2	1:A:944:TRP:H	1.86	0.40
1:A:1086:LEU:HB3	1:B:1085:LEU:HD22	2.04	0.40
1:B:769:LEU:CD1	1:B:1003:PHE:CE2	2.94	0.40
1:C:361:SER:OG	1:C:362:GLU:N	2.54	0.40
1:A:292:ILE:HB	1:A:316:PRO:HB3	2.04	0.40
1:B:635:LEU:HD22	1:B:648:LEU:HG	2.03	0.40
1:C:1046:GLU:HA	1:C:1049:MET:HB2	2.03	0.40
1:B:344:CYS:O	1:B:348:SER:N	2.50	0.40
1:B:448:ASP:N	1:B:448:ASP:OD1	2.46	0.40
1:C:392:ASP:N	1:C:392:ASP:OD1	2.54	0.40
1:A:769:LEU:HD13	1:A:1003:PHE:HZ	1.73	0.40
1:B:281:ILE:HD13	1:B:281:ILE:HA	1.89	0.40
1:B:769:LEU:HD13	1:B:1003:PHE:CE2	2.52	0.40
1:C:131:LYS:HB2	1:C:131:LYS:HE3	1.93	0.40
1:D:281:ILE:HD13	1:D:281:ILE:HA	1.89	0.40
1:D:595:VAL:HG12	1:D:597:ASN:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	813/1098 (74%)	751 (92%)	62 (8%)	0	100	100
1	B	813/1098 (74%)	751 (92%)	62 (8%)	0	100	100
1	C	813/1098 (74%)	752 (92%)	61 (8%)	0	100	100
1	D	813/1098 (74%)	752 (92%)	61 (8%)	0	100	100
All	All	3252/4392 (74%)	3006 (92%)	246 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	743/984 (76%)	739 (100%)	4 (0%)	86	93
1	B	743/984 (76%)	739 (100%)	4 (0%)	86	93
1	C	743/984 (76%)	739 (100%)	4 (0%)	86	93
1	D	743/984 (76%)	739 (100%)	4 (0%)	86	93
All	All	2972/3936 (76%)	2956 (100%)	16 (0%)	85	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	131	LYS
1	A	763	TYR
1	A	779	MET
1	B	110	ARG
1	B	131	LYS
1	B	763	TYR
1	B	779	MET
1	C	110	ARG
1	C	131	LYS
1	C	763	TYR
1	C	779	MET
1	D	110	ARG

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Mol	Chain	Res	Type
1	D	131	LYS
1	D	763	TYR
1	D	779	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	271	GLN
1	A	297	GLN
1	A	308	ASN
1	A	574	GLN
1	A	597	ASN
1	A	610	ASN
1	A	1058	ASN
1	B	248	HIS
1	B	271	GLN
1	B	297	GLN
1	B	308	ASN
1	B	474	ASN
1	B	574	GLN
1	B	597	ASN
1	B	610	ASN
1	B	1058	ASN
1	C	248	HIS
1	C	271	GLN
1	C	297	GLN
1	C	308	ASN
1	C	474	ASN
1	C	574	GLN
1	C	597	ASN
1	C	610	ASN
1	C	1058	ASN
1	D	248	HIS
1	D	271	GLN
1	D	297	GLN
1	D	308	ASN
1	D	471	ASN
1	D	574	GLN
1	D	597	ASN
1	D	610	ASN
1	D	1058	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
5	LQ7	B	1305	-	30,30,30	1.90	6 (20%)	33,39,39	1.40	5 (15%)
3	UND	B	1304	-	10,10,10	0.29	0	9,9,9	0.80	0
2	Y01	C	1301	-	38,38,38	4.66	14 (36%)	57,57,57	2.08	19 (33%)
3	UND	C	1302	-	10,10,10	0.28	0	9,9,9	0.83	0
2	Y01	D	1301	-	38,38,38	4.66	14 (36%)	57,57,57	2.08	20 (35%)
4	9PE	C	1303	-	36,36,39	1.02	4 (11%)	39,41,44	1.04	3 (7%)
3	UND	A	1304	-	10,10,10	0.29	0	9,9,9	0.80	0
4	9PE	D	1303	-	36,36,39	1.02	4 (11%)	39,41,44	1.04	3 (7%)
3	UND	D	1304	-	10,10,10	0.29	0	9,9,9	0.80	0
5	LQ7	C	1305	-	30,30,30	1.90	6 (20%)	33,39,39	1.40	5 (15%)
3	UND	B	1302	-	10,10,10	0.28	0	9,9,9	0.83	0
5	LQ7	A	1305	-	30,30,30	1.90	6 (20%)	33,39,39	1.40	5 (15%)
2	Y01	A	1301	-	38,38,38	4.66	14 (36%)	57,57,57	2.08	19 (33%)
5	LQ7	D	1305	-	30,30,30	1.91	6 (20%)	33,39,39	1.41	5 (15%)
3	UND	C	1304	-	10,10,10	0.30	0	9,9,9	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UND	A	1302	-	10,10,10	0.28	0	9,9,9	0.83	0
3	UND	D	1302	-	10,10,10	0.28	0	9,9,9	0.83	0
2	Y01	B	1301	-	38,38,38	4.66	14 (36%)	57,57,57	2.08	19 (33%)
4	9PE	B	1303	-	36,36,39	1.02	4 (11%)	39,41,44	1.04	3 (7%)
4	9PE	A	1303	-	36,36,39	1.02	4 (11%)	39,41,44	1.04	3 (7%)

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	LQ7	B	1305	-	-	2/20/21/21	0/3/3/3
3	UND	B	1304	-	-	2/8/8/8	-
2	Y01	C	1301	-	-	8/19/77/77	0/4/4/4
3	UND	C	1302	-	-	2/8/8/8	-
2	Y01	D	1301	-	-	8/19/77/77	0/4/4/4
4	9PE	C	1303	-	-	17/40/40/43	-
3	UND	A	1304	-	-	2/8/8/8	-
4	9PE	D	1303	-	-	17/40/40/43	-
3	UND	D	1304	-	-	2/8/8/8	-
5	LQ7	C	1305	-	-	2/20/21/21	0/3/3/3
3	UND	B	1302	-	-	2/8/8/8	-
5	LQ7	A	1305	-	-	2/20/21/21	0/3/3/3
2	Y01	A	1301	-	-	8/19/77/77	0/4/4/4
5	LQ7	D	1305	-	-	2/20/21/21	0/3/3/3
3	UND	C	1304	-	-	2/8/8/8	-
3	UND	A	1302	-	-	2/8/8/8	-
3	UND	D	1302	-	-	2/8/8/8	-
2	Y01	B	1301	-	-	8/19/77/77	0/4/4/4
4	9PE	B	1303	-	-	17/40/40/43	-
4	9PE	A	1303	-	-	17/40/40/43	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	Y01	CAI-CAZ	17.78	1.69	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	Y01	CAI-CAZ	17.76	1.69	1.33
2	C	1301	Y01	CAI-CAZ	17.75	1.69	1.33
2	D	1301	Y01	CAI-CAZ	17.74	1.69	1.33
2	D	1301	Y01	CBH-CBF	10.05	1.72	1.56
2	A	1301	Y01	CBH-CBF	10.04	1.72	1.56
2	C	1301	Y01	CBH-CBF	10.02	1.72	1.56
2	B	1301	Y01	CBH-CBF	10.01	1.72	1.56
2	B	1301	Y01	CBB-CBE	-9.90	1.37	1.54
2	C	1301	Y01	CBB-CBE	-9.90	1.37	1.54
2	A	1301	Y01	CBB-CBE	-9.87	1.37	1.54
2	D	1301	Y01	CBB-CBE	-9.85	1.37	1.54
2	D	1301	Y01	CBI-CBE	8.34	1.70	1.55
2	A	1301	Y01	CBI-CBE	8.31	1.70	1.55
2	B	1301	Y01	CBI-CBE	8.31	1.70	1.55
2	C	1301	Y01	CBI-CBE	8.31	1.70	1.55
2	C	1301	Y01	CAK-CBD	7.59	1.65	1.53
2	B	1301	Y01	CAK-CBD	7.59	1.65	1.53
2	D	1301	Y01	CAK-CBD	7.58	1.65	1.53
2	A	1301	Y01	CAK-CBD	7.57	1.65	1.53
2	D	1301	Y01	CAU-CBI	-7.48	1.41	1.54
2	C	1301	Y01	CAU-CBI	-7.44	1.41	1.54
2	A	1301	Y01	CAU-CBI	-7.43	1.41	1.54
2	B	1301	Y01	CAU-CBI	-7.41	1.41	1.54
2	C	1301	Y01	CAP-CBE	6.28	1.67	1.54
2	A	1301	Y01	CAP-CBE	6.27	1.67	1.54
2	D	1301	Y01	CAP-CBE	6.26	1.67	1.54
2	B	1301	Y01	CAP-CBE	6.25	1.67	1.54
5	D	1305	LQ7	C05-S09	-5.67	1.62	1.73
5	A	1305	LQ7	C05-S09	-5.66	1.62	1.73
5	C	1305	LQ7	C05-S09	-5.65	1.62	1.73
5	B	1305	LQ7	C05-S09	-5.63	1.62	1.73
2	C	1301	Y01	CAU-CAS	5.51	1.64	1.53
2	D	1301	Y01	CAU-CAS	5.50	1.64	1.53
2	A	1301	Y01	CAU-CAS	5.48	1.64	1.53
2	B	1301	Y01	CAU-CAS	5.48	1.64	1.53
5	D	1305	LQ7	C02-N03	5.29	1.45	1.34
5	A	1305	LQ7	C02-N03	5.26	1.45	1.34
5	B	1305	LQ7	C02-N03	5.26	1.45	1.34
5	C	1305	LQ7	C02-N03	5.26	1.45	1.34
5	C	1305	LQ7	C07-C06	4.13	1.52	1.39
5	A	1305	LQ7	C07-C06	4.11	1.52	1.39
5	B	1305	LQ7	C07-C06	4.09	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1305	LQ7	C07-C06	4.09	1.52	1.39
2	B	1301	Y01	CAQ-CBG	3.16	1.60	1.54
2	C	1301	Y01	CAQ-CBG	3.13	1.60	1.54
2	D	1301	Y01	CAQ-CBG	3.11	1.60	1.54
2	A	1301	Y01	CAQ-CBG	3.11	1.60	1.54
5	B	1305	LQ7	C07-C08	2.96	1.43	1.34
5	D	1305	LQ7	C07-C08	2.96	1.43	1.34
5	C	1305	LQ7	C07-C08	2.96	1.43	1.34
5	A	1305	LQ7	C07-C08	2.94	1.43	1.34
2	C	1301	Y01	CBD-CBF	-2.91	1.48	1.53
2	B	1301	Y01	CBD-CBF	-2.91	1.48	1.53
2	A	1301	Y01	CBD-CBF	-2.90	1.48	1.53
2	D	1301	Y01	CBD-CBF	-2.88	1.48	1.53
4	B	1303	9PE	O21-C2	-2.72	1.40	1.46
4	D	1303	9PE	O21-C2	-2.71	1.40	1.46
4	A	1303	9PE	O21-C2	-2.70	1.40	1.46
4	C	1303	9PE	O21-C2	-2.69	1.40	1.46
2	C	1301	Y01	CAC-CBB	2.64	1.59	1.53
2	B	1301	Y01	CAC-CBB	2.64	1.59	1.53
2	D	1301	Y01	CAC-CBB	2.64	1.59	1.53
2	A	1301	Y01	CAC-CBB	2.63	1.59	1.53
2	B	1301	Y01	CAO-CBB	2.58	1.60	1.54
2	D	1301	Y01	CAO-CBB	2.55	1.60	1.54
2	A	1301	Y01	CAO-CBB	2.55	1.60	1.54
2	C	1301	Y01	CAO-CBB	2.54	1.60	1.54
4	A	1303	9PE	O31-C31	2.45	1.40	1.33
4	D	1303	9PE	O31-C31	2.45	1.40	1.33
4	C	1303	9PE	O31-C31	2.44	1.40	1.33
4	B	1303	9PE	O31-C31	2.43	1.40	1.33
2	D	1301	Y01	CBH-CAZ	-2.42	1.48	1.52
2	A	1301	Y01	CBH-CAZ	-2.40	1.48	1.52
2	C	1301	Y01	CBH-CAZ	-2.37	1.48	1.52
2	B	1301	Y01	CBH-CAZ	-2.37	1.48	1.52
5	B	1305	LQ7	C06-C05	2.22	1.43	1.37
4	B	1303	9PE	O31-C3	-2.22	1.40	1.45
4	C	1303	9PE	O31-C3	-2.21	1.40	1.45
4	D	1303	9PE	O31-C3	-2.21	1.40	1.45
5	A	1305	LQ7	C06-C05	2.20	1.43	1.37
4	A	1303	9PE	O31-C3	-2.19	1.40	1.45
5	D	1305	LQ7	C06-C05	2.19	1.43	1.37
5	C	1305	LQ7	C06-C05	2.19	1.43	1.37
4	B	1303	9PE	O21-C21	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1303	9PE	O21-C21	2.08	1.40	1.34
4	A	1303	9PE	O21-C21	2.07	1.40	1.34
4	D	1303	9PE	O21-C21	2.06	1.40	1.34
2	B	1301	Y01	OAW-CAY	2.02	1.40	1.34
2	D	1301	Y01	OAW-CAY	2.02	1.40	1.34
5	B	1305	LQ7	O01-C02	-2.01	1.18	1.22
5	A	1305	LQ7	O01-C02	-2.01	1.18	1.22
2	C	1301	Y01	OAW-CAY	2.01	1.39	1.34
5	C	1305	LQ7	O01-C02	-2.01	1.18	1.22
2	A	1301	Y01	OAW-CAY	2.01	1.39	1.34
5	D	1305	LQ7	O01-C02	-2.00	1.18	1.22

