



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 01:55 AM JST

PDB ID : 7DXE  
EMDB ID : EMD-30906  
Title : Structure of TRPC3 gain of function mutation R803C at 3.2 angstrom in 1340nM free calcium state  
Authors : Chen, L.; Guo, W.  
Deposited on : 2021-01-18  
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:

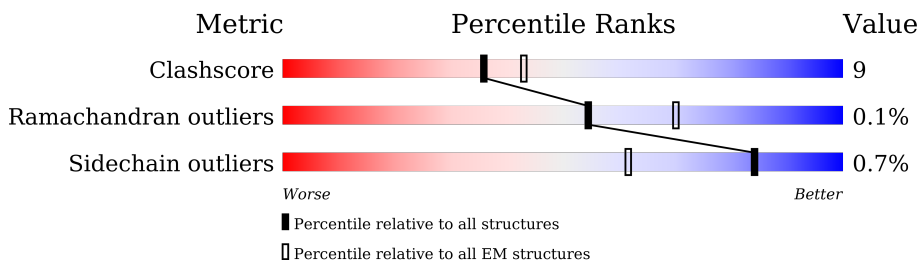
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	836	
1	B	836	
1	C	836	
1	D	836	

## 2 Entry composition [i](#)

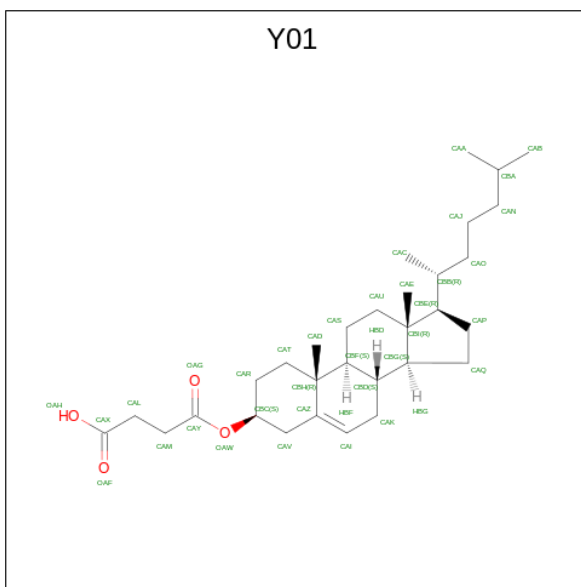
There are 5 unique types of molecules in this entry. The entry contains 22280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	685	Total	C	N	O	S	0	0
			5434	3559	886	961	28		
1	A	685	Total	C	N	O	S	0	0
			5434	3559	886	961	28		
1	B	685	Total	C	N	O	S	0	0
			5434	3559	886	961	28		
1	C	685	Total	C	N	O	S	0	0
			5434	3559	886	961	28		

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
2	D	1	Total	C	O	0
			70	62	8	
2	D	1	Total	C	O	0
			70	62	8	
2	A	1	Total	C	O	0
			70	62	8	

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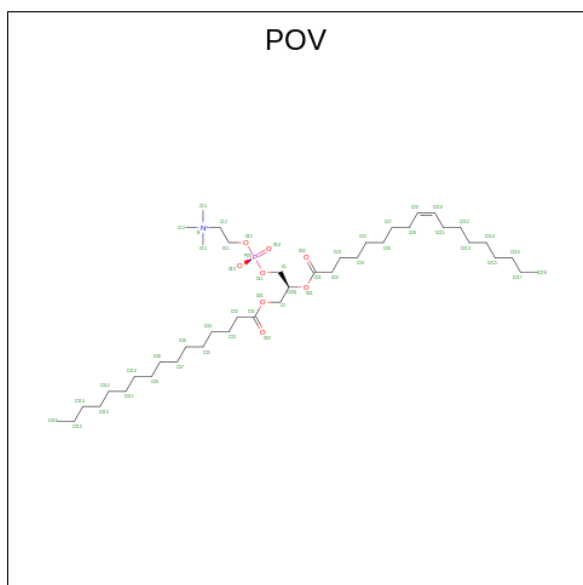
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Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			70	62	8	
2	B	1	Total	C	O	0
			70	62	8	
2	B	1	Total	C	O	0
			70	62	8	
2	C	1	Total	C	O	0
			70	62	8	
2	C	1	Total	C	O	0
			70	62	8	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

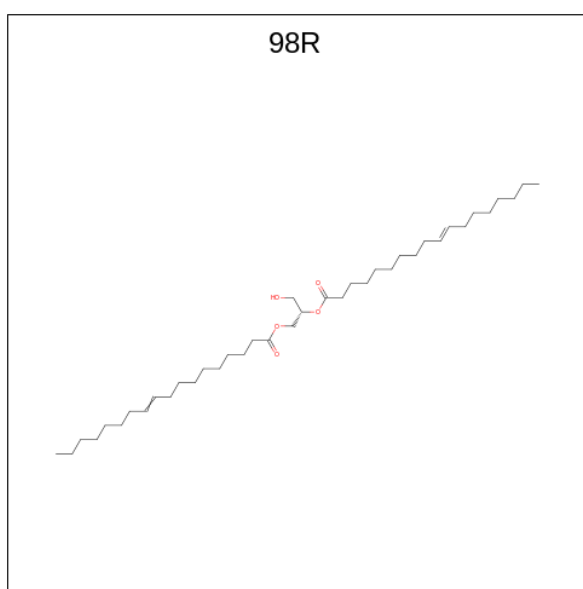
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms			AltConf
4	D	1	Total	C	O	0
			36	32	4	
4	A	1	Total	C	O	0
			36	32	4	
4	B	1	Total	C	O	0
			36	32	4	
4	C	1	Total	C	O	0
			36	32	4	

- Molecule 5 is [(2S)-2-[(E)-octadec-10-enoyl]oxy-3-oxidanyl-propyl] octadec-10-enoate (three-letter code: 98R) (formula: C<sub>39</sub>H<sub>72</sub>O<sub>5</sub>).

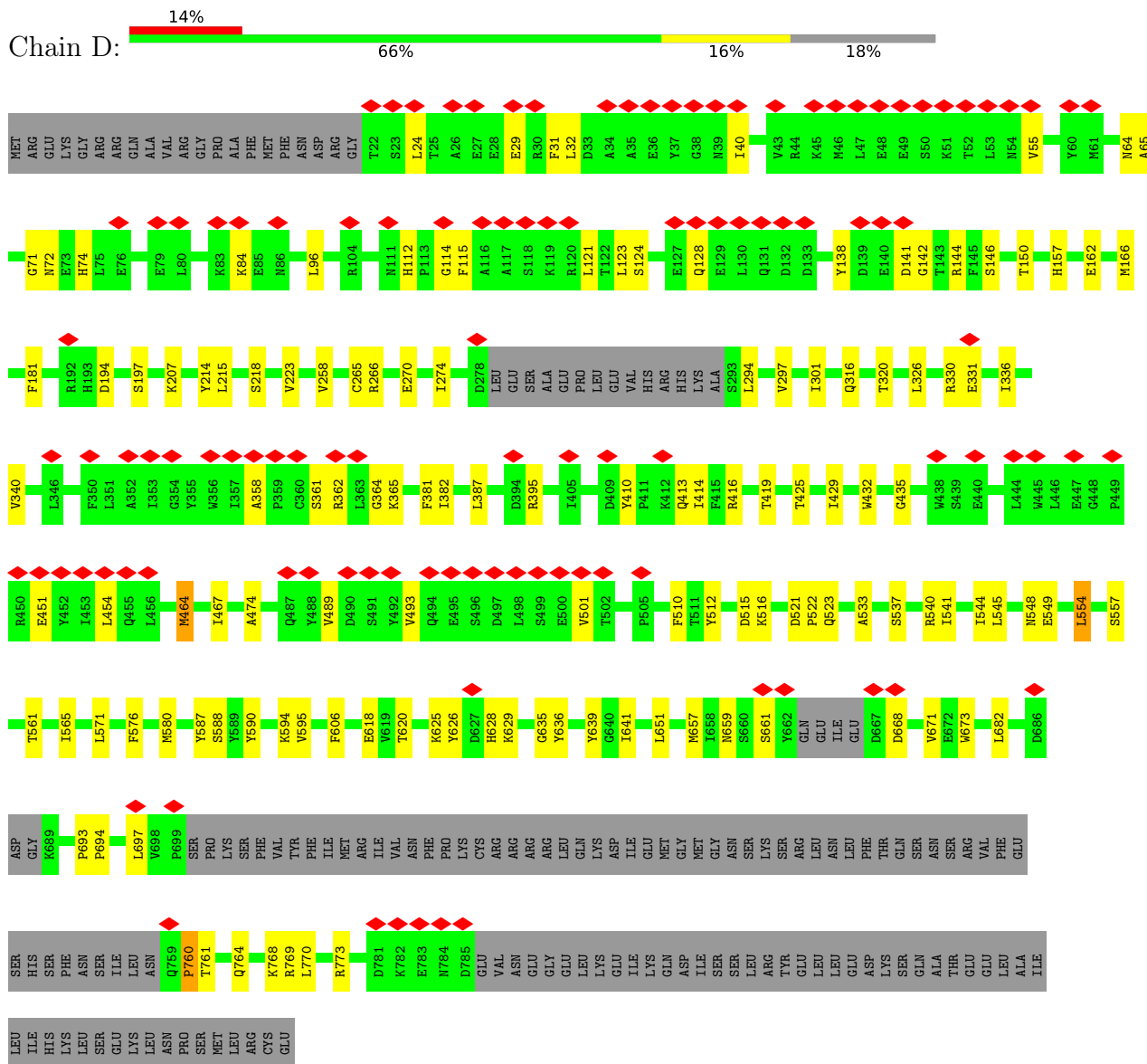


Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	C	O	0
			29	24	5	
5	A	1	Total	C	O	0
			29	24	5	
5	B	1	Total	C	O	0
			29	24	5	
5	C	1	Total	C	O	0
			29	24	5	