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	Y01	CAK-CAI-CAZ	-4.98	116.61	125.02
2	A	1301	Y01	CAK-CAI-CAZ	-4.96	116.64	125.02
2	B	1301	Y01	CAK-CAI-CAZ	-4.96	116.65	125.02
2	D	1301	Y01	CAK-CAI-CAZ	-4.94	116.67	125.02
2	B	1301	Y01	CBH-CAZ-CAI	-4.55	116.29	122.93
2	A	1301	Y01	CBH-CAZ-CAI	-4.53	116.32	122.93
2	C	1301	Y01	CBH-CAZ-CAI	-4.53	116.32	122.93
2	D	1301	Y01	CBH-CAZ-CAI	-4.52	116.33	122.93
5	D	1305	LQ7	C07-C08-S09	-4.38	109.43	112.98
4	C	1303	9PE	O21-C21-C22	4.36	120.91	111.48
4	A	1303	9PE	O21-C21-C22	4.35	120.88	111.48
4	B	1303	9PE	O21-C21-C22	4.34	120.88	111.48
4	D	1303	9PE	O21-C21-C22	4.34	120.87	111.48
5	C	1305	LQ7	C07-C08-S09	-4.34	109.46	112.98
5	B	1305	LQ7	C07-C08-S09	-4.33	109.47	112.98
5	A	1305	LQ7	C07-C08-S09	-4.30	109.49	112.98
2	A	1301	Y01	CAE-CBI-CBG	-3.61	105.13	111.68
2	C	1301	Y01	CAE-CBI-CBG	-3.59	105.16	111.68
2	D	1301	Y01	CAE-CBI-CBG	-3.59	105.16	111.68
2	B	1301	Y01	CAE-CBI-CBG	-3.59	105.17	111.68
2	B	1301	Y01	CAD-CBH-CBF	-3.53	107.69	111.66
2	A	1301	Y01	CAD-CBH-CBF	-3.53	107.70	111.66
2	D	1301	Y01	CAD-CBH-CBF	-3.53	107.70	111.66
2	C	1301	Y01	CAD-CBH-CBF	-3.50	107.73	111.66
2	A	1301	Y01	CAU-CBI-CBE	3.50	121.75	116.60
2	B	1301	Y01	CAU-CBI-CBE	3.49	121.73	116.60
2	D	1301	Y01	CAU-CBI-CBE	3.48	121.73	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	Y01	CAU-CBI-CBE	3.47	121.72	116.60
2	C	1301	Y01	CBF-CBH-CAZ	3.43	114.67	109.65
2	A	1301	Y01	CBF-CBH-CAZ	3.42	114.66	109.65
2	B	1301	Y01	CBF-CBH-CAZ	3.41	114.64	109.65
2	D	1301	Y01	CBF-CBH-CAZ	3.40	114.64	109.65
2	B	1301	Y01	CAT-CAR-CBC	3.35	115.80	110.33
2	A	1301	Y01	CAT-CAR-CBC	3.35	115.79	110.33
2	C	1301	Y01	CAT-CAR-CBC	3.34	115.78	110.33
2	D	1301	Y01	CAT-CAR-CBC	3.33	115.77	110.33
2	D	1301	Y01	CAE-CBI-CAU	-3.31	105.73	110.61
2	A	1301	Y01	CAE-CBI-CAU	-3.31	105.73	110.61
2	B	1301	Y01	CAE-CBI-CAU	-3.31	105.73	110.61
2	C	1301	Y01	CAE-CBI-CAU	-3.30	105.73	110.61
5	D	1305	LQ7	C14-C02-N03	3.26	123.31	118.24
5	A	1305	LQ7	C14-C02-N03	3.26	123.31	118.24
5	B	1305	LQ7	C14-C02-N03	3.25	123.29	118.24
5	C	1305	LQ7	C14-C02-N03	3.25	123.28	118.24
2	D	1301	Y01	OAW-CAY-CAM	3.24	118.49	111.48
2	A	1301	Y01	OAW-CAY-CAM	3.23	118.48	111.48
2	C	1301	Y01	OAW-CAY-CAM	3.23	118.48	111.48
2	B	1301	Y01	OAW-CAY-CAM	3.23	118.46	111.48
2	A	1301	Y01	CAS-CAU-CBI	3.12	118.00	112.74
2	B	1301	Y01	CAS-CAU-CBI	3.12	118.00	112.74
2	D	1301	Y01	CAS-CAU-CBI	3.12	118.00	112.74
2	C	1301	Y01	CAS-CAU-CBI	3.10	117.97	112.74
2	B	1301	Y01	CBG-CBI-CBE	3.06	103.61	100.10
2	C	1301	Y01	CBG-CBI-CBE	3.05	103.60	100.10
2	A	1301	Y01	CBG-CBI-CBE	3.05	103.59	100.10
2	D	1301	Y01	CBG-CBI-CBE	3.02	103.56	100.10
2	B	1301	Y01	CAC-CBB-CAO	-2.98	105.73	110.34
2	C	1301	Y01	CAC-CBB-CAO	-2.94	105.79	110.34
2	A	1301	Y01	CAC-CBB-CAO	-2.94	105.79	110.34
2	D	1301	Y01	CAC-CBB-CAO	-2.93	105.81	110.34
2	C	1301	Y01	CAU-CBI-CBG	2.74	111.34	107.25
2	D	1301	Y01	CAU-CBI-CBG	2.73	111.33	107.25
2	A	1301	Y01	CAU-CBI-CBG	2.71	111.31	107.25
2	B	1301	Y01	CAU-CBI-CBG	2.70	111.29	107.25
4	C	1303	9PE	O31-C31-C32	2.41	119.17	111.83
5	A	1305	LQ7	O01-C02-N03	-2.40	118.57	122.35
4	D	1303	9PE	O31-C31-C32	2.39	119.13	111.83
5	D	1305	LQ7	O01-C02-N03	-2.39	118.59	122.35
4	B	1303	9PE	O31-C31-C32	2.39	119.12	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1303	9PE	O31-C31-C32	2.39	119.12	111.83
5	C	1305	LQ7	C15-C14-C02	-2.39	118.13	122.26
5	B	1305	LQ7	O01-C02-N03	-2.38	118.60	122.35
5	B	1305	LQ7	C15-C14-C02	-2.38	118.14	122.26
5	A	1305	LQ7	C15-C14-C02	-2.38	118.14	122.26
5	D	1305	LQ7	C15-C14-C02	-2.37	118.16	122.26
5	C	1305	LQ7	O01-C02-N03	-2.37	118.62	122.35
2	D	1301	Y01	CAC-CBB-CBE	-2.37	109.33	112.88
2	A	1301	Y01	CAC-CBB-CBE	-2.35	109.35	112.88
2	C	1301	Y01	CAC-CBB-CBE	-2.35	109.36	112.88
2	B	1301	Y01	CAC-CBB-CBE	-2.32	109.40	112.88
2	C	1301	Y01	CAV-CAZ-CBH	-2.32	113.46	116.42
2	B	1301	Y01	CBF-CBD-CBG	2.31	112.10	109.09
2	B	1301	Y01	CAV-CAZ-CBH	-2.30	113.48	116.42
2	A	1301	Y01	CAV-CAZ-CBH	-2.29	113.49	116.42
2	D	1301	Y01	CAV-CAZ-CBH	-2.29	113.49	116.42
2	A	1301	Y01	CBF-CBD-CBG	2.28	112.07	109.09
2	A	1301	Y01	CAU-CAS-CBF	2.28	117.02	113.14
2	D	1301	Y01	CBF-CBD-CBG	2.28	112.07	109.09
2	B	1301	Y01	CAU-CAS-CBF	2.28	117.00	113.14
2	D	1301	Y01	CAU-CAS-CBF	2.27	117.00	113.14
2	C	1301	Y01	CBF-CBD-CBG	2.27	112.06	109.09
2	C	1301	Y01	CAU-CAS-CBF	2.26	116.98	113.14
2	B	1301	Y01	CAV-CAZ-CAI	-2.19	117.60	120.57
4	C	1303	9PE	C2-O21-C21	-2.19	112.56	117.80
4	B	1303	9PE	C2-O21-C21	-2.18	112.57	117.80
2	D	1301	Y01	CAV-CAZ-CAI	-2.18	117.61	120.57
4	A	1303	9PE	C2-O21-C21	-2.18	112.58	117.80
4	D	1303	9PE	C2-O21-C21	-2.18	112.59	117.80
2	A	1301	Y01	CAV-CAZ-CAI	-2.18	117.62	120.57
5	D	1305	LQ7	C04-N03-C10	2.16	121.18	116.45
5	B	1305	LQ7	C04-N03-C10	2.16	121.18	116.45
2	C	1301	Y01	CAV-CAZ-CAI	-2.15	117.65	120.57
5	C	1305	LQ7	C04-N03-C10	2.14	121.14	116.45
5	A	1305	LQ7	C04-N03-C10	2.14	121.14	116.45
2	C	1301	Y01	CBH-CBF-CBD	-2.10	109.64	112.71
2	A	1301	Y01	CBH-CBF-CBD	-2.09	109.67	112.71
2	D	1301	Y01	CBH-CBF-CBD	-2.07	109.68	112.71
2	B	1301	Y01	CBH-CBF-CBD	-2.05	109.72	112.71
2	D	1301	Y01	CBD-CAK-CAI	-2.02	109.97	112.76

There are no chirality outliers.