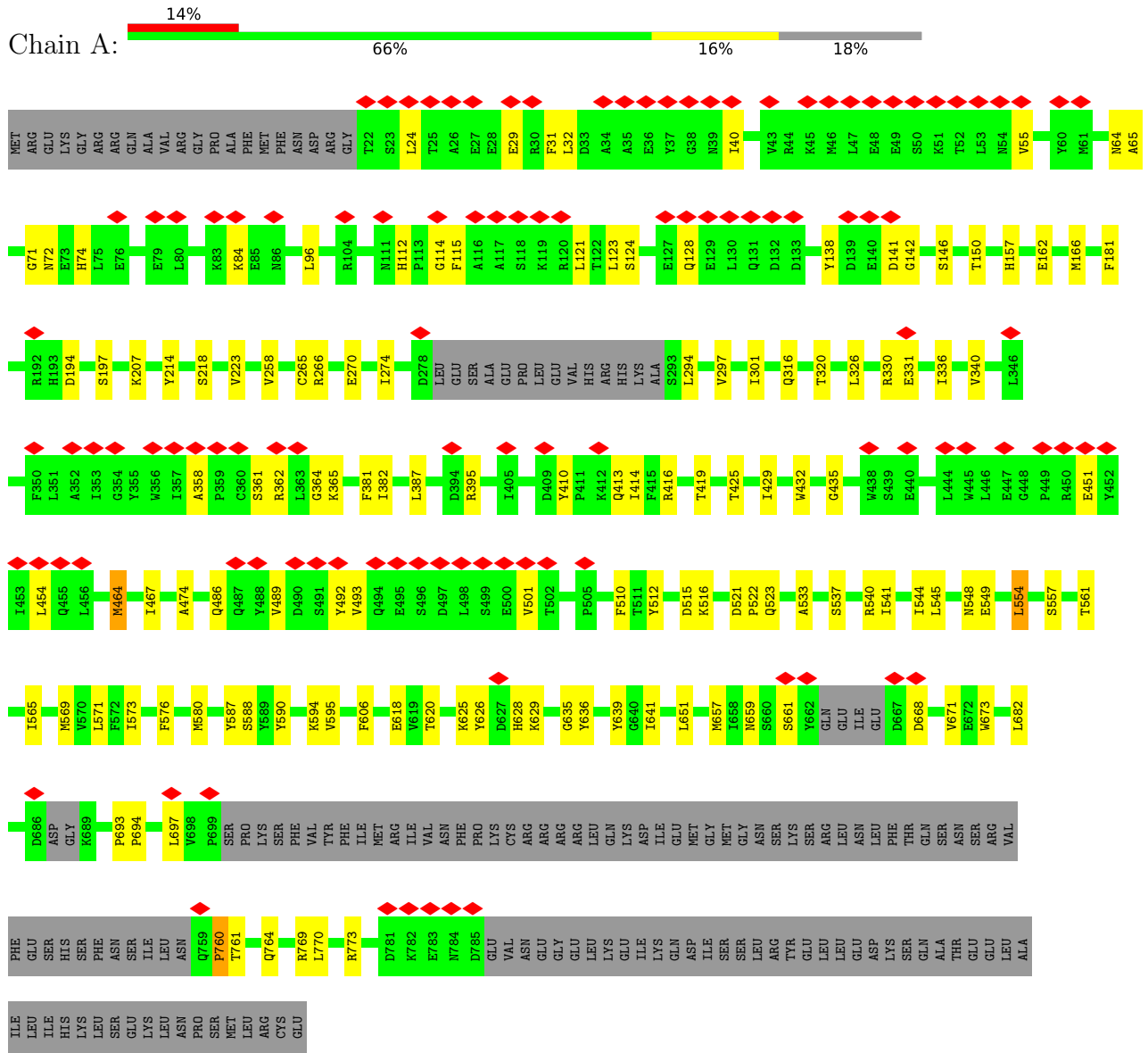
### 3 Residue-property plots i

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

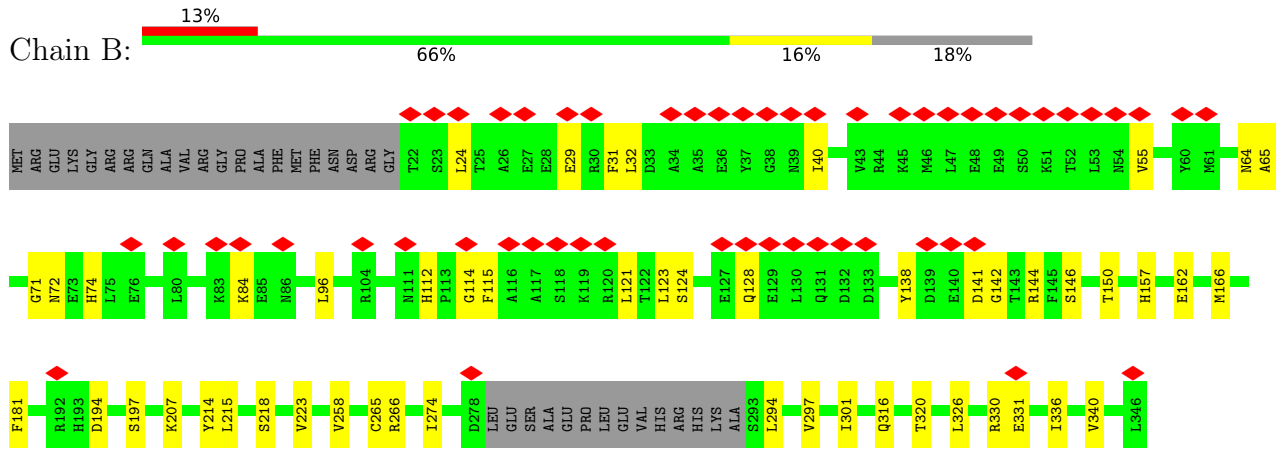
- Molecule 1: Short transient receptor potential channel 3

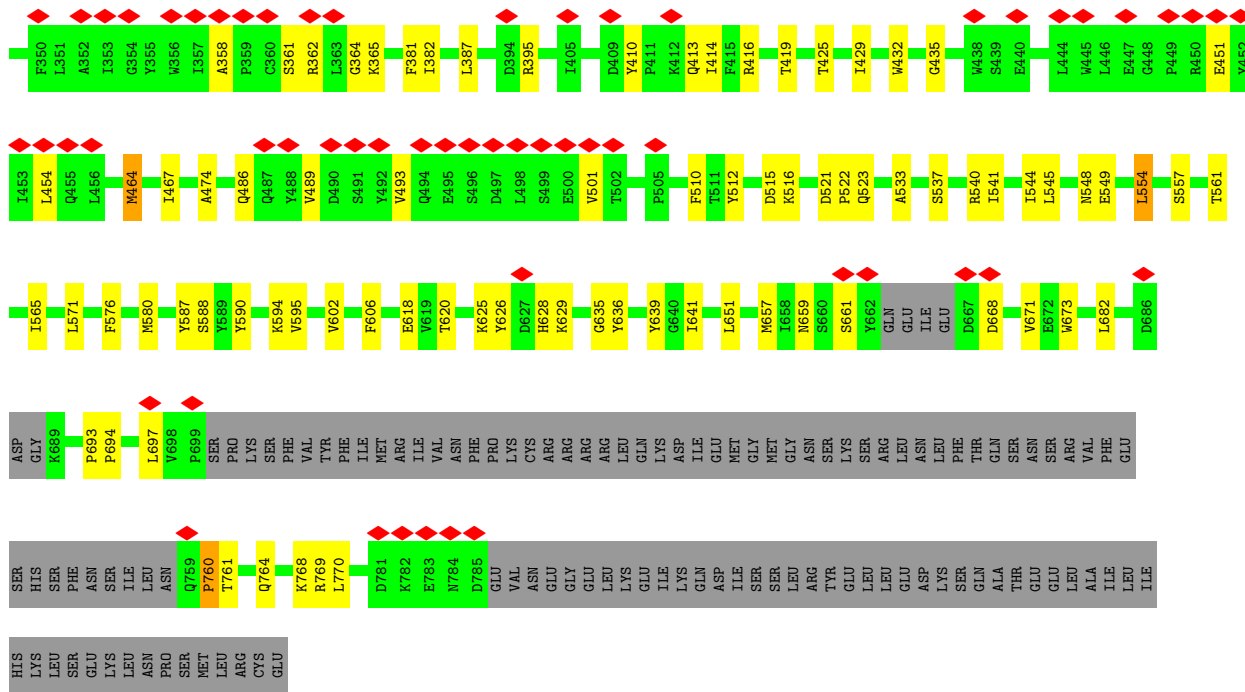


- Molecule 1: Short transient receptor potential channel 3

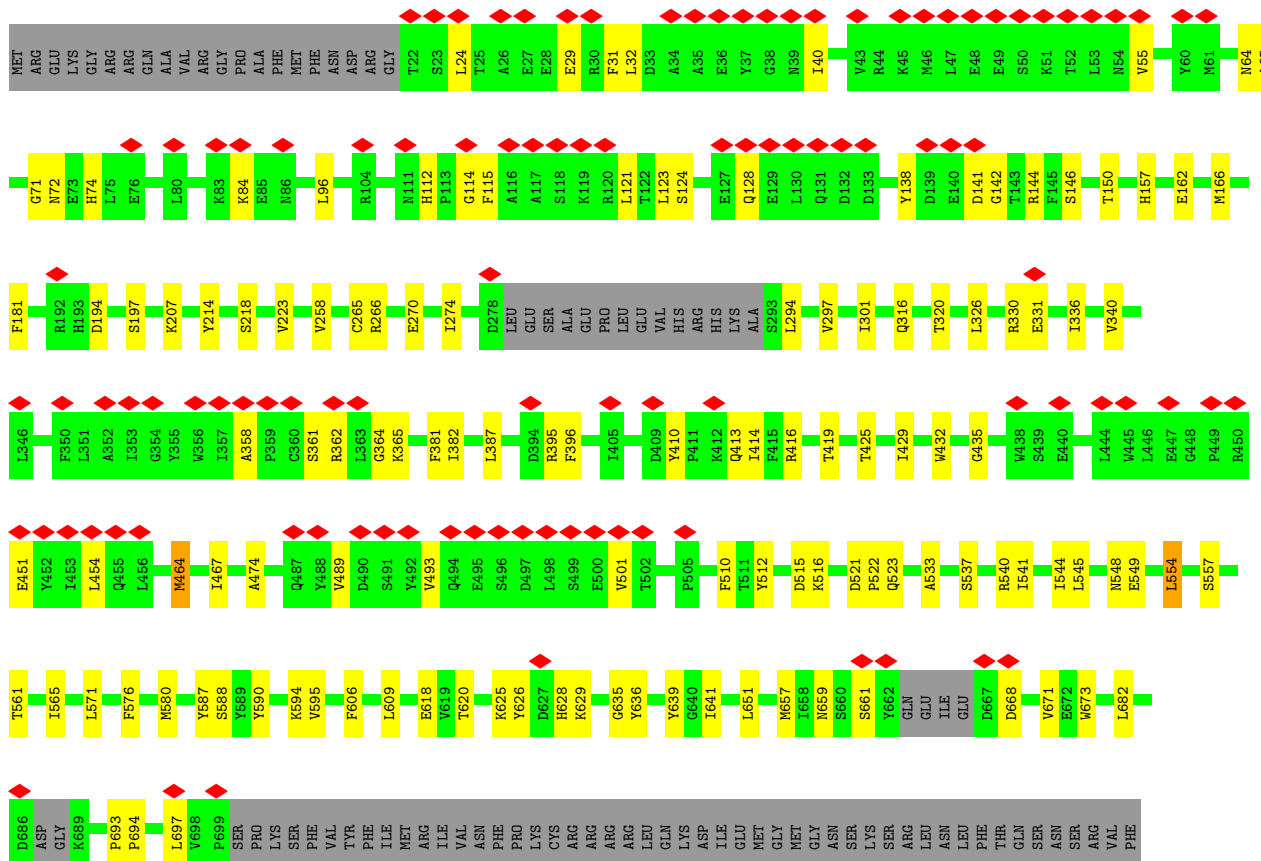


• Molecule 1: Short transient receptor potential channel 3

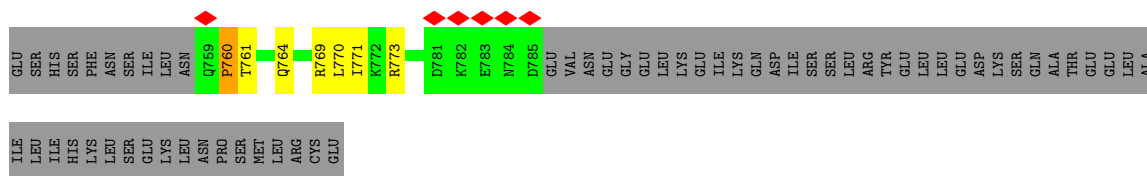




• Molecule 1: Short transient receptor potential channel 3







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.612	Depositor
Minimum map value	-1.713	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.8	Depositor
Map size ( $\text{\AA}$ )	292.59998, 292.59998, 292.59998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.045, 1.045, 1.045	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, ZN, Y01, 98R

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	0.27	0/5557	0.42	0/7536
1	B	0.27	0/5557	0.42	0/7536
1	C	0.27	0/5557	0.42	0/7536
1	D	0.27	0/5557	0.42	0/7536
All	All	0.27	0/22228	0.42	0/30144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5434	0	5443	100	0
1	B	5434	0	5443	101	0
1	C	5434	0	5443	101	0
1	D	5434	0	5443	98	0
2	A	70	0	98	6	0
2	B	70	0	98	8	0
2	C	70	0	98	9	0
2	D	70	0	98	10	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	36	0	51	2	0
4	B	36	0	51	2	0
4	C	36	0	51	2	0
4	D	36	0	51	2	0
5	A	29	0	0	5	0
5	B	29	0	0	5	0
5	C	29	0	0	5	0
5	D	29	0	0	5	0
All	All	22280	0	22368	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (381) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:PHE:CE1	1:C:606:PHE:CE2	2.39	1.04
1:B:606:PHE:CE1	1:B:606:PHE:CE2	2.39	1.03
1:C:576:PHE:CE1	1:C:576:PHE:CE2	2.38	1.02
1:A:576:PHE:CE2	1:A:576:PHE:CE1	2.38	1.01
1:D:576:PHE:CE1	1:D:576:PHE:CE2	2.38	1.01
1:B:576:PHE:CE1	1:B:576:PHE:CE2	2.38	1.01
1:D:606:PHE:CE1	1:D:606:PHE:CE2	2.39	0.99
1:A:606:PHE:CE1	1:A:606:PHE:CE2	2.39	0.96
1:A:661:SER:HB2	1:C:659:ASN:HD21	1.30	0.95
1:D:659:ASN:HD21	1:B:661:SER:HB2	1.30	0.94
1:B:659:ASN:HD21	1:C:661:SER:HB2	1.30	0.94
1:D:661:SER:HB2	1:A:659:ASN:HD21	1.30	0.93
1:A:419:THR:HG22	1:A:523:GLN:HE22	1.58	0.69
1:C:419:THR:HG22	1:C:523:GLN:HE22	1.58	0.69
1:C:493:VAL:HG21	1:C:501:VAL:HG11	1.74	0.69
1:B:493:VAL:HG21	1:B:501:VAL:HG11	1.74	0.69
1:D:419:THR:HG22	1:D:523:GLN:HE22	1.58	0.68
1:D:493:VAL:HG21	1:D:501:VAL:HG11	1.74	0.68
1:A:493:VAL:HG21	1:A:501:VAL:HG11	1.74	0.68
1:B:419:THR:HG22	1:B:523:GLN:HE22	1.58	0.68
1:B:659:ASN:HD21	1:C:661:SER:CB	2.08	0.66
1:D:659:ASN:HD21	1:B:661:SER:CB	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:LYS:NZ	1:D:594:LYS:HB3	2.13	0.64
1:D:661:SER:CB	1:A:659:ASN:HD21	2.08	0.64
1:A:594:LYS:NZ	1:A:594:LYS:HB3	2.13	0.63
1:A:435:GLY:HA2	1:A:697:LEU:HD21	1.80	0.63
1:B:435:GLY:HA2	1:B:697:LEU:HD21	1.80	0.63
1:C:594:LYS:NZ	1:C:594:LYS:HB3	2.13	0.63
1:B:594:LYS:NZ	1:B:594:LYS:HB3	2.13	0.62
1:D:435:GLY:HA2	1:D:697:LEU:HD21	1.80	0.62
1:C:435:GLY:HA2	1:C:697:LEU:HD21	1.80	0.62
1:C:362:ARG:HG2	1:C:365:LYS:HE2	1.83	0.61
1:A:362:ARG:HG2	1:A:365:LYS:HE2	1.83	0.61
1:A:661:SER:CB	1:C:659:ASN:HD21	2.08	0.60
1:B:64:ASN:OD1	1:B:65:ALA:N	2.35	0.60
1:B:362:ARG:HG2	1:B:365:LYS:HE2	1.83	0.60
1:D:64:ASN:OD1	1:D:65:ALA:N	2.35	0.60
1:D:362:ARG:HG2	1:D:365:LYS:HE2	1.83	0.59
1:A:64:ASN:OD1	1:A:65:ALA:N	2.35	0.59
1:C:64:ASN:OD1	1:C:65:ALA:N	2.35	0.59
1:C:194:ASP:HB3	1:C:197:SER:HB3	1.84	0.59
1:D:194:ASP:HB3	1:D:197:SER:HB3	1.84	0.58
1:D:769:ARG:NH2	1:A:141:ASP:OD1	2.34	0.58
1:A:72:ASN:O	1:A:74:HIS:ND1	2.31	0.58
1:D:141:ASP:OD1	1:B:769:ARG:NH2	2.34	0.58
1:B:194:ASP:HB3	1:B:197:SER:HB3	1.84	0.58
1:A:194:ASP:HB3	1:A:197:SER:HB3	1.84	0.58
1:B:760:PRO:O	1:B:761:THR:OG1	2.21	0.58
1:D:760:PRO:O	1:D:761:THR:OG1	2.21	0.58
1:A:595:VAL:HG12	1:A:625:LYS:HG3	1.86	0.58
1:B:72:ASN:O	1:B:74:HIS:ND1	2.31	0.58
1:C:595:VAL:HG12	1:C:625:LYS:HG3	1.86	0.58
1:D:571:LEU:HD12	1:B:554:LEU:HD21	1.86	0.58
1:C:31:PHE:HD1	1:C:32:LEU:HD23	1.69	0.58
1:A:31:PHE:HD1	1:A:32:LEU:HD23	1.69	0.58
1:D:554:LEU:HD21	1:A:571:LEU:HD12	1.86	0.57
1:B:595:VAL:HG12	1:B:625:LYS:HG3	1.86	0.57
1:D:467:ILE:HG22	1:D:533:ALA:HB2	1.87	0.57
1:B:301:ILE:HD12	1:B:682:LEU:HD22	1.86	0.57
1:B:31:PHE:HD1	1:B:32:LEU:HD23	1.69	0.57
1:D:31:PHE:HD1	1:D:32:LEU:HD23	1.69	0.57
1:C:301:ILE:HD12	1:C:682:LEU:HD22	1.86	0.57
1:A:760:PRO:O	1:A:761:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ILE:HG22	1:B:533:ALA:HB2	1.87	0.57
1:D:595:VAL:HG12	1:D:625:LYS:HG3	1.86	0.57
1:A:769:ARG:NH2	1:C:141:ASP:OD1	2.34	0.57
1:D:72:ASN:O	1:D:74:HIS:ND1	2.31	0.56
1:B:571:LEU:HD12	1:C:554:LEU:HD21	1.86	0.56
1:A:301:ILE:HD12	1:A:682:LEU:HD22	1.86	0.56
1:A:467:ILE:HG22	1:A:533:ALA:HB2	1.87	0.56
1:D:301:ILE:HD12	1:D:682:LEU:HD22	1.86	0.56
1:A:554:LEU:HD21	1:C:571:LEU:HD12	1.86	0.56
1:B:636:TYR:HB3	5:B:905:98R:O2	2.06	0.56
1:C:467:ILE:HG22	1:C:533:ALA:HB2	1.87	0.56
1:C:636:TYR:HB3	5:C:902:98R:O2	2.06	0.56
1:D:641:ILE:HD13	5:D:905:98R:C40	2.37	0.55
1:A:636:TYR:HB3	5:A:902:98R:O2	2.06	0.55
1:B:141:ASP:OD1	1:C:769:ARG:NH2	2.34	0.55
1:C:71:GLY:HA2	1:C:96:LEU:HD21	1.89	0.55
1:A:641:ILE:HD13	5:A:902:98R:C40	2.37	0.55
1:B:641:ILE:HD13	5:B:905:98R:C40	2.37	0.55
1:C:641:ILE:HD13	5:C:902:98R:C40	2.37	0.55
1:D:71:GLY:HA2	1:D:96:LEU:HD21	1.89	0.55
1:B:71:GLY:HA2	1:B:96:LEU:HD21	1.89	0.55
1:D:636:TYR:HB3	5:D:905:98R:O2	2.06	0.55
1:A:71:GLY:HA2	1:A:96:LEU:HD21	1.89	0.55
1:C:72:ASN:O	1:C:74:HIS:ND1	2.31	0.55
1:C:760:PRO:O	1:C:761:THR:OG1	2.21	0.55
5:C:902:98R:C19	5:C:902:98R:C42	2.85	0.54
5:C:902:98R:C42	5:C:902:98R:C18	2.86	0.54
5:D:905:98R:C18	5:D:905:98R:C42	2.86	0.54
1:B:410:TYR:CZ	1:B:413:GLN:HB3	2.43	0.54
1:D:410:TYR:CZ	1:D:413:GLN:HB3	2.43	0.54
1:C:410:TYR:CZ	1:C:413:GLN:HB3	2.43	0.54
1:A:410:TYR:CZ	1:A:413:GLN:HB3	2.43	0.54
5:B:905:98R:C19	5:B:905:98R:C42	2.85	0.54
5:A:902:98R:C42	5:A:902:98R:C18	2.86	0.53
5:B:905:98R:C42	5:B:905:98R:C18	2.86	0.53
5:D:905:98R:C42	5:D:905:98R:C19	2.85	0.53
5:A:902:98R:C42	5:A:902:98R:C19	2.85	0.53
1:D:618:GLU:HB3	1:D:620:THR:HG22	1.91	0.53
1:D:214:TYR:O	1:D:218:SER:CB	2.57	0.53
1:B:214:TYR:O	1:B:218:SER:CB	2.57	0.53
1:A:618:GLU:HB3	1:A:620:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:GLU:HA	1:D:673:TRP:CZ2	2.45	0.52
1:C:387:LEU:HB3	1:C:429:ILE:HD11	1.91	0.52
1:A:214:TYR:O	1:A:218:SER:CB	2.57	0.52
1:C:382:ILE:HD11	2:C:903:Y01:HAK2	1.92	0.52
1:D:668:ASP:HA	1:D:671:VAL:HG22	1.92	0.52
1:B:382:ILE:HD11	2:B:901:Y01:HAK2	1.91	0.52
1:C:214:TYR:O	1:C:218:SER:CB	2.57	0.52
1:C:668:ASP:HA	1:C:671:VAL:HG22	1.92	0.52
1:D:223:VAL:HG23	1:D:258:VAL:HG13	1.91	0.52
1:A:668:ASP:HA	1:A:671:VAL:HG22	1.92	0.52
1:D:561:THR:O	1:D:565:ILE:HG12	2.10	0.52
1:A:387:LEU:HB3	1:A:429:ILE:HD11	1.91	0.52
1:A:223:VAL:HG23	1:A:258:VAL:HG13	1.91	0.51
1:B:223:VAL:HG23	1:B:258:VAL:HG13	1.91	0.51
1:D:382:ILE:HD11	2:D:901:Y01:HAK2	1.92	0.51
1:D:387:LEU:HB3	1:D:429:ILE:HD11	1.91	0.51
1:A:561:THR:O	1:A:565:ILE:HG12	2.11	0.51
1:B:618:GLU:HB3	1:B:620:THR:HG22	1.91	0.51
1:B:668:ASP:HA	1:B:671:VAL:HG22	1.92	0.51
1:C:223:VAL:HG23	1:C:258:VAL:HG13	1.91	0.51
1:C:549:GLU:HA	1:C:673:TRP:CZ2	2.45	0.51
1:B:387:LEU:HB3	1:B:429:ILE:HD11	1.91	0.51
1:A:549:GLU:HA	1:A:673:TRP:CZ2	2.45	0.51
1:D:138:TYR:HB3	1:D:142:GLY:O	2.11	0.51
1:A:138:TYR:HB3	1:A:142:GLY:O	2.11	0.51
1:C:561:THR:O	1:C:565:ILE:HG12	2.11	0.51
1:C:618:GLU:HB3	1:C:620:THR:HG22	1.91	0.51
1:A:214:TYR:O	1:A:218:SER:HB2	2.11	0.51
1:B:138:TYR:HB3	1:B:142:GLY:O	2.11	0.51
1:B:549:GLU:HA	1:B:673:TRP:CZ2	2.45	0.51
1:A:382:ILE:HD11	2:A:903:Y01:HAK2	1.92	0.51
1:B:561:THR:O	1:B:565:ILE:HG12	2.10	0.51
1:C:214:TYR:O	1:C:218:SER:HB2	2.11	0.51
1:D:214:TYR:O	1:D:218:SER:HB2	2.11	0.50
1:A:594:LYS:NZ	1:A:594:LYS:CB	2.73	0.50
1:C:138:TYR:HB3	1:C:142:GLY:O	2.11	0.50
1:C:557:SER:O	1:C:561:THR:HG23	2.12	0.50
1:A:557:SER:O	1:A:561:THR:HG23	2.12	0.49
1:B:557:SER:O	1:B:561:THR:HG23	2.12	0.49
1:D:557:SER:O	1:D:561:THR:HG23	2.12	0.49
1:B:214:TYR:O	1:B:218:SER:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:OD1	1:A:516:LYS:HG2	2.13	0.49
1:B:157:HIS:CD2	1:B:207:LYS:HD2	2.48	0.49
1:C:157:HIS:CD2	1:C:207:LYS:HD2	2.48	0.48
1:C:515:ASP:OD1	1:C:516:LYS:HG2	2.13	0.48
2:B:903:Y01:HAO1	2:B:903:Y01:HAP1	1.70	0.48
1:A:157:HIS:CD2	1:A:207:LYS:HD2	2.48	0.48
1:D:157:HIS:CD2	1:D:207:LYS:HD2	2.48	0.48
1:A:636:TYR:CD2	5:A:902:98R:C1	2.97	0.48
1:B:414:ILE:HD11	1:B:489:VAL:HG21	1.96	0.48
1:D:515:ASP:OD1	1:D:516:LYS:HG2	2.13	0.48
1:B:636:TYR:CD2	5:B:905:98R:C1	2.97	0.48
1:D:112:HIS:CD2	1:D:114:GLY:H	2.32	0.48
1:B:515:ASP:OD1	1:B:516:LYS:HG2	2.13	0.47
1:D:636:TYR:CD2	5:D:905:98R:C1	2.97	0.47
1:B:512:TYR:HB3	1:B:516:LYS:HB2	1.97	0.47
1:D:414:ILE:HD11	1:D:489:VAL:HG21	1.96	0.47
1:A:414:ILE:HD11	1:A:489:VAL:HG21	1.96	0.47
1:A:112:HIS:CD2	1:A:114:GLY:H	2.32	0.47
1:C:414:ILE:HD11	1:C:489:VAL:HG21	1.96	0.47
1:C:636:TYR:CD2	5:C:902:98R:C1	2.97	0.47
1:B:112:HIS:CD2	1:B:114:GLY:H	2.32	0.47
1:C:512:TYR:HB3	1:C:516:LYS:HB2	1.97	0.47
1:D:512:TYR:HB3	1:D:516:LYS:HB2	1.97	0.47
2:D:903:Y01:HAO1	2:D:903:Y01:HAP1	1.70	0.47
1:A:512:TYR:HB3	1:A:516:LYS:HB2	1.97	0.47
1:B:594:LYS:HB3	1:B:594:LYS:HZ1	1.79	0.47
1:C:112:HIS:CD2	1:C:114:GLY:H	2.32	0.47
1:D:651:LEU:HD23	1:B:657:MET:HE1	1.96	0.46
1:B:358:ALA:O	1:B:361:SER:N	2.48	0.46
1:B:590:TYR:OH	1:B:628:HIS:ND1	2.38	0.46
1:C:358:ALA:O	1:C:361:SER:N	2.48	0.46
1:B:651:LEU:HD23	1:C:657:MET:HE1	1.97	0.46
1:D:124:SER:HA	1:D:150:THR:HG22	1.98	0.46
1:B:320:THR:HG22	1:B:330:ARG:HH12	1.81	0.46
1:D:657:MET:HE1	1:A:651:LEU:HD23	1.96	0.46
1:C:521:ASP:OD1	1:C:522:PRO:HD2	2.16	0.46
1:C:594:LYS:HB3	1:C:594:LYS:HZ1	1.78	0.46
2:C:905:Y01:HAA1	2:C:905:Y01:HAJ1	1.80	0.46
1:C:115:PHE:HD2	1:C:121:LEU:HB2	1.81	0.46
1:C:294:LEU:HB3	1:C:297:VAL:HB	1.98	0.46