All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1303	9PE	C31-C32-C33-C34
4	B	1303	9PE	C31-C32-C33-C34
4	C	1303	9PE	C31-C32-C33-C34
4	D	1303	9PE	C31-C32-C33-C34
2	A	1301	Y01	CAX-CAL-CAM-CAY
2	B	1301	Y01	CAX-CAL-CAM-CAY
2	C	1301	Y01	CAX-CAL-CAM-CAY
2	D	1301	Y01	CAX-CAL-CAM-CAY
2	A	1301	Y01	CAJ-CAN-CBA-CAA
2	B	1301	Y01	CAJ-CAN-CBA-CAA
2	C	1301	Y01	CAJ-CAN-CBA-CAA
2	D	1301	Y01	CAJ-CAN-CBA-CAA
4	A	1303	9PE	C23-C24-C25-C26
4	B	1303	9PE	C23-C24-C25-C26
4	C	1303	9PE	C23-C24-C25-C26
4	D	1303	9PE	C23-C24-C25-C26
2	A	1301	Y01	CAJ-CAN-CBA-CAB
2	B	1301	Y01	CAJ-CAN-CBA-CAB
2	C	1301	Y01	CAJ-CAN-CBA-CAB
2	D	1301	Y01	CAJ-CAN-CBA-CAB
4	A	1303	9PE	C22-C21-O21-C2
4	B	1303	9PE	C22-C21-O21-C2
4	C	1303	9PE	C22-C21-O21-C2
4	D	1303	9PE	C22-C21-O21-C2
2	A	1301	Y01	CAO-CAJ-CAN-CBA
2	B	1301	Y01	CAO-CAJ-CAN-CBA
2	C	1301	Y01	CAO-CAJ-CAN-CBA
2	D	1301	Y01	CAO-CAJ-CAN-CBA
2	B	1301	Y01	CAC-CBB-CBE-CBI
3	A	1302	UND	C6-C7-C8-C9
3	B	1302	UND	C6-C7-C8-C9
3	C	1302	UND	C6-C7-C8-C9
3	D	1302	UND	C6-C7-C8-C9
3	C	1302	UND	C5-C6-C7-C8
3	A	1302	UND	C5-C6-C7-C8
3	B	1302	UND	C5-C6-C7-C8
3	D	1302	UND	C5-C6-C7-C8
2	A	1301	Y01	CAC-CBB-CBE-CBI
2	C	1301	Y01	CAC-CBB-CBE-CBI
2	D	1301	Y01	CAC-CBB-CBE-CBI
4	A	1303	9PE	C33-C34-C35-C36
4	B	1303	9PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	D	1303	9PE	C33-C34-C35-C36
4	C	1303	9PE	C33-C34-C35-C36
4	C	1303	9PE	C29-C2A-C2B-C2C
2	A	1301	Y01	CAC-CBB-CBE-CAP
2	B	1301	Y01	CAC-CBB-CBE-CAP
2	C	1301	Y01	CAC-CBB-CBE-CAP
2	D	1301	Y01	CAC-CBB-CBE-CAP
4	A	1303	9PE	C29-C2A-C2B-C2C
4	B	1303	9PE	C29-C2A-C2B-C2C
4	D	1303	9PE	C29-C2A-C2B-C2C
4	A	1303	9PE	C26-C27-C28-C29
4	B	1303	9PE	C26-C27-C28-C29
4	C	1303	9PE	C26-C27-C28-C29
4	D	1303	9PE	C26-C27-C28-C29
4	B	1303	9PE	C25-C26-C27-C28
4	C	1303	9PE	C25-C26-C27-C28
4	A	1303	9PE	C25-C26-C27-C28
4	D	1303	9PE	C25-C26-C27-C28
4	A	1303	9PE	C22-C23-C24-C25
4	C	1303	9PE	C22-C23-C24-C25
4	B	1303	9PE	C22-C23-C24-C25
4	D	1303	9PE	C22-C23-C24-C25
4	A	1303	9PE	O22-C21-O21-C2
4	C	1303	9PE	O22-C21-O21-C2
4	D	1303	9PE	O22-C21-O21-C2
4	B	1303	9PE	O22-C21-O21-C2
4	A	1303	9PE	C1-C2-C3-O31
4	B	1303	9PE	C1-C2-C3-O31
4	C	1303	9PE	C1-C2-C3-O31
4	D	1303	9PE	C1-C2-C3-O31
4	B	1303	9PE	C2A-C2B-C2C-C2D
4	D	1303	9PE	C2A-C2B-C2C-C2D
4	A	1303	9PE	C2A-C2B-C2C-C2D
4	C	1303	9PE	C2A-C2B-C2C-C2D
4	A	1303	9PE	C24-C25-C26-C27
4	B	1303	9PE	C24-C25-C26-C27
4	C	1303	9PE	C24-C25-C26-C27
4	D	1303	9PE	C24-C25-C26-C27
4	A	1303	9PE	O21-C2-C3-O31
4	B	1303	9PE	O21-C2-C3-O31
4	C	1303	9PE	O21-C2-C3-O31
4	D	1303	9PE	O21-C2-C3-O31

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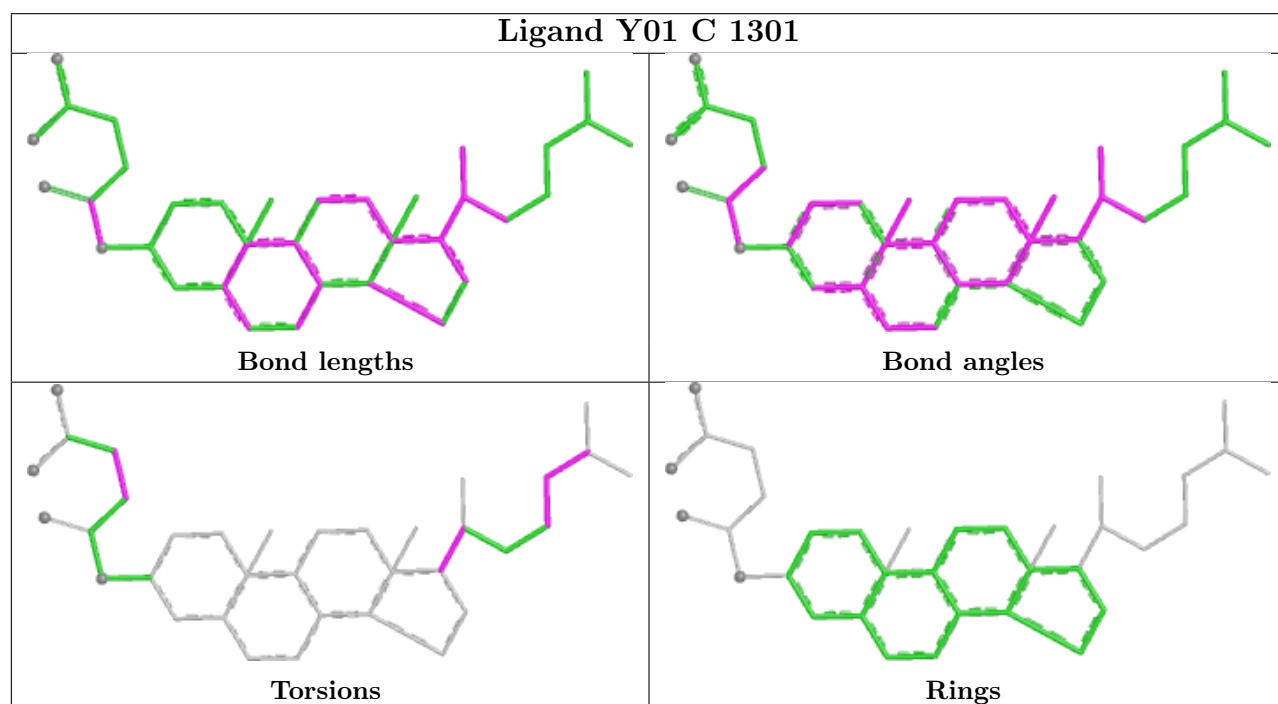
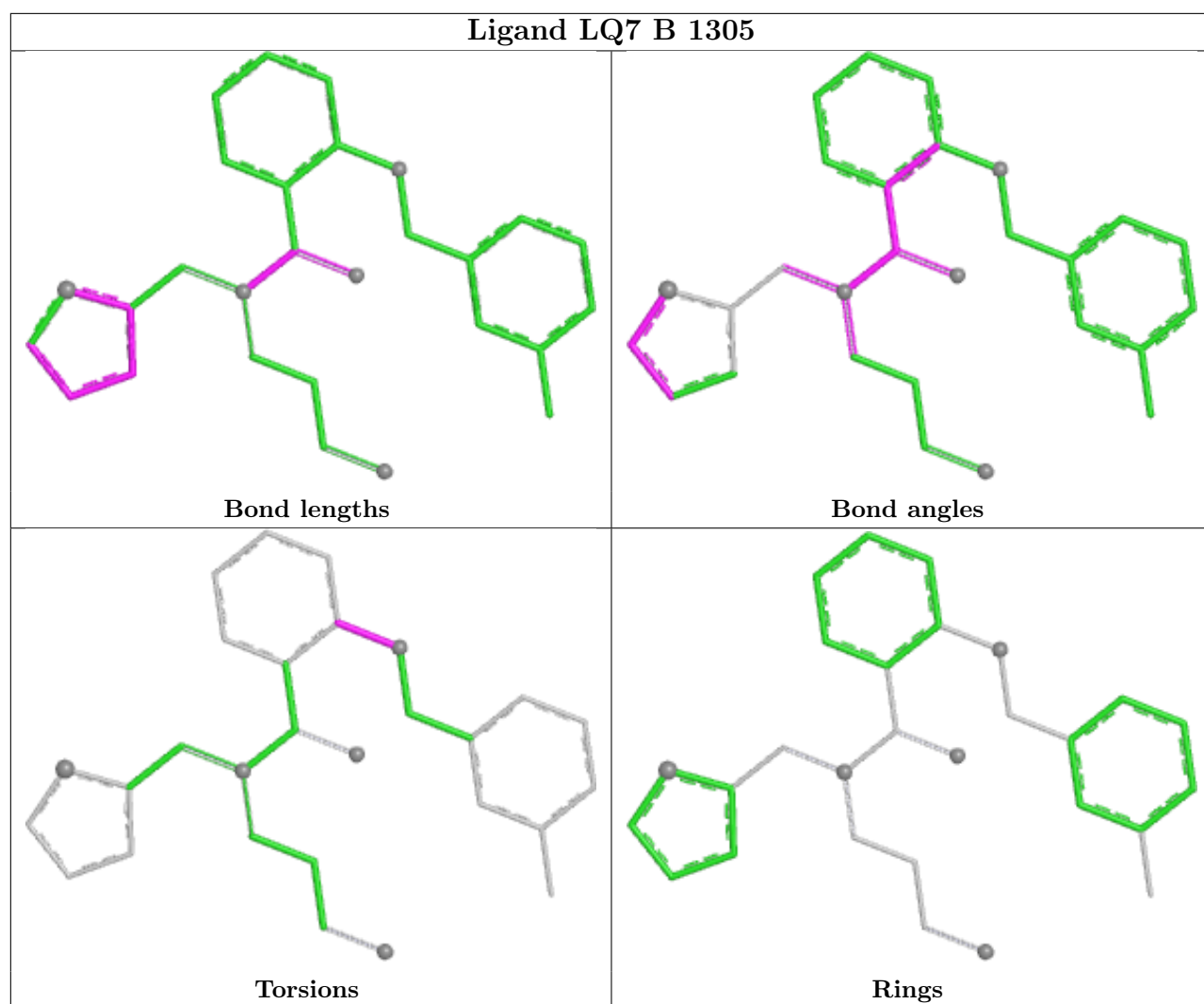
Mol	Chain	Res	Type	Atoms
2	A	1301	Y01	CAO-CBB-CBE-CBI
2	B	1301	Y01	CAO-CBB-CBE-CBI
2	C	1301	Y01	CAO-CBB-CBE-CBI
2	D	1301	Y01	CAO-CBB-CBE-CBI
4	B	1303	9PE	C28-C29-C2A-C2B
4	C	1303	9PE	C28-C29-C2A-C2B
4	A	1303	9PE	C28-C29-C2A-C2B
4	D	1303	9PE	C28-C29-C2A-C2B
4	A	1303	9PE	C11-O13-P-O14
4	B	1303	9PE	C11-O13-P-O14
4	C	1303	9PE	C11-O13-P-O14
4	D	1303	9PE	C11-O13-P-O14
2	A	1301	Y01	CAO-CBB-CBE-CAP
2	B	1301	Y01	CAO-CBB-CBE-CAP
2	C	1301	Y01	CAO-CBB-CBE-CAP
2	D	1301	Y01	CAO-CBB-CBE-CAP
3	C	1304	UND	C2-C3-C4-C5
3	A	1304	UND	C2-C3-C4-C5
3	B	1304	UND	C2-C3-C4-C5
3	D	1304	UND	C2-C3-C4-C5
5	B	1305	LQ7	C25-C15-O16-C17
5	A	1305	LQ7	C25-C15-O16-C17
5	D	1305	LQ7	C25-C15-O16-C17
5	C	1305	LQ7	C25-C15-O16-C17
5	D	1305	LQ7	C14-C15-O16-C17
5	A	1305	LQ7	C14-C15-O16-C17
5	B	1305	LQ7	C14-C15-O16-C17
5	C	1305	LQ7	C14-C15-O16-C17
4	B	1303	9PE	O31-C31-C32-C33
4	C	1303	9PE	O31-C31-C32-C33
4	A	1303	9PE	O31-C31-C32-C33
4	D	1303	9PE	O31-C31-C32-C33
3	B	1304	UND	C3-C4-C5-C6
3	D	1304	UND	C3-C4-C5-C6
3	A	1304	UND	C3-C4-C5-C6
3	C	1304	UND	C3-C4-C5-C6
4	A	1303	9PE	O32-C31-C32-C33
4	B	1303	9PE	O32-C31-C32-C33
4	C	1303	9PE	O32-C31-C32-C33
4	D	1303	9PE	O32-C31-C32-C33