1:A:657:MET:HE1	1:C:651:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PHE:HD2	1:B:121:LEU:HB2	1.81	0.46
1:A:521:ASP:OD1	1:A:522:PRO:HD2	2.16	0.45
1:B:294:LEU:HB3	1:B:297:VAL:HB	1.98	0.45
4:B:904:POV:H21B	2:C:905:Y01:HAQ1	1.99	0.45
1:C:124:SER:HA	1:C:150:THR:HG22	1.97	0.45
1:D:629:LYS:HA	1:D:629:LYS:HD3	1.77	0.45
1:D:358:ALA:HB1	1:D:364:GLY:CA	2.46	0.45
2:D:903:Y01:HAQ1	4:A:901:POV:H21B	1.99	0.45
2:D:903:Y01:HBB	2:D:903:Y01:HAE2	1.66	0.45
1:C:358:ALA:HB1	1:C:364:GLY:CA	2.46	0.45
1:D:521:ASP:OD1	1:D:522:PRO:HD2	2.16	0.45
1:C:594:LYS:NZ	1:C:594:LYS:CB	2.73	0.45
2:A:905:Y01:HAO1	2:A:905:Y01:HAP1	1.71	0.45
1:B:124:SER:HA	1:B:150:THR:HG22	1.97	0.45
1:D:358:ALA:O	1:D:361:SER:N	2.48	0.45
1:D:464:MET:SD	1:D:537:SER:HA	2.57	0.45
1:A:761:THR:HB	1:A:764:GLN:H	1.82	0.45
1:C:320:THR:HG22	1:C:330:ARG:HH12	1.81	0.45
1:D:320:THR:HG22	1:D:330:ARG:HH12	1.81	0.45
4:D:904:POV:H21B	2:B:903:Y01:HAQ1	1.99	0.45
1:A:320:THR:HG22	1:A:330:ARG:HH12	1.81	0.45
1:A:358:ALA:HB1	1:A:364:GLY:CA	2.46	0.45
1:B:521:ASP:OD1	1:B:522:PRO:HD2	2.16	0.45
1:C:464:MET:SD	1:C:537:SER:HA	2.57	0.45
1:A:124:SER:HA	1:A:150:THR:HG22	1.98	0.45
1:A:358:ALA:O	1:A:361:SER:N	2.48	0.45
1:B:358:ALA:HB1	1:B:364:GLY:CA	2.46	0.45
1:B:464:MET:SD	1:B:537:SER:HA	2.57	0.45
1:A:115:PHE:HD2	1:A:121:LEU:HB2	1.81	0.45
1:A:425:THR:O	1:A:429:ILE:HG12	2.17	0.45
1:C:425:THR:O	1:C:429:ILE:HG12	2.17	0.45
1:D:294:LEU:HB3	1:D:297:VAL:HB	1.98	0.45
1:A:541:ILE:HG22	1:A:545:LEU:HG	1.99	0.45
2:A:905:Y01:HAQ1	4:C:901:POV:H21B	1.99	0.45
1:D:590:TYR:OH	1:D:628:HIS:ND1	2.38	0.44
1:D:115:PHE:HD2	1:D:121:LEU:HB2	1.81	0.44
1:A:464:MET:SD	1:A:537:SER:HA	2.57	0.44
1:B:541:ILE:HG22	1:B:545:LEU:HG	1.99	0.44
1:C:416:ARG:HG2	1:C:510:PHE:O	2.18	0.44
1:C:544:ILE:HG22	2:C:903:Y01:HAR1	1.99	0.44
1:D:693:PRO:N	1:D:694:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HB3	1:A:297:VAL:HB	1.98	0.44
1:C:629:LYS:HA	1:C:629:LYS:HD3	1.77	0.44
1:C:761:THR:HB	1:C:764:GLN:H	1.82	0.44
1:A:544:ILE:HG22	2:A:903:Y01:HAR1	1.99	0.44
1:D:425:THR:O	1:D:429:ILE:HG12	2.17	0.44
1:C:693:PRO:N	1:C:694:PRO:HD2	2.32	0.44
1:C:587:TYR:OH	1:C:635:GLY:HA3	2.18	0.44
1:D:761:THR:HB	1:D:764:GLN:H	1.82	0.44
1:B:416:ARG:HG2	1:B:510:PHE:O	2.18	0.44
1:B:425:THR:O	1:B:429:ILE:HG12	2.17	0.44
1:D:544:ILE:HG22	2:D:901:Y01:HAR1	1.99	0.44
1:B:761:THR:HB	1:B:764:GLN:H	1.82	0.44
1:C:365:LYS:HB2	1:C:365:LYS:HE3	1.80	0.44
1:D:395:ARG:NE	1:A:588:SER:OG	2.50	0.43
1:A:587:TYR:OH	1:A:635:GLY:HA3	2.18	0.43
1:D:162:GLU:O	1:D:166:MET:HG3	2.18	0.43
1:D:541:ILE:HG22	1:D:545:LEU:HG	1.99	0.43
2:D:903:Y01:HAC3	2:D:903:Y01:HAJ1	1.85	0.43
1:A:416:ARG:HG2	1:A:510:PHE:O	2.18	0.43
1:B:587:TYR:OH	1:B:635:GLY:HA3	2.18	0.43
1:C:541:ILE:HG22	1:C:545:LEU:HG	1.99	0.43
1:A:769:ARG:HH21	1:C:141:ASP:CG	2.21	0.43
1:C:162:GLU:O	1:C:166:MET:HG3	2.18	0.43
1:A:162:GLU:O	1:A:166:MET:HG3	2.18	0.43
1:A:590:TYR:OH	1:A:628:HIS:ND1	2.38	0.43
2:A:905:Y01:HAK1	4:C:901:POV:H211	2.01	0.43
1:B:162:GLU:O	1:B:166:MET:HG3	2.18	0.43
1:B:544:ILE:HG22	2:B:901:Y01:HAR1	1.99	0.43
1:A:693:PRO:N	1:A:694:PRO:HD2	2.32	0.43
1:B:123:LEU:HD23	1:B:128:GLN:HA	2.01	0.43
1:B:588:SER:OG	1:C:395:ARG:NE	2.50	0.43
1:C:123:LEU:HD23	1:C:128:GLN:HA	2.01	0.43
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.88	0.43
1:A:594:LYS:HB3	1:A:594:LYS:HZ1	1.84	0.43
1:C:40:ILE:HD12	1:C:40:ILE:H	1.84	0.43
1:D:416:ARG:HG2	1:D:510:PHE:O	2.18	0.43
2:D:903:Y01:HAK1	4:A:901:POV:H211	2.01	0.43
1:B:40:ILE:HD12	1:B:40:ILE:H	1.84	0.43
4:B:904:POV:H211	2:C:905:Y01:HAK1	2.01	0.43
4:D:904:POV:H211	2:B:903:Y01:HAK1	2.01	0.43
1:B:548:ASN:OD1	1:B:549:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:PRO:N	1:B:694:PRO:HD2	2.32	0.43
1:C:24:LEU:HD13	1:C:29:GLU:HB2	2.01	0.43
1:D:587:TYR:OH	1:D:635:GLY:HA3	2.18	0.42
1:D:141:ASP:CG	1:B:769:ARG:HH21	2.21	0.42
1:D:336:ILE:O	1:D:340:VAL:HG23	2.19	0.42
1:A:331:GLU:HG3	1:C:181:PHE:HE1	1.85	0.42
1:C:414:ILE:HG22	1:C:416:ARG:H	1.84	0.42
2:C:905:Y01:HAP1	2:C:905:Y01:HAO1	1.71	0.42
1:D:40:ILE:H	1:D:40:ILE:HD12	1.84	0.42
1:D:548:ASN:OD1	1:D:549:GLU:N	2.52	0.42
1:A:414:ILE:HG22	1:A:416:ARG:H	1.84	0.42
1:B:336:ILE:O	1:B:340:VAL:HG23	2.19	0.42
1:D:123:LEU:HD23	1:D:128:GLN:HA	2.01	0.42
1:A:40:ILE:HD12	1:A:40:ILE:H	1.84	0.42
1:A:336:ILE:O	1:A:340:VAL:HG23	2.19	0.42
1:A:432:TRP:CH2	1:A:694:PRO:HG3	2.55	0.42
1:C:548:ASN:OD1	1:C:549:GLU:N	2.52	0.42
1:C:590:TYR:OH	1:C:628:HIS:ND1	2.38	0.42
1:D:146:SER:HA	1:B:266:ARG:HD2	2.01	0.42
1:D:432:TRP:CH2	1:D:694:PRO:HG3	2.55	0.42
1:D:588:SER:OG	1:B:395:ARG:NE	2.50	0.42
1:A:207:LYS:HB2	1:A:207:LYS:HE3	1.80	0.42
1:D:769:ARG:HH21	1:A:141:ASP:CG	2.21	0.42
2:D:903:Y01:HAJ1	2:D:903:Y01:HAA1	1.80	0.42
1:A:123:LEU:HD23	1:A:128:GLN:HA	2.01	0.42
1:A:545:LEU:HD23	1:A:545:LEU:HA	1.88	0.42
1:C:336:ILE:O	1:C:340:VAL:HG23	2.19	0.42
1:A:24:LEU:HD13	1:A:29:GLU:HB2	2.01	0.42
1:A:266:ARG:HD2	1:C:146:SER:HA	2.01	0.42
1:A:451:GLU:HA	1:A:454:LEU:HD12	2.01	0.42
1:D:414:ILE:HG22	1:D:416:ARG:H	1.84	0.42
1:B:768:LYS:HB2	1:B:768:LYS:HE3	1.83	0.42
2:B:903:Y01:HAA1	2:B:903:Y01:HAJ1	1.80	0.42
1:C:432:TRP:CH2	1:C:694:PRO:HG3	2.55	0.42
2:C:905:Y01:HAE2	2:C:905:Y01:HBB	1.67	0.42
1:D:55:VAL:HG11	1:D:84:LYS:HG3	2.02	0.42
1:A:395:ARG:NE	1:C:588:SER:OG	2.50	0.42
1:B:365:LYS:HB2	1:B:365:LYS:HE3	1.80	0.42
1:C:580:MET:SD	1:C:606:PHE:HB2	2.60	0.42
1:D:554:LEU:HD21	1:A:571:LEU:CD1	2.49	0.41
1:B:24:LEU:HD13	1:B:29:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.88	0.41
1:B:580:MET:SD	1:B:606:PHE:HB2	2.60	0.41
1:B:629:LYS:HD3	1:B:629:LYS:HA	1.77	0.41
2:B:903:Y01:HAE2	2:B:903:Y01:HBB	1.66	0.41
1:C:381:PHE:CE1	1:C:540:ARG:HB2	2.55	0.41
1:D:266:ARG:HD2	1:A:146:SER:HA	2.02	0.41
1:D:571:LEU:CD1	1:B:554:LEU:HD21	2.49	0.41
1:B:146:SER:HA	1:C:266:ARG:HD2	2.01	0.41
1:B:571:LEU:CD1	1:C:554:LEU:HD21	2.49	0.41
1:D:331:GLU:HG3	1:A:181:PHE:HE1	1.85	0.41
1:A:548:ASN:OD1	1:A:549:GLU:N	2.52	0.41
1:B:414:ILE:HG22	1:B:416:ARG:H	1.84	0.41
1:A:55:VAL:HG11	1:A:84:LYS:HG3	2.02	0.41
1:A:381:PHE:CE1	1:A:540:ARG:HB2	2.55	0.41
1:A:629:LYS:HA	1:A:629:LYS:HD3	1.77	0.41
1:B:432:TRP:CH2	1:B:694:PRO:HG3	2.55	0.41
1:D:451:GLU:HA	1:D:454:LEU:HD12	2.02	0.41
1:A:580:MET:SD	1:A:606:PHE:HB2	2.60	0.41
1:B:274:ILE:HD11	1:B:770:LEU:HD13	2.02	0.41
1:B:381:PHE:CE1	1:B:540:ARG:HB2	2.55	0.41
1:C:274:ILE:HD11	1:C:770:LEU:HD13	2.02	0.41
1:D:381:PHE:CE1	1:D:540:ARG:HB2	2.55	0.41
1:D:626:TYR:CZ	1:B:515:ASP:HB3	2.56	0.41
1:D:768:LYS:HE3	1:D:768:LYS:HB2	1.83	0.41
1:B:181:PHE:HE1	1:C:331:GLU:HG3	1.85	0.41
1:B:451:GLU:HA	1:B:454:LEU:HD12	2.01	0.41
1:D:474:ALA:HB2	2:D:903:Y01:HAD1	2.02	0.41
1:A:474:ALA:HB2	2:A:905:Y01:HAD1	2.02	0.41
1:B:141:ASP:CG	1:C:769:ARG:HH21	2.21	0.41
1:C:316:GLN:O	1:C:320:THR:HG23	2.21	0.41
1:C:265:CYS:SG	1:C:274:ILE:HD12	2.61	0.41
1:C:771:ILE:HD13	1:C:771:ILE:HA	1.89	0.41
1:D:24:LEU:HD13	1:D:29:GLU:HB2	2.01	0.41
1:D:265:CYS:SG	1:D:274:ILE:HD12	2.61	0.41
1:D:270:GLU:OE1	1:D:773:ARG:NH1	2.54	0.41
1:D:515:ASP:HB3	1:A:626:TYR:CZ	2.56	0.41
1:B:112:HIS:HD2	1:B:114:GLY:H	1.69	0.41
1:C:55:VAL:HG11	1:C:84:LYS:HG3	2.02	0.41
1:C:270:GLU:OE1	1:C:773:ARG:NH1	2.54	0.41
1:C:451:GLU:HA	1:C:454:LEU:HD12	2.01	0.41
1:D:274:ILE:HD11	1:D:770:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:GLN:O	1:D:320:THR:HG23	2.21	0.41
1:D:580:MET:SD	1:D:606:PHE:HB2	2.60	0.41
1:A:274:ILE:HD11	1:A:770:LEU:HD13	2.02	0.41
1:B:55:VAL:HG11	1:B:84:LYS:HG3	2.02	0.41
1:B:474:ALA:HB2	2:B:903:Y01:HAD1	2.02	0.41
1:B:626:TYR:CZ	1:C:515:ASP:HB3	2.56	0.41
1:D:594:LYS:HB3	1:D:594:LYS:HZ1	1.86	0.40
1:A:569:MET:O	1:A:573:ILE:HG13	2.22	0.40
1:C:609:LEU:HD23	1:C:609:LEU:HA	1.82	0.40
2:C:905:Y01:HAJ1	2:C:905:Y01:HAC3	1.85	0.40
1:D:181:PHE:HE1	1:B:331:GLU:HG3	1.85	0.40
2:D:901:Y01:HAS1	2:D:901:Y01:HAT1	1.96	0.40
1:A:554:LEU:HD21	1:C:571:LEU:CD1	2.49	0.40
1:B:626:TYR:CE2	1:C:515:ASP:HB3	2.57	0.40
1:C:545:LEU:HD23	1:C:545:LEU:HA	1.88	0.40
1:A:265:CYS:SG	1:A:274:ILE:HD12	2.61	0.40
1:A:316:GLN:O	1:A:320:THR:HG23	2.21	0.40
1:A:413:GLN:HA	1:A:486:GLN:OE1	2.22	0.40
1:B:96:LEU:HD12	1:B:144:ARG:NH2	2.36	0.40
1:B:413:GLN:HA	1:B:486:GLN:OE1	2.22	0.40
1:C:96:LEU:HD12	1:C:144:ARG:NH2	2.36	0.40
1:D:96:LEU:HD12	1:D:144:ARG:NH2	2.36	0.40
1:D:626:TYR:CE2	1:B:515:ASP:HB3	2.57	0.40
1:A:492:TYR:HD1	1:A:492:TYR:HA	1.78	0.40
1:A:515:ASP:HB3	1:C:626:TYR:CZ	2.56	0.40
1:B:265:CYS:SG	1:B:274:ILE:HD12	2.61	0.40
1:C:474:ALA:HB2	2:C:905:Y01:HAD1	2.02	0.40
1:D:515:ASP:HB3	1:A:626:TYR:CE2	2.57	0.40
1:A:270:GLU:OE1	1:A:773:ARG:NH1	2.54	0.40
1:B:316:GLN:O	1:B:320:THR:HG23	2.20	0.40
1:B:602:VAL:HG12	1:C:396:PHE:O	2.22	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	675/836 (81%)	658 (98%)	16 (2%)	1 (0%)	51	83
1	B	675/836 (81%)	658 (98%)	16 (2%)	1 (0%)	51	83
1	C	675/836 (81%)	658 (98%)	16 (2%)	1 (0%)	51	83
1	D	675/836 (81%)	658 (98%)	16 (2%)	1 (0%)	51	83
All	All	2700/3344 (81%)	2632 (98%)	64 (2%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	760	PRO
1	A	760	PRO
1	B	760	PRO
1	C	760	PRO

### 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	577/744 (78%)	573 (99%)	4 (1%)	84	94
1	B	577/744 (78%)	573 (99%)	4 (1%)	84	94
1	C	577/744 (78%)	573 (99%)	4 (1%)	84	94
1	D	577/744 (78%)	573 (99%)	4 (1%)	84	94
All	All	2308/2976 (78%)	2292 (99%)	16 (1%)	84	94

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

Mol	Chain	Res	Type
1	D	326	LEU
1	D	464	MET
1	D	554	LEU
1	D	639	TYR

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	464	MET
1	A	554	LEU
1	A	639	TYR
1	B	326	LEU
1	B	464	MET
1	B	554	LEU
1	B	639	TYR
1	C	326	LEU
1	C	464	MET
1	C	554	LEU
1	C	639	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	112	HIS
1	D	413	GLN
1	D	659	ASN
1	A	112	HIS
1	A	413	GLN
1	A	659	ASN
1	B	112	HIS
1	B	413	GLN
1	B	659	ASN
1	C	112	HIS
1	C	413	GLN
1	C	659	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
4	POV	B	904	-	35,35,51	1.13	3 (8%)	37,37,59	1.28	3 (8%)
2	Y01	D	901	-	38,38,38	0.93	1 (2%)	57,57,57	1.85	13 (22%)
4	POV	C	901	-	35,35,51	1.13	3 (8%)	37,37,59	1.28	3 (8%)
5	98R	D	905	-	27,27,43	1.18	2 (7%)	27,28,45	1.41	4 (14%)
5	98R	A	902	-	27,27,43	1.18	2 (7%)	27,28,45	1.41	4 (14%)
2	Y01	B	901	-	38,38,38	0.93	1 (2%)	57,57,57	1.84	13 (22%)
2	Y01	B	903	-	38,38,38	0.96	1 (2%)	57,57,57	1.54	10 (17%)
4	POV	A	901	-	35,35,51	1.12	3 (8%)	37,37,59	1.28	3 (8%)
5	98R	C	902	-	27,27,43	1.18	2 (7%)	27,28,45	1.41	4 (14%)
2	Y01	C	903	-	38,38,38	0.94	1 (2%)	57,57,57	1.84	13 (22%)
5	98R	B	905	-	27,27,43	1.19	2 (7%)	27,28,45	1.41	4 (14%)
2	Y01	D	903	-	38,38,38	0.97	1 (2%)	57,57,57	1.54	10 (17%)
2	Y01	A	903	-	38,38,38	0.94	1 (2%)	57,57,57	1.84	13 (22%)
4	POV	D	904	-	35,35,51	1.13	3 (8%)	37,37,59	1.28	3 (8%)
2	Y01	C	905	-	38,38,38	0.96	1 (2%)	57,57,57	1.54	10 (17%)
2	Y01	A	905	-	38,38,38	0.97	1 (2%)	57,57,57	1.54	10 (17%)

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
4	POV	B	904	-	-	11/36/36/55	-
2	Y01	D	901	-	-	11/19/77/77	0/4/4/4
4	POV	C	901	-	-	11/36/36/55	-
5	98R	D	905	-	-	11/27/27/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	98R	A	902	-	-	11/27/27/45	-
2	Y01	B	901	-	-	11/19/77/77	0/4/4/4
2	Y01	B	903	-	-	9/19/77/77	0/4/4/4
4	POV	A	901	-	-	11/36/36/55	-
5	98R	C	902	-	-	11/27/27/45	-
2	Y01	C	903	-	-	11/19/77/77	0/4/4/4
5	98R	B	905	-	-	11/27/27/45	-
2	Y01	D	903	-	-	9/19/77/77	0/4/4/4
2	Y01	A	903	-	-	11/19/77/77	0/4/4/4
4	POV	D	904	-	-	11/36/36/55	-
2	Y01	C	905	-	-	9/19/77/77	0/4/4/4
2	Y01	A	905	-	-	9/19/77/77	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	POV	O31-C31	4.24	1.45	1.33
4	A	901	POV	O31-C31	4.24	1.45	1.33
4	B	904	POV	O31-C31	4.24	1.45	1.33
4	C	901	POV	O31-C31	4.24	1.45	1.33
2	D	901	Y01	OAW-CAY	4.23	1.46	1.34
2	A	903	Y01	OAW-CAY	4.23	1.46	1.34
2	B	901	Y01	OAW-CAY	4.23	1.46	1.34
2	C	903	Y01	OAW-CAY	4.23	1.46	1.34
4	A	901	POV	O21-C21	4.18	1.46	1.34
4	B	904	POV	O21-C21	4.18	1.46	1.34
4	D	904	POV	O21-C21	4.17	1.46	1.34
4	C	901	POV	O21-C21	4.17	1.46	1.34
2	D	903	Y01	OAW-CAY	4.15	1.46	1.34
2	A	905	Y01	OAW-CAY	4.15	1.46	1.34
2	B	903	Y01	OAW-CAY	4.15	1.46	1.34
2	C	905	Y01	OAW-CAY	4.15	1.46	1.34
5	D	905	98R	O3-C11	4.08	1.45	1.33
5	A	902	98R	O3-C11	4.08	1.45	1.33
5	B	905	98R	O3-C11	4.08	1.45	1.33
5	C	902	98R	O3-C11	4.08	1.45	1.33
5	D	905	98R	O2-C31	3.96	1.45	1.34
5	A	902	98R	O2-C31	3.96	1.45	1.34
5	B	905	98R	O2-C31	3.96	1.45	1.34
5	C	902	98R	O2-C31	3.96	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	POV	O21-C2	-2.30	1.43	1.47
4	B	904	POV	O21-C2	-2.30	1.43	1.47
4	C	901	POV	O21-C2	-2.30	1.43	1.47
4	A	901	POV	O21-C2	-2.27	1.43	1.47