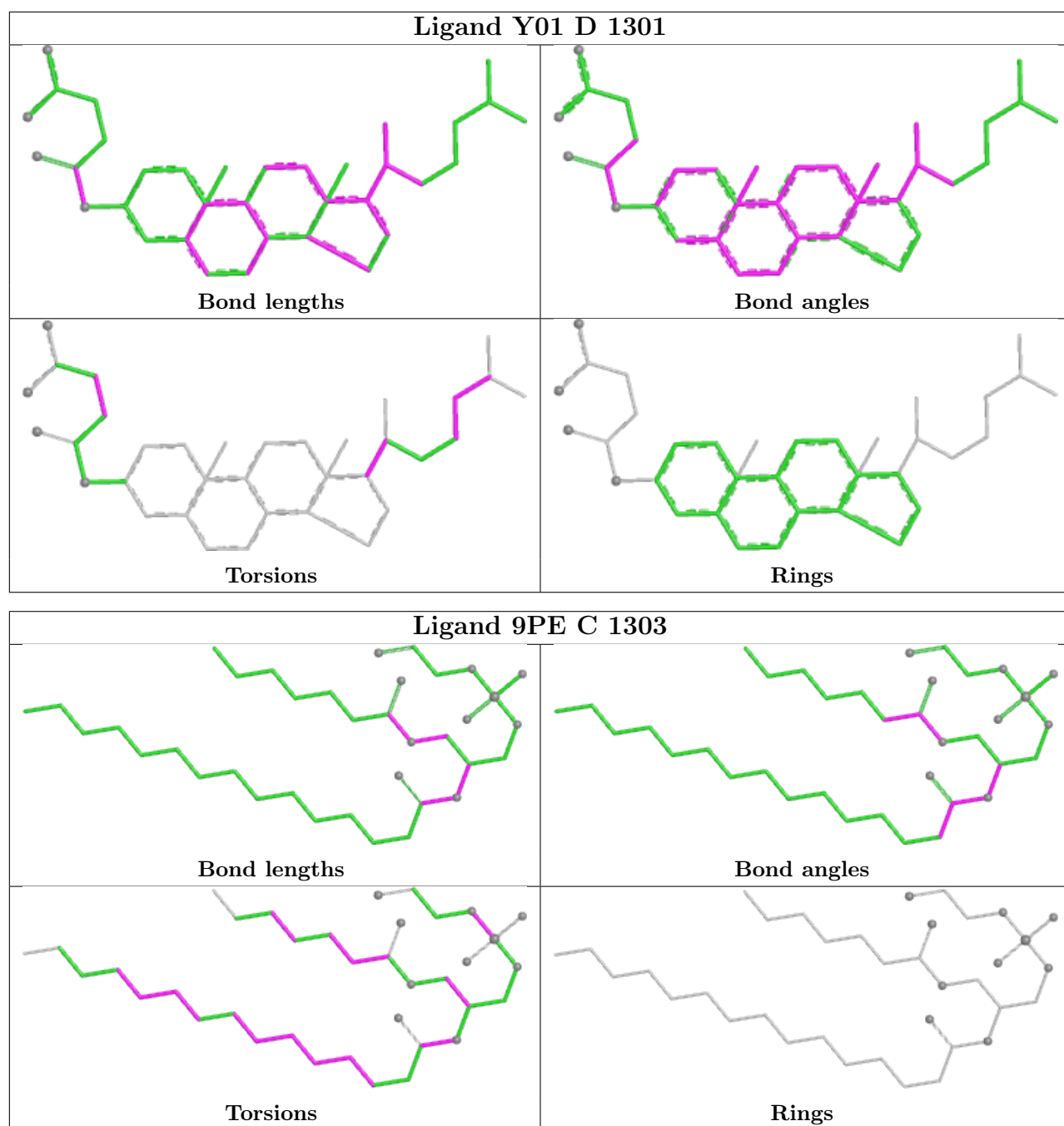
There are no ring outliers.

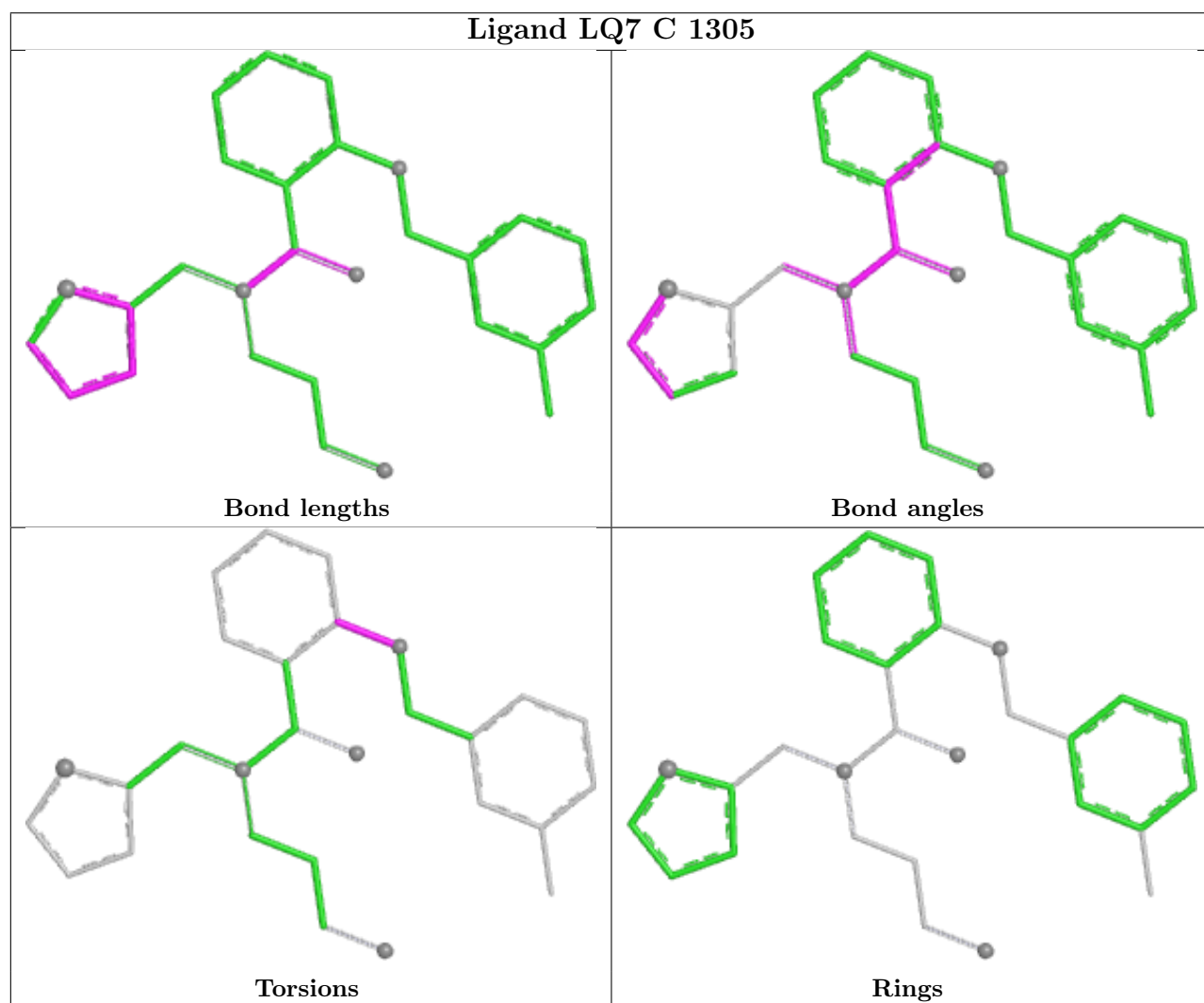
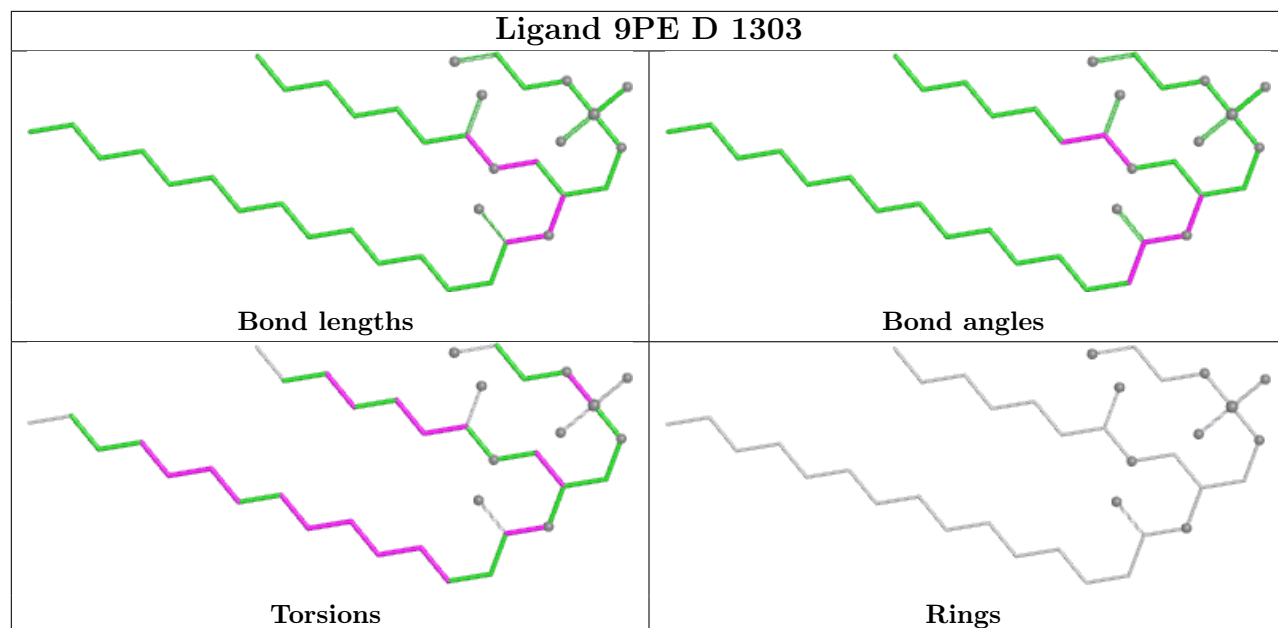
8 monomers are involved in 22 short contacts:

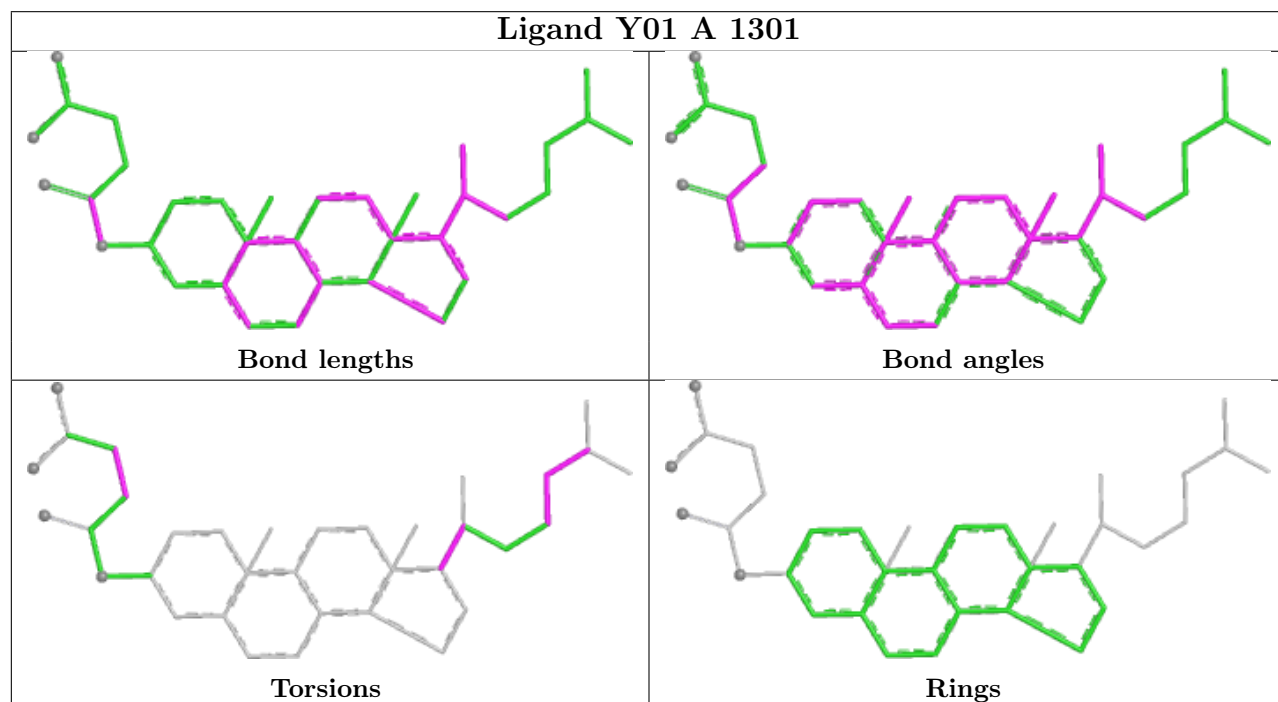
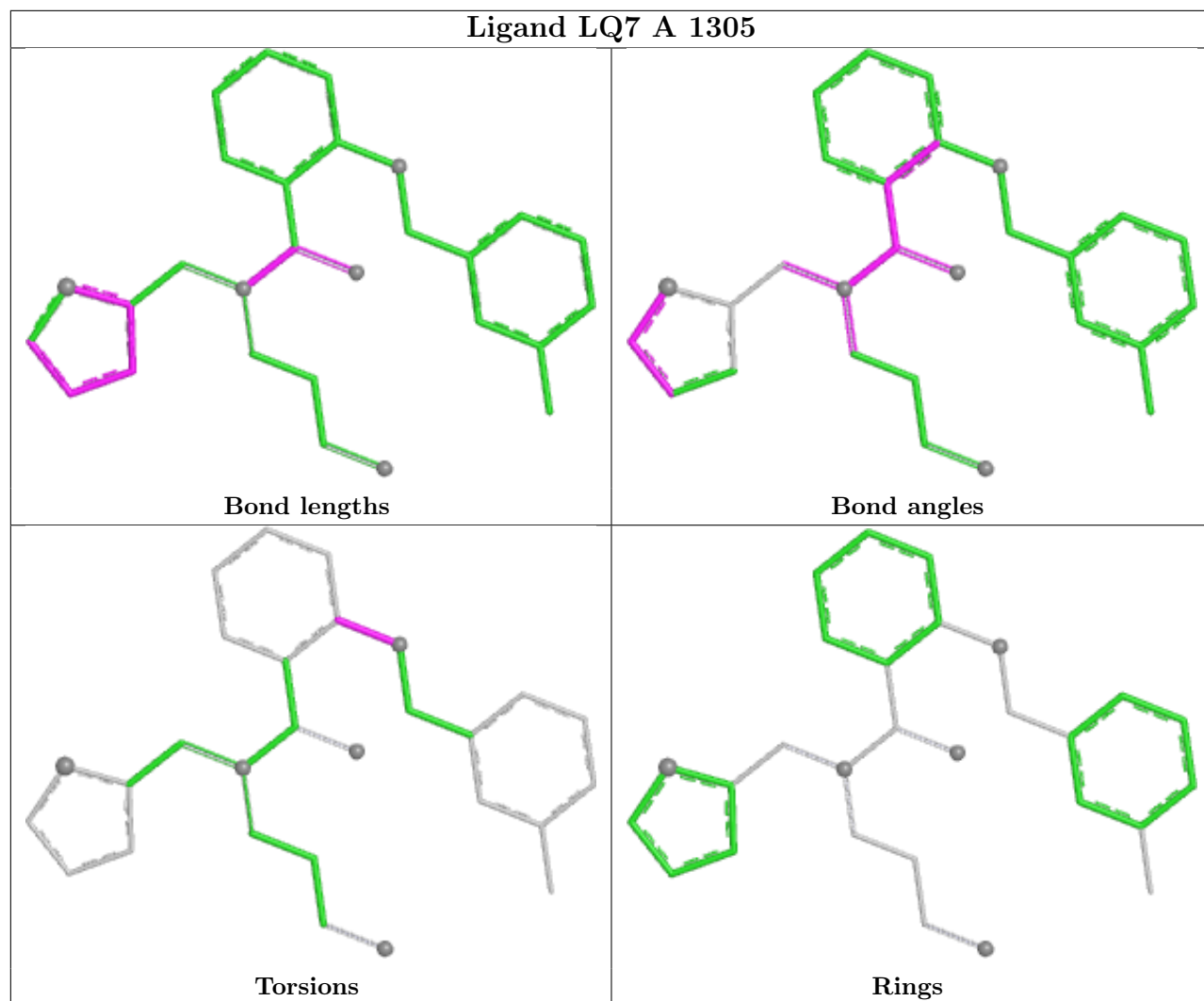
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	Y01	4	0
2	D	1301	Y01	4	0
4	C	1303	9PE	2	0
4	D	1303	9PE	2	0
2	A	1301	Y01	5	0
2	B	1301	Y01	5	0
4	B	1303	9PE	2	0
4	A	1303	9PE	2	0

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.

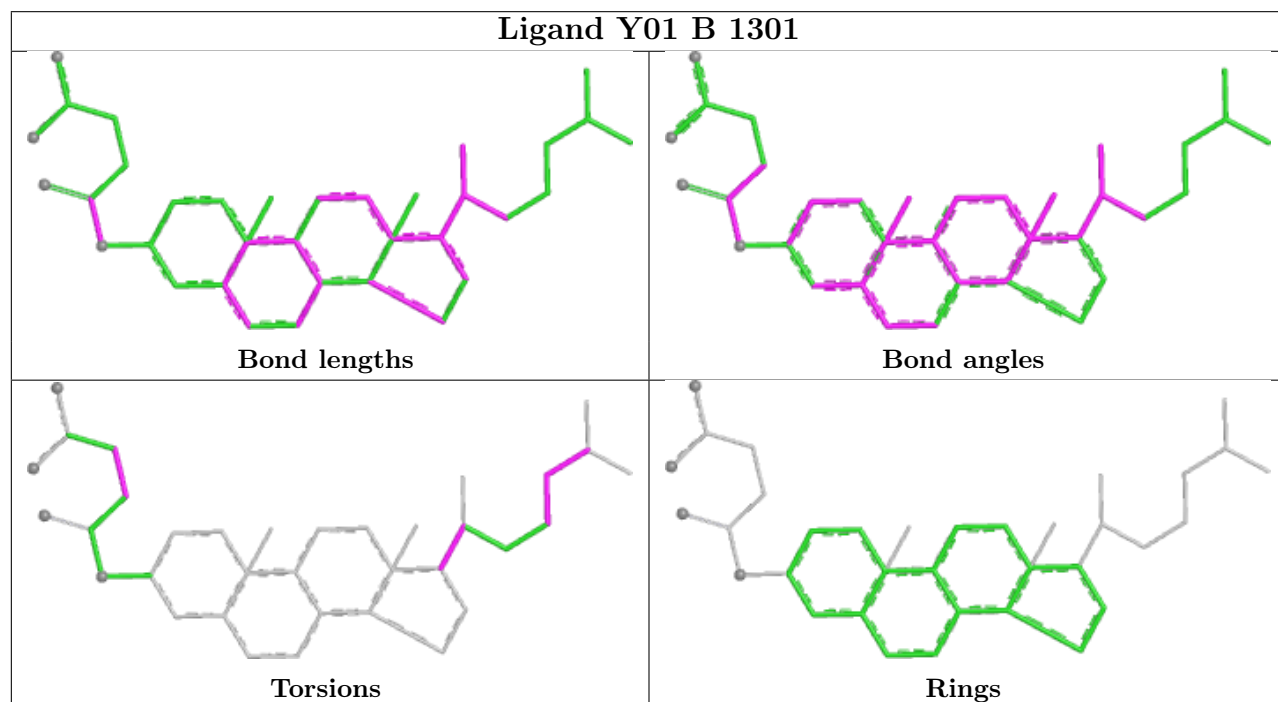
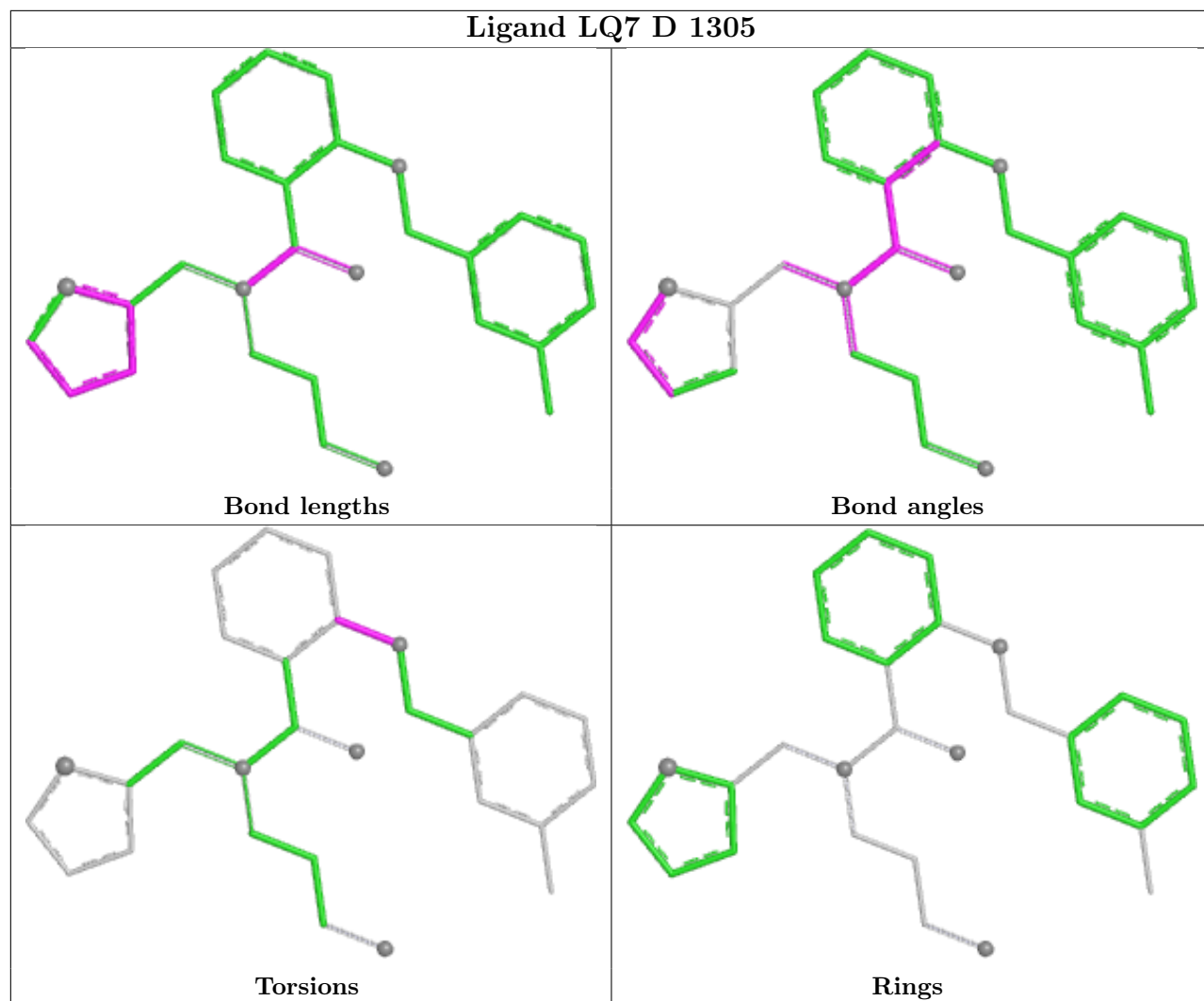