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	Y01	CAV-CAZ-CBH	6.93	125.62	116.42
2	A	903	Y01	CAV-CAZ-CBH	6.90	125.59	116.42
2	C	903	Y01	CAV-CAZ-CBH	6.90	125.59	116.42
2	B	901	Y01	CAV-CAZ-CBH	6.88	125.57	116.42
5	D	905	98R	O2-C31-C32	4.37	120.92	111.50
5	A	902	98R	O2-C31-C32	4.37	120.92	111.50
5	B	905	98R	O2-C31-C32	4.37	120.92	111.50
5	C	902	98R	O2-C31-C32	4.37	120.92	111.50
2	D	901	Y01	OAW-CAY-CAM	4.21	120.58	111.50
2	A	903	Y01	OAW-CAY-CAM	4.21	120.58	111.50
2	B	901	Y01	OAW-CAY-CAM	4.21	120.58	111.50
2	C	903	Y01	OAW-CAY-CAM	4.20	120.56	111.50
2	A	905	Y01	CAV-CAZ-CBH	4.14	121.92	116.42
2	B	903	Y01	CAV-CAZ-CBH	4.14	121.92	116.42
2	C	905	Y01	CAV-CAZ-CBH	4.14	121.92	116.42
2	D	903	Y01	CAV-CAZ-CBH	4.14	121.92	116.42
4	B	904	POV	C2-O21-C21	-4.06	112.65	117.88
4	A	901	POV	C2-O21-C21	-4.04	112.68	117.88
4	D	904	POV	C2-O21-C21	-4.04	112.69	117.88
4	C	901	POV	C2-O21-C21	-4.04	112.69	117.88
2	D	901	Y01	CBH-CAZ-CAI	-3.91	116.92	122.90
2	A	903	Y01	CBH-CAZ-CAI	-3.90	116.93	122.90
2	C	903	Y01	CBH-CAZ-CAI	-3.90	116.93	122.90
2	D	903	Y01	OAW-CAY-CAM	3.89	119.89	111.50
2	A	905	Y01	OAW-CAY-CAM	3.89	119.89	111.50
2	B	903	Y01	OAW-CAY-CAM	3.89	119.89	111.50
2	C	905	Y01	OAW-CAY-CAM	3.89	119.89	111.50
2	B	901	Y01	CBH-CAZ-CAI	-3.88	116.96	122.90
4	D	904	POV	O21-C21-C22	3.80	119.68	111.50
4	C	901	POV	O21-C21-C22	3.80	119.68	111.50
4	A	901	POV	O21-C21-C22	3.79	119.66	111.50
4	B	904	POV	O21-C21-C22	3.79	119.66	111.50
2	D	903	Y01	CBI-CBE-CBB	-3.73	113.64	119.49
2	A	905	Y01	CBI-CBE-CBB	-3.73	113.64	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	Y01	CBI-CBE-CBB	-3.73	113.64	119.49
2	C	905	Y01	CBI-CBE-CBB	-3.73	113.65	119.49
2	D	901	Y01	CAK-CAI-CAZ	-3.45	118.70	125.06
2	A	903	Y01	CAK-CAI-CAZ	-3.45	118.70	125.06
2	B	901	Y01	CAK-CAI-CAZ	-3.45	118.70	125.06
2	C	903	Y01	CAK-CAI-CAZ	-3.45	118.70	125.06
2	C	905	Y01	CBG-CBI-CBE	3.25	103.92	100.07
2	A	905	Y01	CBG-CBI-CBE	3.24	103.91	100.07
2	D	903	Y01	CBG-CBI-CBE	3.22	103.89	100.07
2	B	903	Y01	CBG-CBI-CBE	3.22	103.89	100.07
2	B	901	Y01	CBD-CAK-CAI	-3.04	108.36	112.73
2	D	901	Y01	CBD-CAK-CAI	-3.01	108.41	112.73
2	A	903	Y01	CBD-CAK-CAI	-3.01	108.41	112.73
2	C	903	Y01	CBD-CAK-CAI	-3.01	108.41	112.73
5	D	905	98R	O3-C11-C12	2.81	120.71	111.91
5	A	902	98R	O3-C11-C12	2.81	120.71	111.91
5	B	905	98R	O3-C11-C12	2.81	120.71	111.91
5	C	902	98R	O3-C11-C12	2.81	120.71	111.91
4	D	904	POV	O31-C31-C32	2.73	120.47	111.91
4	A	901	POV	O31-C31-C32	2.73	120.47	111.91
4	B	904	POV	O31-C31-C32	2.73	120.47	111.91
4	C	901	POV	O31-C31-C32	2.73	120.47	111.91
2	B	901	Y01	CAT-CBH-CBF	2.70	112.50	108.73
2	D	901	Y01	CAT-CBH-CBF	2.69	112.49	108.73
2	C	903	Y01	CAT-CBH-CBF	2.69	112.48	108.73
2	A	903	Y01	CAT-CBH-CBF	2.68	112.47	108.73
2	A	905	Y01	CBD-CAK-CAI	-2.60	109.00	112.73
2	B	903	Y01	CBD-CAK-CAI	-2.60	109.00	112.73
2	C	905	Y01	CBD-CAK-CAI	-2.60	109.00	112.73
2	D	903	Y01	CBD-CAK-CAI	-2.59	109.01	112.73
2	A	903	Y01	CBC-OAW-CAY	-2.44	111.78	117.79
2	B	901	Y01	CBC-OAW-CAY	-2.44	111.80	117.79
2	D	901	Y01	CBC-OAW-CAY	-2.43	111.80	117.79
2	C	903	Y01	CBC-OAW-CAY	-2.43	111.81	117.79
2	A	903	Y01	CBC-CAV-CAZ	2.38	115.22	111.52
2	B	901	Y01	CBC-CAV-CAZ	2.38	115.22	111.52
2	D	901	Y01	CBH-CBF-CBD	-2.38	109.17	112.73
2	B	901	Y01	CBF-CBH-CAZ	-2.38	105.93	109.65
2	A	903	Y01	CBH-CBF-CBD	-2.37	109.17	112.73
2	B	901	Y01	CBH-CBF-CBD	-2.37	109.17	112.73
2	C	903	Y01	CBH-CBF-CBD	-2.37	109.17	112.73
2	D	901	Y01	CBC-CAV-CAZ	2.37	115.20	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	903	Y01	CBC-CAV-CAZ	2.37	115.19	111.52
2	D	901	Y01	CBF-CBH-CAZ	-2.35	105.97	109.65
2	A	903	Y01	CBF-CBH-CAZ	-2.34	105.98	109.65
2	C	903	Y01	CBF-CBH-CAZ	-2.34	105.98	109.65
2	D	903	Y01	CBI-CBG-CBD	-2.28	111.01	114.38
2	B	903	Y01	CBI-CBG-CBD	-2.26	111.04	114.38
2	A	905	Y01	CBI-CBG-CBD	-2.24	111.06	114.38
2	C	905	Y01	CAV-CAZ-CAI	-2.24	117.38	120.61
2	B	903	Y01	CBC-OAW-CAY	-2.24	112.28	117.79
2	C	905	Y01	CBI-CBG-CBD	-2.24	111.07	114.38
2	D	903	Y01	CBC-OAW-CAY	-2.23	112.31	117.79
2	A	905	Y01	CBC-OAW-CAY	-2.23	112.31	117.79
2	C	905	Y01	CBC-OAW-CAY	-2.23	112.31	117.79
2	D	903	Y01	CAV-CAZ-CAI	-2.22	117.41	120.61
2	A	905	Y01	CAV-CAZ-CAI	-2.22	117.41	120.61
2	B	903	Y01	CAV-CAZ-CAI	-2.22	117.41	120.61
2	C	905	Y01	CAS-CAU-CBI	-2.21	109.00	112.78
2	B	903	Y01	CAS-CAU-CBI	-2.20	109.01	112.78
2	D	903	Y01	CAS-CAU-CBI	-2.19	109.02	112.78
2	A	905	Y01	CAS-CAU-CBI	-2.19	109.02	112.78
2	D	901	Y01	CAV-CAZ-CAI	-2.19	117.46	120.61
2	A	903	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
2	B	901	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
2	C	903	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
2	C	903	Y01	CAT-CBH-CAZ	2.13	112.64	108.75
2	B	901	Y01	CAT-CBH-CAZ	2.12	112.63	108.75
2	A	903	Y01	CAT-CBH-CAZ	2.11	112.62	108.75
5	D	905	98R	O2-C31-O31	-2.10	118.62	123.70
5	A	902	98R	O2-C31-O31	-2.10	118.62	123.70
2	D	901	Y01	CAT-CBH-CAZ	2.10	112.60	108.75
5	B	905	98R	O2-C31-O31	-2.10	118.62	123.70
5	C	902	98R	O2-C31-O31	-2.10	118.62	123.70
5	D	905	98R	C2-O2-C31	-2.09	112.66	117.79
5	A	902	98R	C2-O2-C31	-2.08	112.67	117.79
5	B	905	98R	C2-O2-C31	-2.08	112.67	117.79
5	C	902	98R	C2-O2-C31	-2.08	112.67	117.79
2	D	901	Y01	OAH-CAX-CAL	2.08	120.70	114.03
2	A	903	Y01	OAH-CAX-CAL	2.06	120.66	114.03
2	B	901	Y01	OAH-CAX-CAL	2.06	120.66	114.03
2	C	903	Y01	OAH-CAX-CAL	2.05	120.62	114.03
2	D	903	Y01	OAH-CAX-CAL	2.02	120.50	114.03
2	A	905	Y01	OAH-CAX-CAL	2.02	120.50	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	Y01	OAH-CAX-CAL	2.02	120.50	114.03
2	C	905	Y01	OAH-CAX-CAL	2.01	120.49	114.03

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	905	98R	O3P-C1-C2-O2
5	D	905	98R	C32-C31-O2-C2
5	A	902	98R	O3P-C1-C2-O2
5	A	902	98R	C32-C31-O2-C2
5	B	905	98R	O3P-C1-C2-O2
5	B	905	98R	C32-C31-O2-C2
5	C	902	98R	O3P-C1-C2-O2
5	C	902	98R	C32-C31-O2-C2
5	D	905	98R	C12-C11-O3-C3
5	A	902	98R	C12-C11-O3-C3
5	B	905	98R	C12-C11-O3-C3
5	C	902	98R	C12-C11-O3-C3
5	D	905	98R	O11-C11-O3-C3
5	A	902	98R	O11-C11-O3-C3
5	B	905	98R	O11-C11-O3-C3
5	C	902	98R	O11-C11-O3-C3
5	D	905	98R	O31-C31-O2-C2
5	A	902	98R	O31-C31-O2-C2
5	B	905	98R	O31-C31-O2-C2
5	C	902	98R	O31-C31-O2-C2
2	D	901	Y01	CAC-CBB-CBE-CAP
2	A	903	Y01	CAC-CBB-CBE-CAP
2	B	901	Y01	CAC-CBB-CBE-CAP
2	C	903	Y01	CAC-CBB-CBE-CAP
2	D	901	Y01	CAC-CBB-CBE-CBI
2	A	903	Y01	CAC-CBB-CBE-CBI
2	B	901	Y01	CAC-CBB-CBE-CBI
2	C	903	Y01	CAC-CBB-CBE-CBI
2	D	901	Y01	CAX-CAL-CAM-CAY
2	A	903	Y01	CAX-CAL-CAM-CAY
2	B	901	Y01	CAX-CAL-CAM-CAY
2	C	903	Y01	CAX-CAL-CAM-CAY
2	D	901	Y01	CAO-CBB-CBE-CAP
2	A	903	Y01	CAO-CBB-CBE-CAP
2	B	901	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	C	903	Y01	CAO-CBB-CBE-CAP
2	D	901	Y01	CAO-CBB-CBE-CBI
2	A	903	Y01	CAO-CBB-CBE-CBI
2	B	901	Y01	CAO-CBB-CBE-CBI
2	C	903	Y01	CAO-CBB-CBE-CBI
2	D	901	Y01	CAM-CAY-OAW-CBC
2	A	903	Y01	CAM-CAY-OAW-CBC
2	B	901	Y01	CAM-CAY-OAW-CBC
2	C	903	Y01	CAM-CAY-OAW-CBC
2	D	903	Y01	CAO-CBB-CBE-CBI
2	A	905	Y01	CAO-CBB-CBE-CBI
2	B	903	Y01	CAO-CBB-CBE-CBI
2	C	905	Y01	CAO-CBB-CBE-CBI
2	D	901	Y01	OAG-CAY-OAW-CBC
2	A	903	Y01	OAG-CAY-OAW-CBC
2	B	901	Y01	OAG-CAY-OAW-CBC
2	C	903	Y01	OAG-CAY-OAW-CBC
4	D	904	POV	C24-C25-C26-C27
4	A	901	POV	C24-C25-C26-C27
4	B	904	POV	C24-C25-C26-C27
4	C	901	POV	C24-C25-C26-C27
4	D	904	POV	C22-C21-O21-C2
4	A	901	POV	C22-C21-O21-C2
4	B	904	POV	C22-C21-O21-C2
4	C	901	POV	C22-C21-O21-C2
2	D	901	Y01	CAJ-CAN-CBA-CAB
2	A	903	Y01	CAJ-CAN-CBA-CAB
2	B	901	Y01	CAJ-CAN-CBA-CAB
2	C	903	Y01	CAJ-CAN-CBA-CAB
4	D	904	POV	O22-C21-O21-C2
4	A	901	POV	O22-C21-O21-C2
4	B	904	POV	O22-C21-O21-C2
4	C	901	POV	O22-C21-O21-C2
2	D	903	Y01	CAC-CBB-CBE-CBI
2	A	905	Y01	CAC-CBB-CBE-CBI
2	B	903	Y01	CAC-CBB-CBE-CBI
2	C	905	Y01	CAC-CBB-CBE-CBI
4	D	904	POV	C33-C34-C35-C36
4	A	901	POV	C33-C34-C35-C36
4	B	904	POV	C33-C34-C35-C36
4	C	901	POV	C33-C34-C35-C36
2	D	903	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	A	905	Y01	CAM-CAY-OAW-CBC
2	B	903	Y01	CAM-CAY-OAW-CBC
2	C	905	Y01	CAM-CAY-OAW-CBC
2	D	901	Y01	CAJ-CAN-CBA-CAA
2	A	903	Y01	CAJ-CAN-CBA-CAA
2	B	901	Y01	CAJ-CAN-CBA-CAA
2	C	903	Y01	CAJ-CAN-CBA-CAA
2	D	903	Y01	OAG-CAY-OAW-CBC
2	A	905	Y01	OAG-CAY-OAW-CBC
2	B	903	Y01	OAG-CAY-OAW-CBC
2	C	905	Y01	OAG-CAY-OAW-CBC
5	D	905	98R	C31-C32-C33-C34
5	A	902	98R	C31-C32-C33-C34
5	B	905	98R	C31-C32-C33-C34
5	C	902	98R	C31-C32-C33-C34
4	D	904	POV	C311-C310-C39-C38
4	A	901	POV	C311-C310-C39-C38
4	B	904	POV	C311-C310-C39-C38
4	C	901	POV	C311-C310-C39-C38
5	D	905	98R	C35-C36-C37-C38
5	A	902	98R	C35-C36-C37-C38
5	B	905	98R	C35-C36-C37-C38
5	C	902	98R	C35-C36-C37-C38
2	D	903	Y01	CAO-CBB-CBE-CAP
2	A	905	Y01	CAO-CBB-CBE-CAP
2	B	903	Y01	CAO-CBB-CBE-CAP
2	C	905	Y01	CAO-CBB-CBE-CAP
2	D	903	Y01	CAC-CBB-CBE-CAP
2	A	905	Y01	CAC-CBB-CBE-CAP
2	B	903	Y01	CAC-CBB-CBE-CAP
2	C	905	Y01	CAC-CBB-CBE-CAP
4	D	904	POV	O21-C2-C3-O31
4	A	901	POV	O21-C2-C3-O31
4	B	904	POV	O21-C2-C3-O31
4	C	901	POV	O21-C2-C3-O31
5	D	905	98R	O3P-C1-C2-C3
5	A	902	98R	O3P-C1-C2-C3
5	B	905	98R	O3P-C1-C2-C3
5	C	902	98R	O3P-C1-C2-C3
4	A	901	POV	C39-C310-C311-C312
4	C	901	POV	C39-C310-C311-C312
4	D	904	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
4	B	904	POV	C39-C310-C311-C312
5	D	905	98R	C32-C33-C34-C35
5	A	902	98R	C32-C33-C34-C35
5	B	905	98R	C32-C33-C34-C35
5	C	902	98R	C32-C33-C34-C35
4	D	904	POV	C22-C23-C24-C25
4	A	901	POV	C22-C23-C24-C25
4	B	904	POV	C22-C23-C24-C25
4	C	901	POV	C22-C23-C24-C25
2	D	903	Y01	CAM-CAL-CAX-OAH
2	A	905	Y01	CAM-CAL-CAX-OAH
2	B	903	Y01	CAM-CAL-CAX-OAH
2	C	905	Y01	CAM-CAL-CAX-OAH
4	D	904	POV	C34-C35-C36-C37
2	D	901	Y01	CAM-CAL-CAX-OAH
2	A	903	Y01	CAM-CAL-CAX-OAH
2	B	901	Y01	CAM-CAL-CAX-OAH
2	C	903	Y01	CAM-CAL-CAX-OAH
4	A	901	POV	C34-C35-C36-C37
4	B	904	POV	C34-C35-C36-C37
4	C	901	POV	C34-C35-C36-C37
2	D	903	Y01	CAM-CAL-CAX-OAF
2	A	905	Y01	CAM-CAL-CAX-OAF
2	B	903	Y01	CAM-CAL-CAX-OAF
2	C	905	Y01	CAM-CAL-CAX-OAF
2	D	901	Y01	CAM-CAL-CAX-OAF
2	C	903	Y01	CAM-CAL-CAX-OAF
2	A	903	Y01	CAM-CAL-CAX-OAF
2	B	901	Y01	CAM-CAL-CAX-OAF
5	D	905	98R	C38-C39-C40-C41
5	A	902	98R	C38-C39-C40-C41
5	B	905	98R	C38-C39-C40-C41
5	C	902	98R	C38-C39-C40-C41
4	D	904	POV	O21-C21-C22-C23
4	A	901	POV	O21-C21-C22-C23
4	B	904	POV	O21-C21-C22-C23
4	C	901	POV	O21-C21-C22-C23
4	D	904	POV	O22-C21-C22-C23
4	A	901	POV	O22-C21-C22-C23
4	B	904	POV	O22-C21-C22-C23
4	C	901	POV	O22-C21-C22-C23
5	D	905	98R	O2-C31-C32-C33

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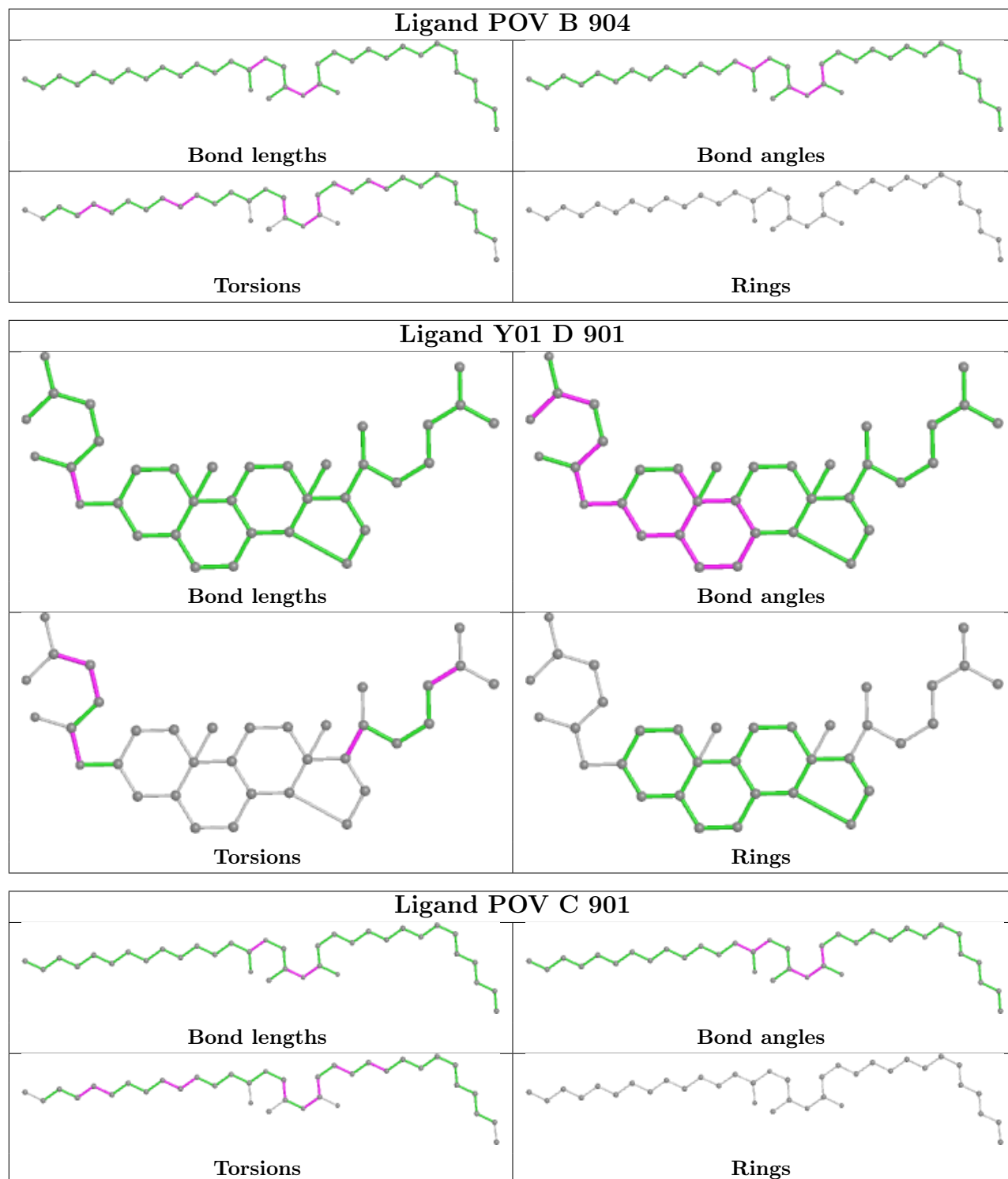
Mol	Chain	Res	Type	Atoms
5	A	902	98R	O2-C31-C32-C33
2	D	903	Y01	CAL-CAM-CAY-OAW
2	A	905	Y01	CAL-CAM-CAY-OAW
2	B	903	Y01	CAL-CAM-CAY-OAW
2	C	905	Y01	CAL-CAM-CAY-OAW
5	B	905	98R	O2-C31-C32-C33
5	C	902	98R	O2-C31-C32-C33