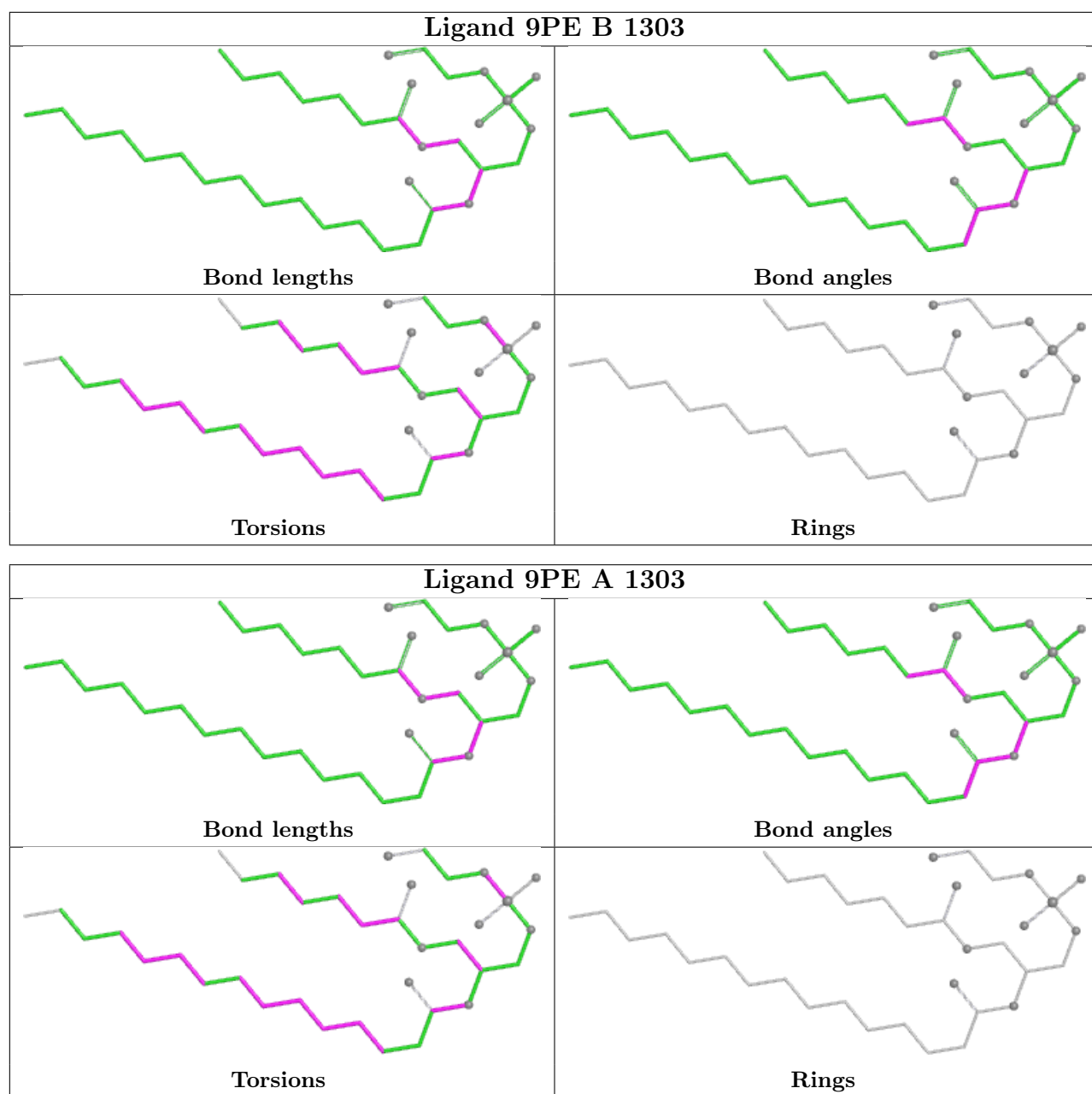












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

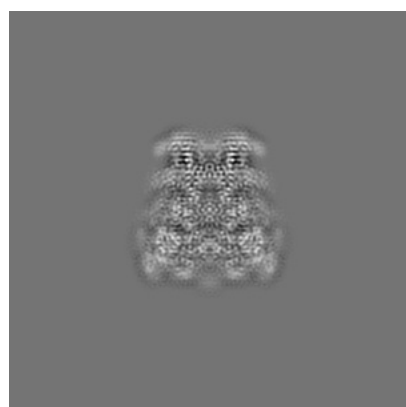
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0636. These allow visual inspection of the internal detail of the map and identification of artifacts.

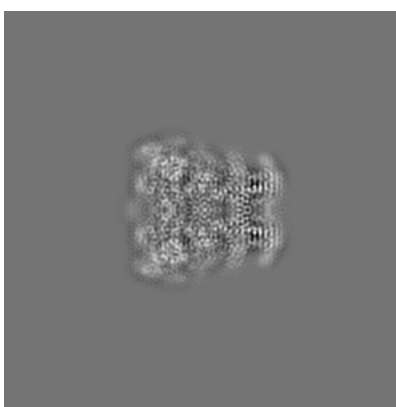
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

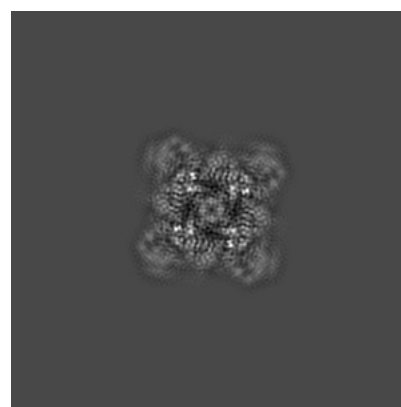
#### 6.1.1 Primary map



X



Y

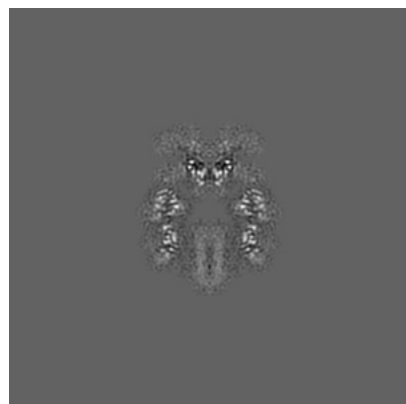


Z

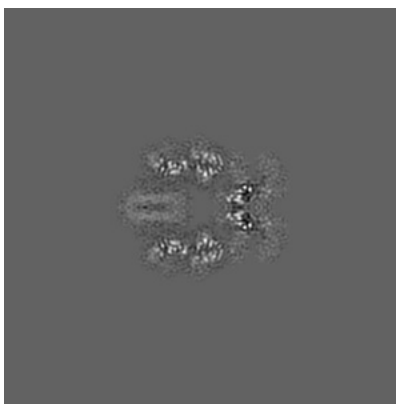
The images above show the map projected in three orthogonal directions.

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

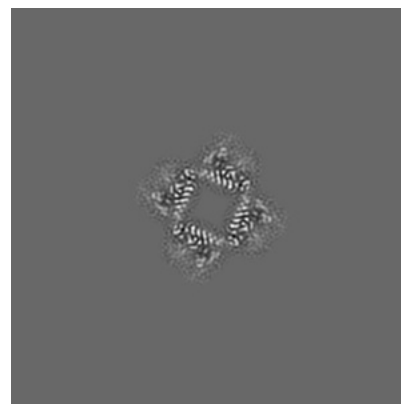
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

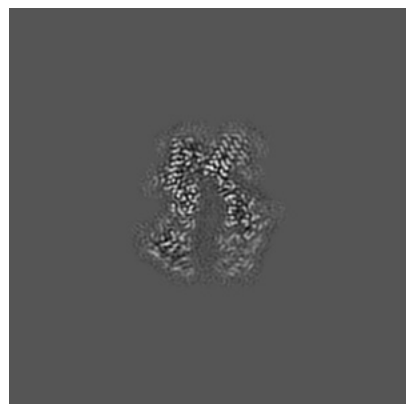


Z Index: 160

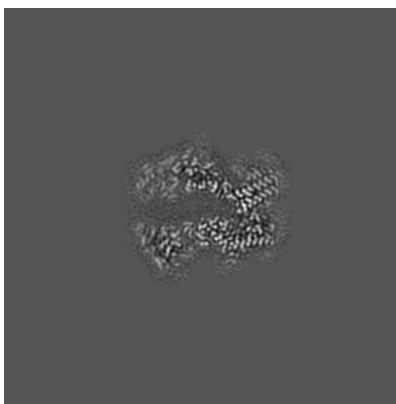
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

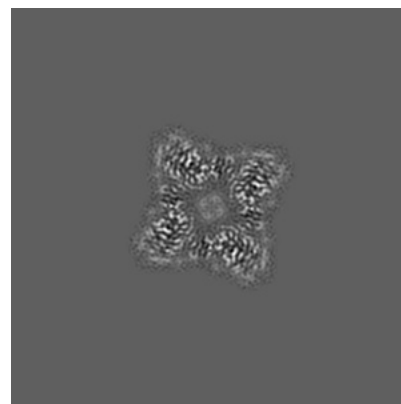
### 6.3.1 Primary map



X Index: 176



Y Index: 144

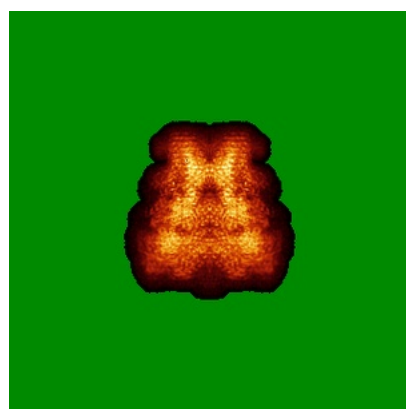


Z Index: 134

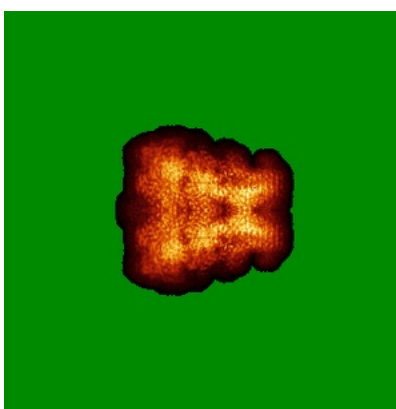
The images above show the largest variance slices of the map in three orthogonal directions.

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

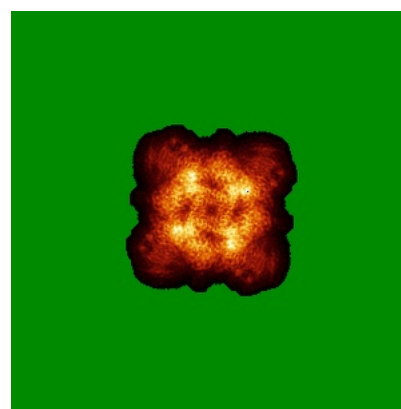
### 6.4.1 Primary map



X



Y

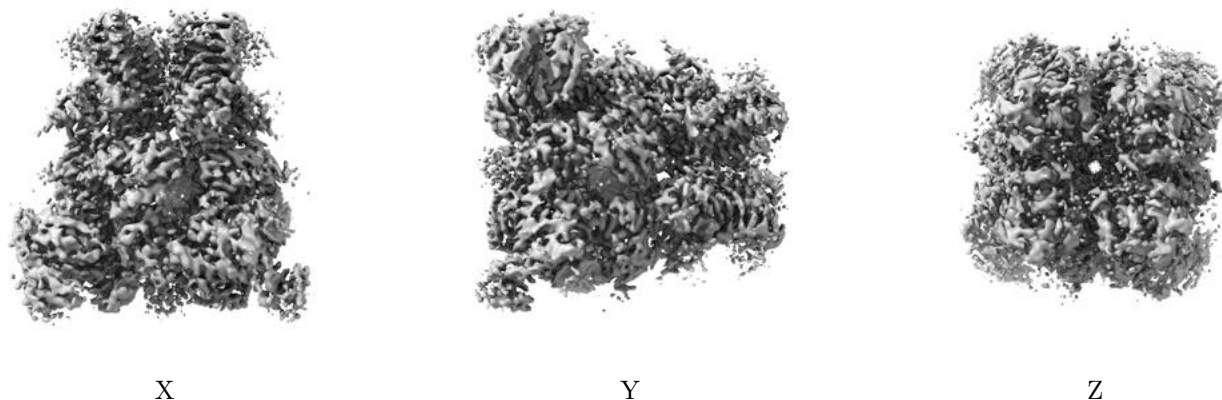


Z

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

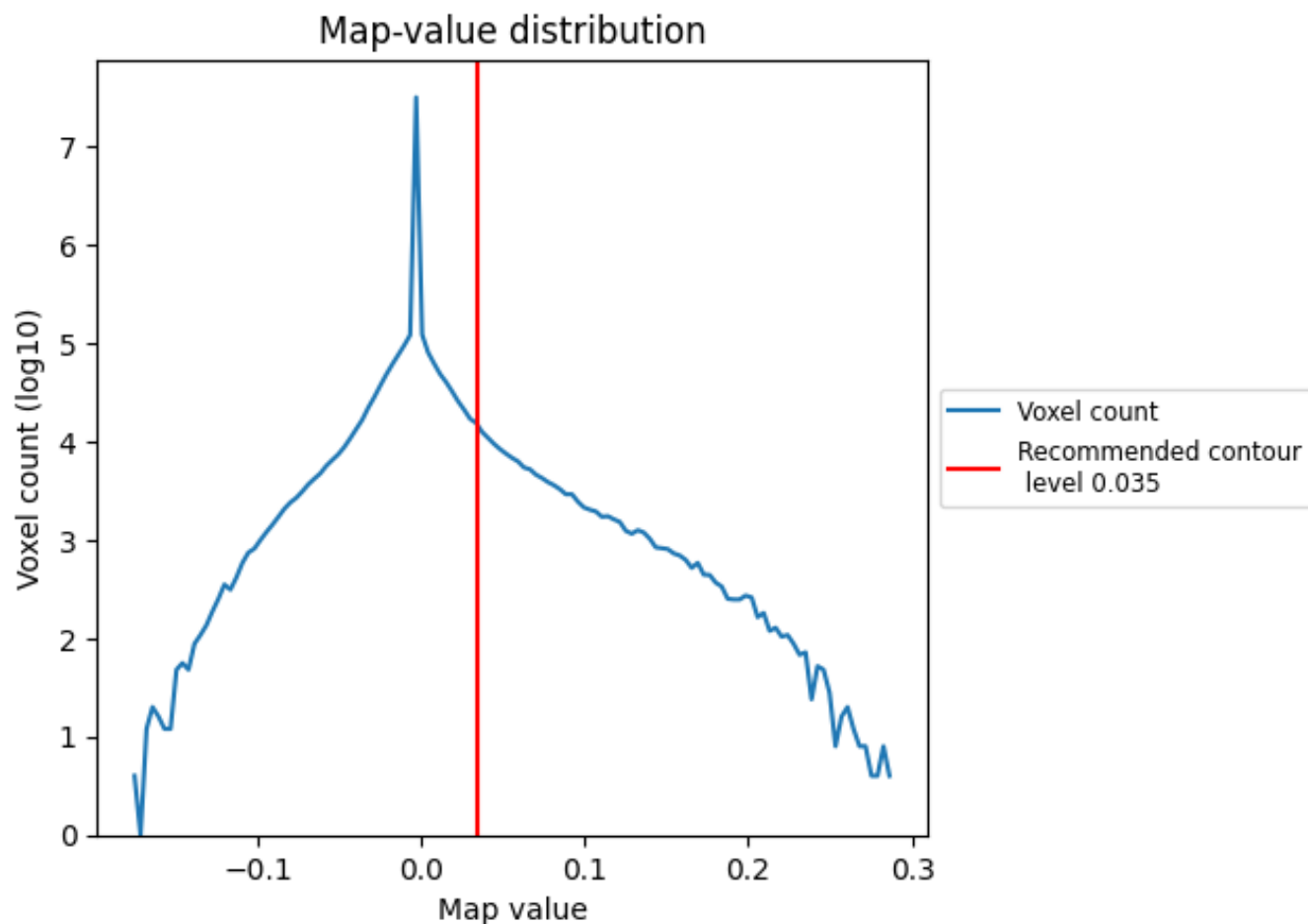
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

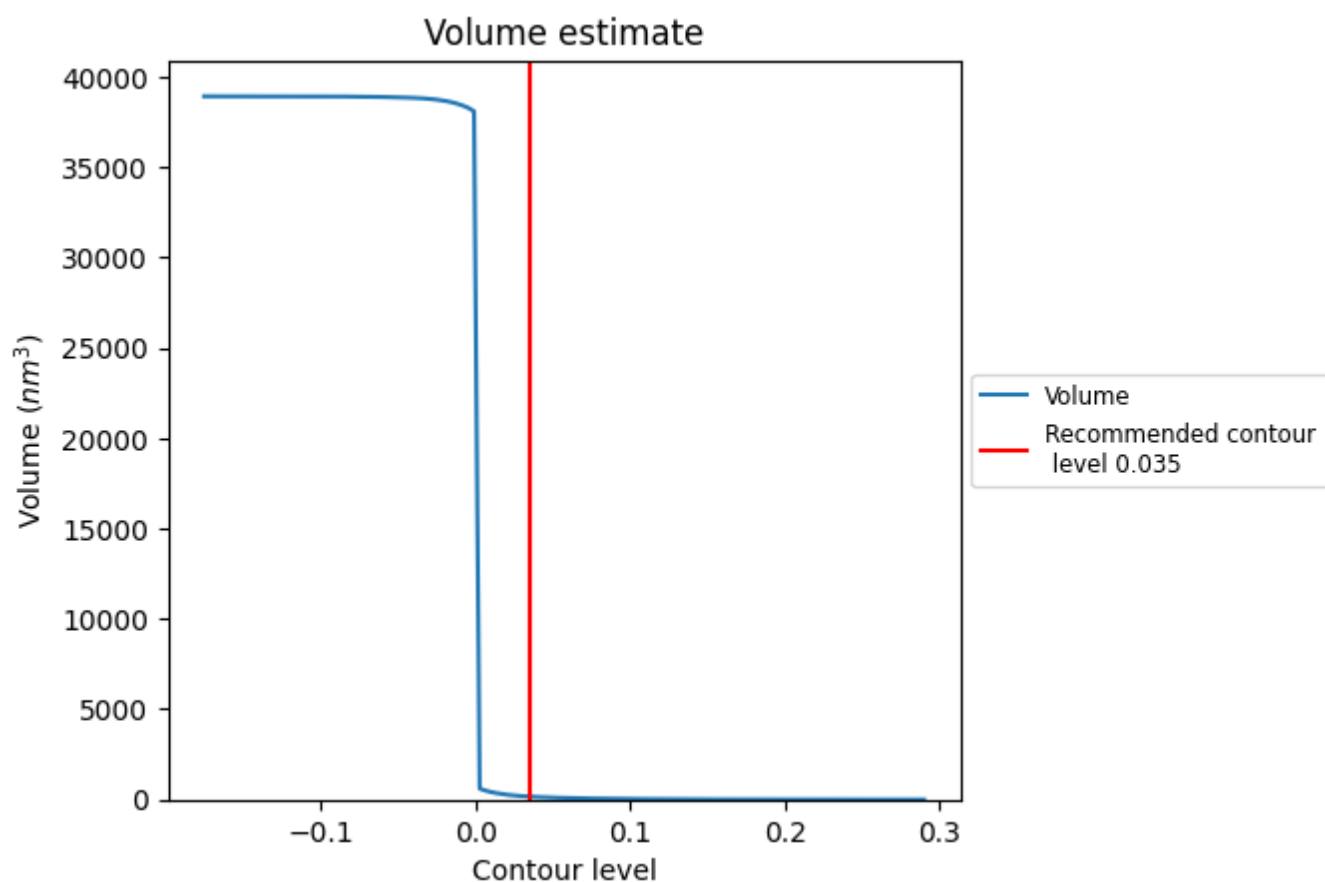
This section contains the results of statistical analysis of the map.

### 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.

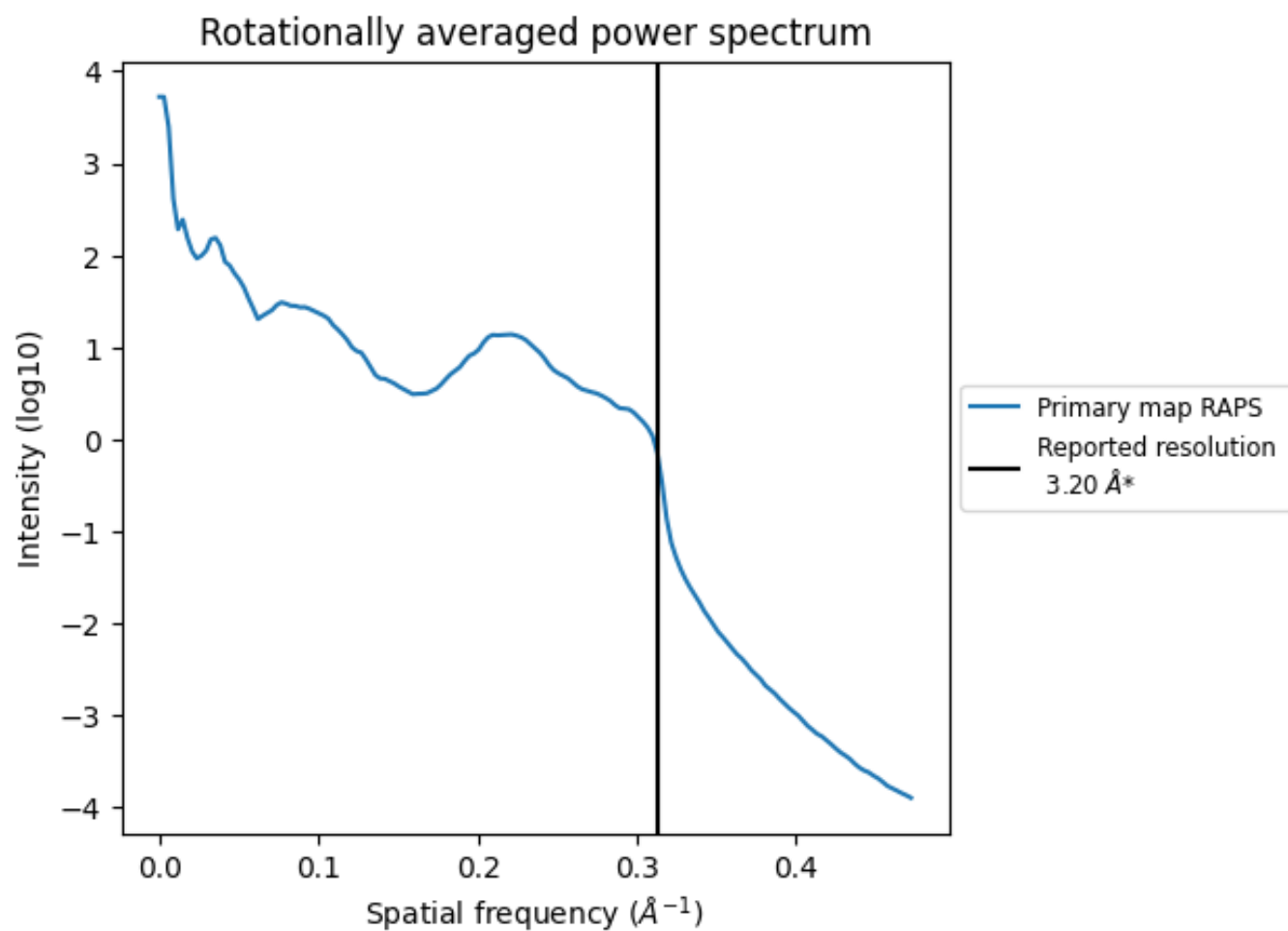
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm<sup>3</sup>; this corresponds to an approximate mass of 148 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 ⓘ



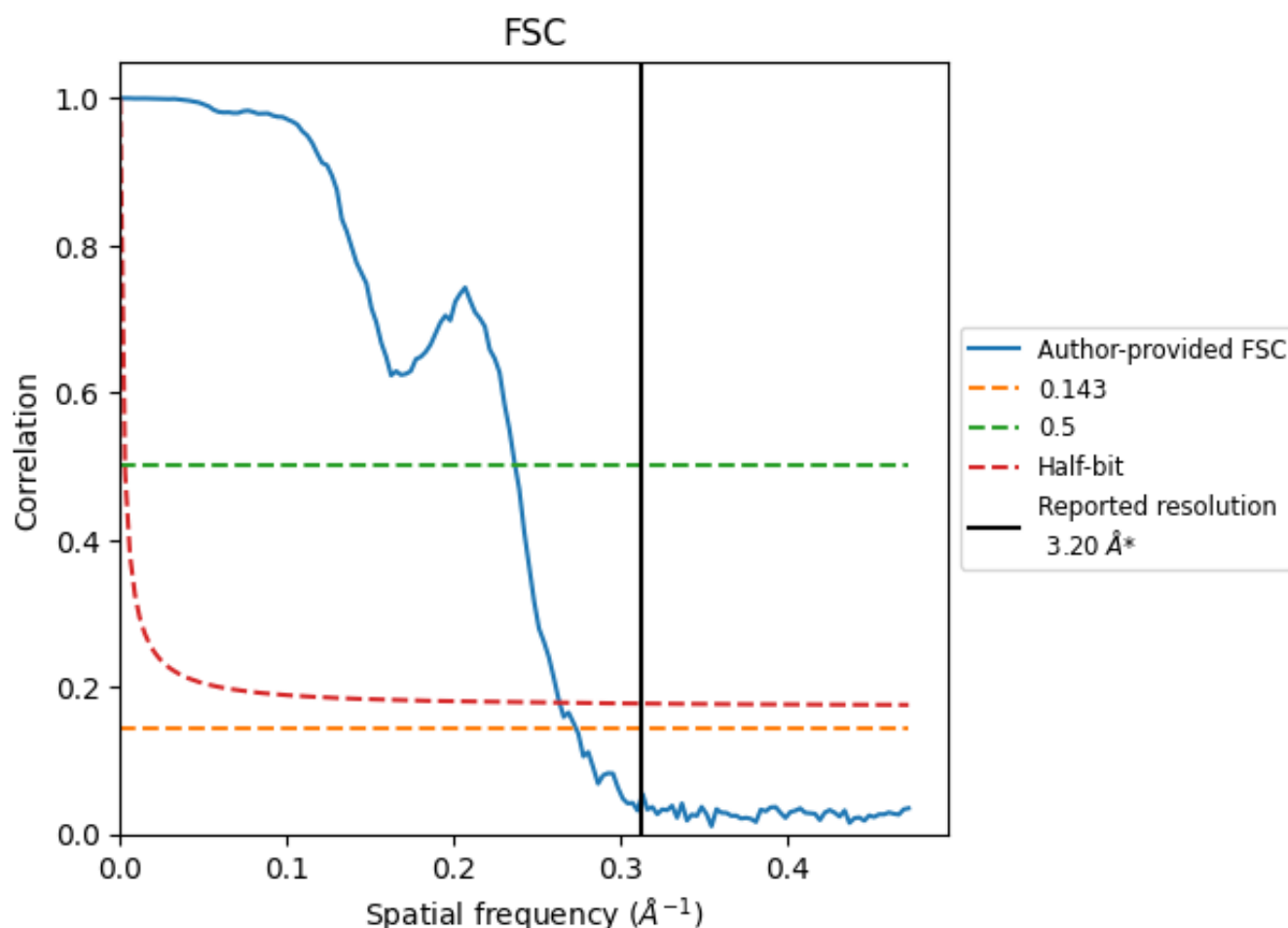
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

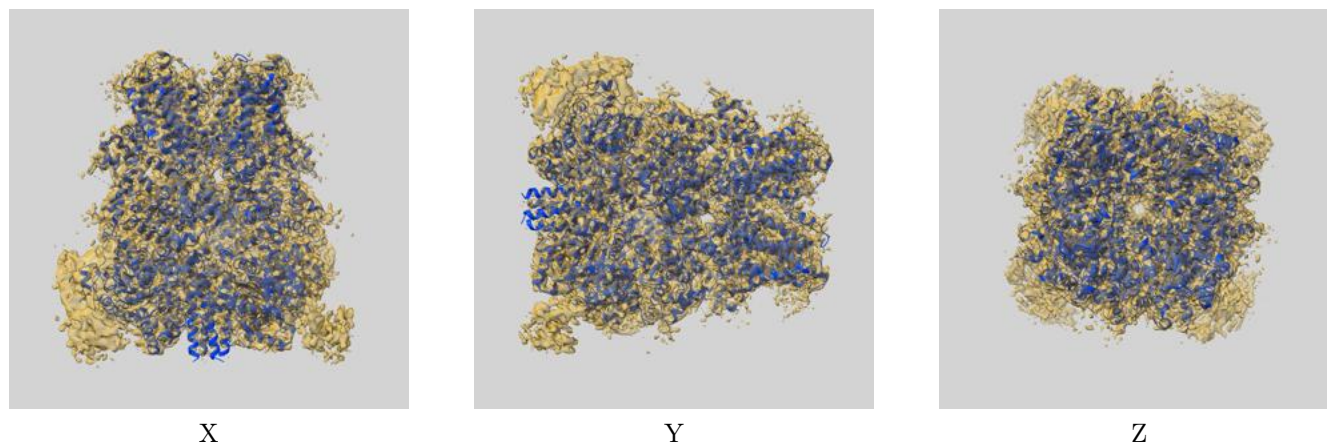
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.66	4.23	3.80
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.2 by more than 10 %

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

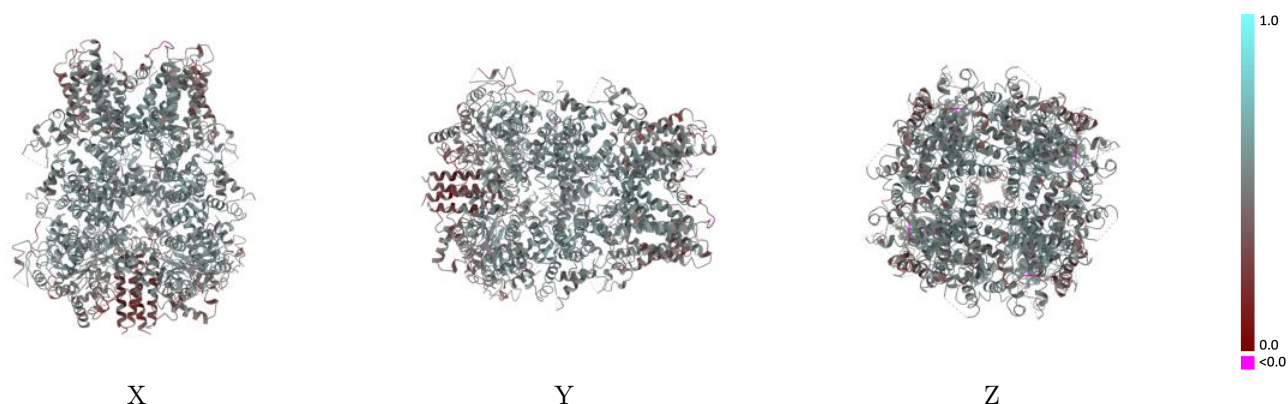
This section contains information regarding the fit between EMDB map EMD-0636 and PDB model 6O6R. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



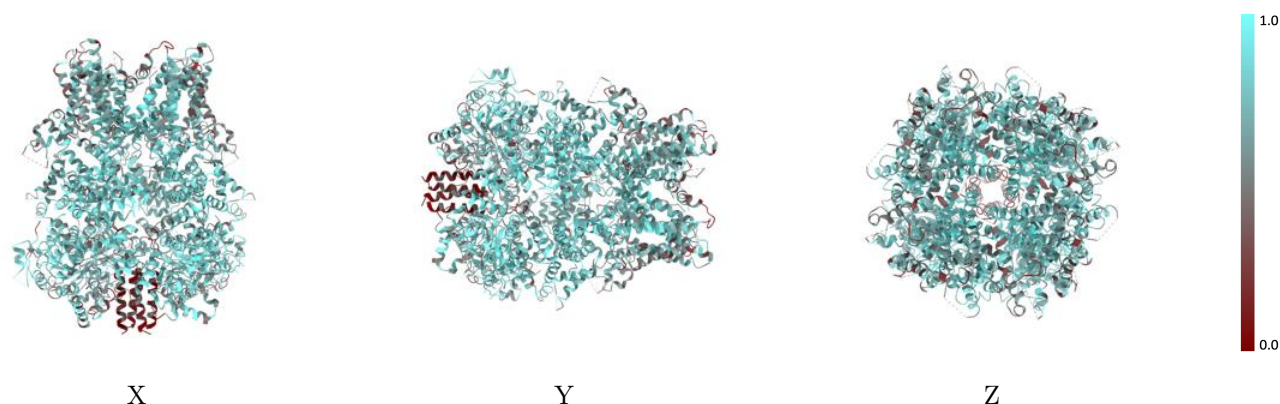
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



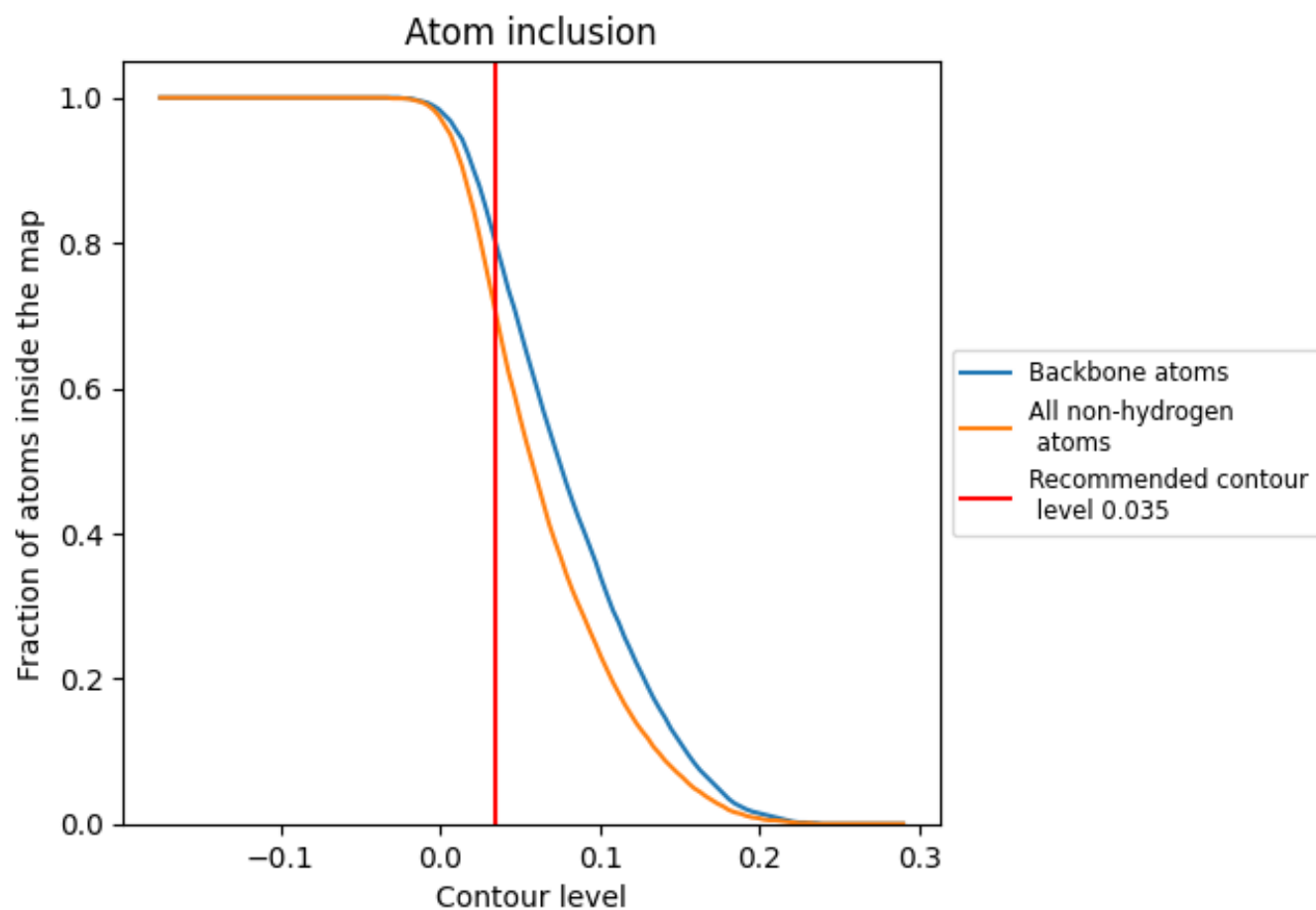
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.4930
A	<div></div> 0.7040	<div></div> 0.4940
B	<div></div> 0.7040	<div></div> 0.4960
C	<div></div> 0.7030	<div></div> 0.4930
D	<div></div> 0.6990	<div></div> 0.4900