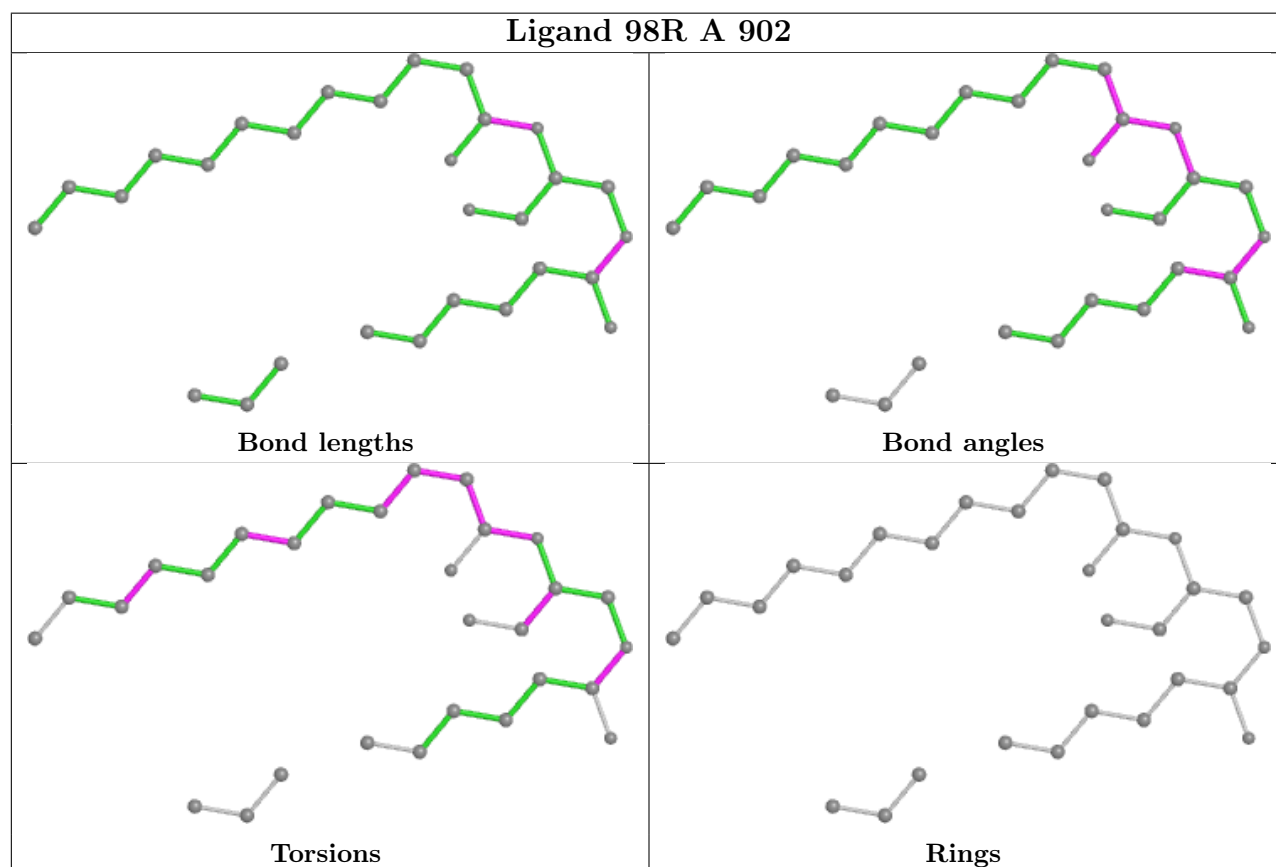
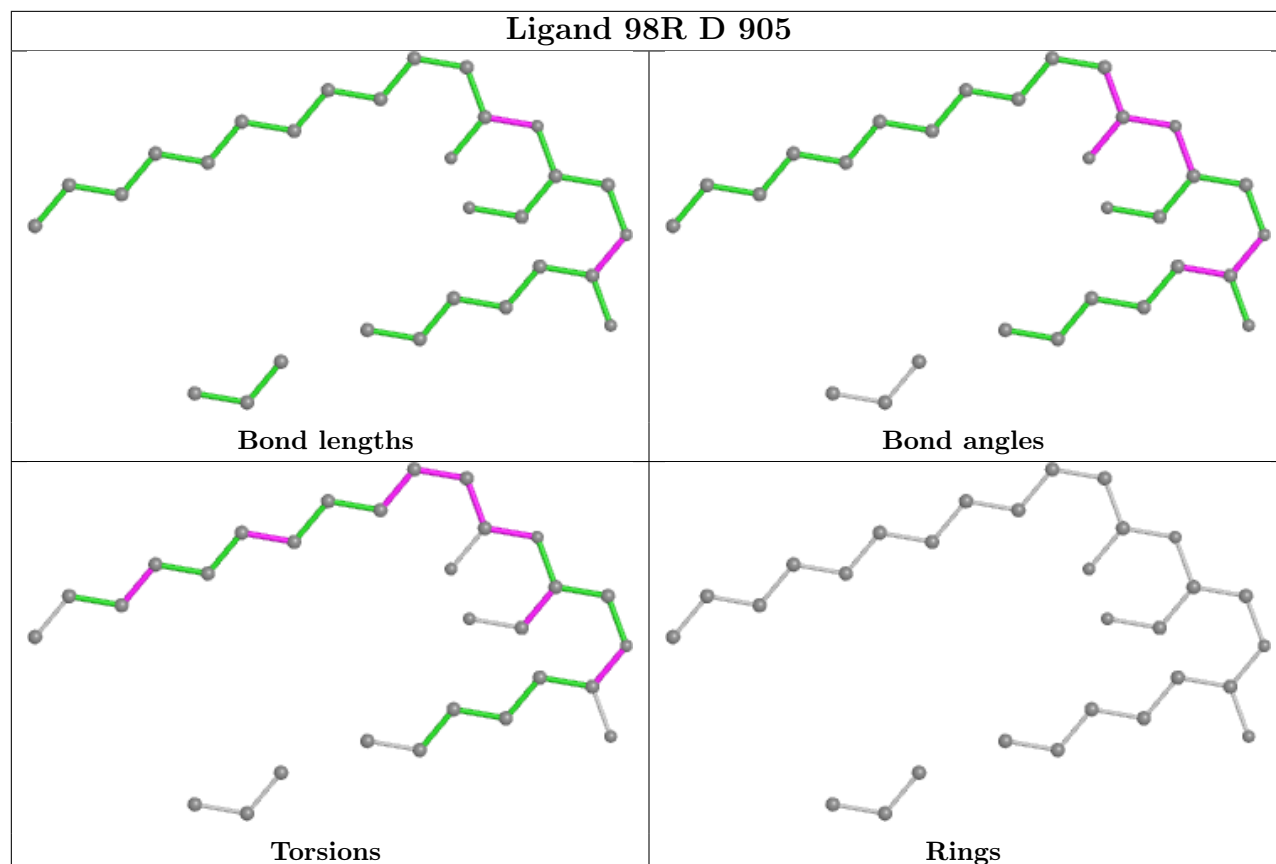
There are no ring outliers.

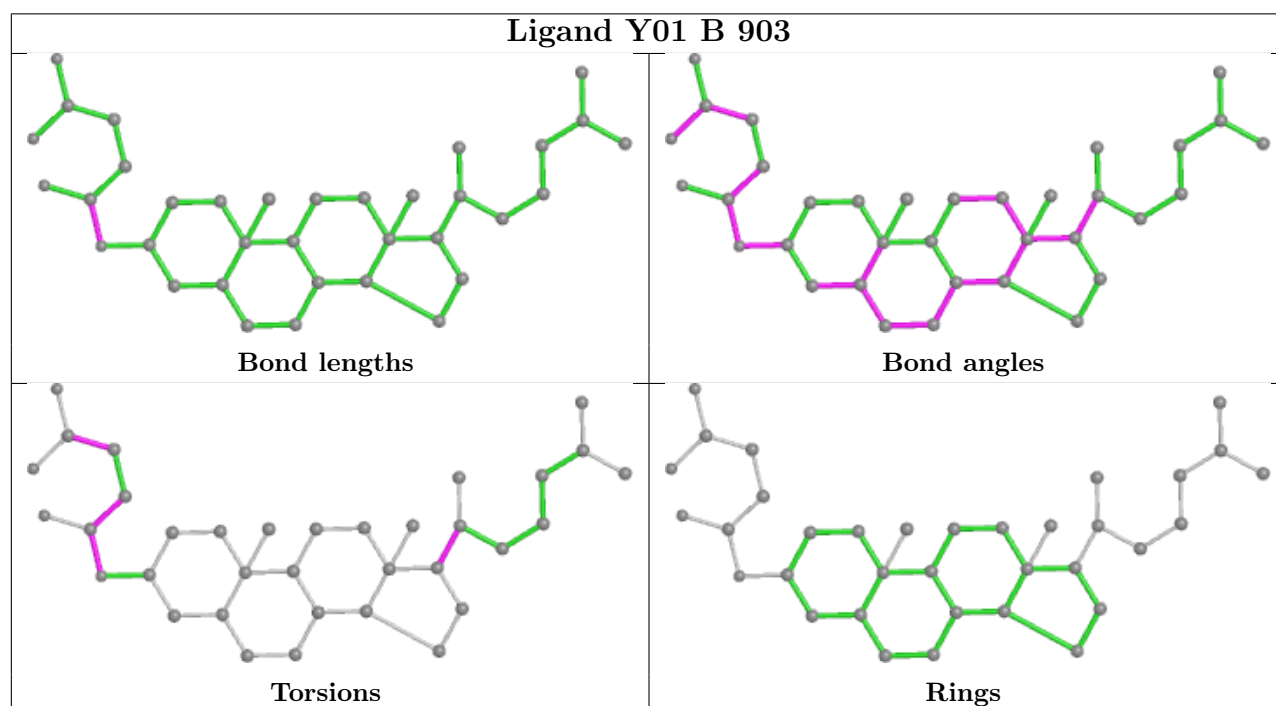
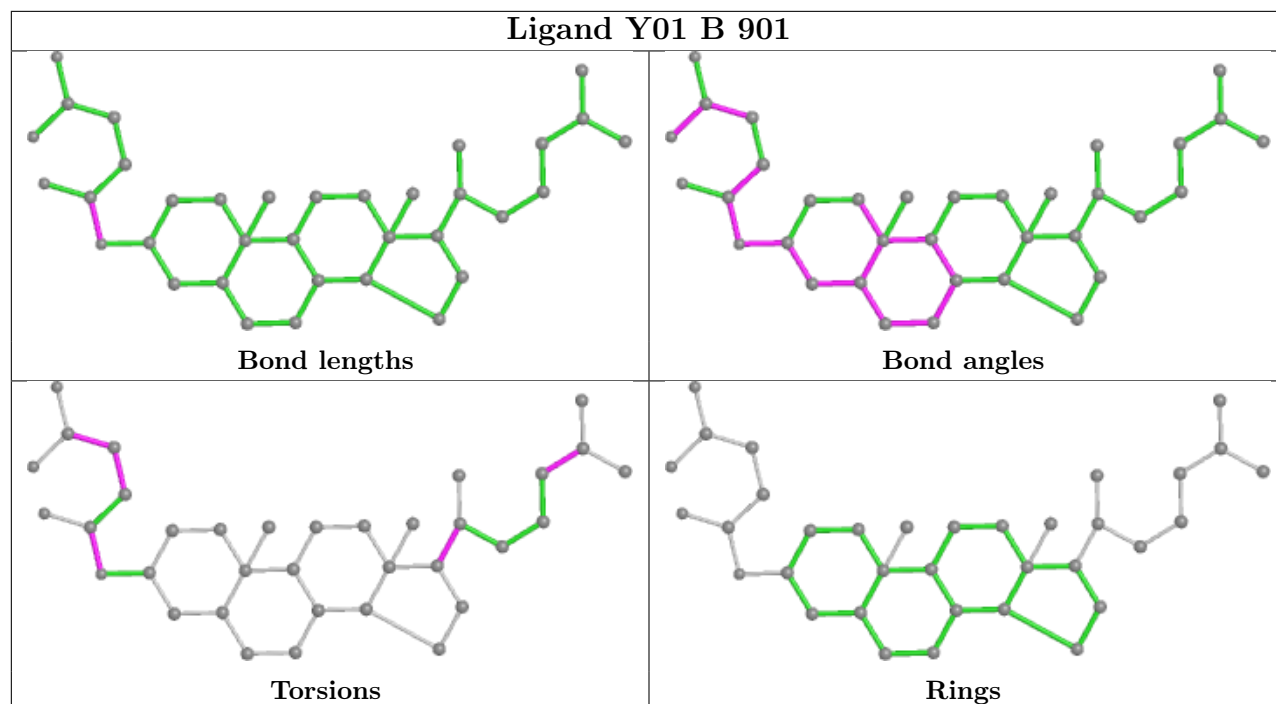
16 monomers are involved in 53 short contacts:

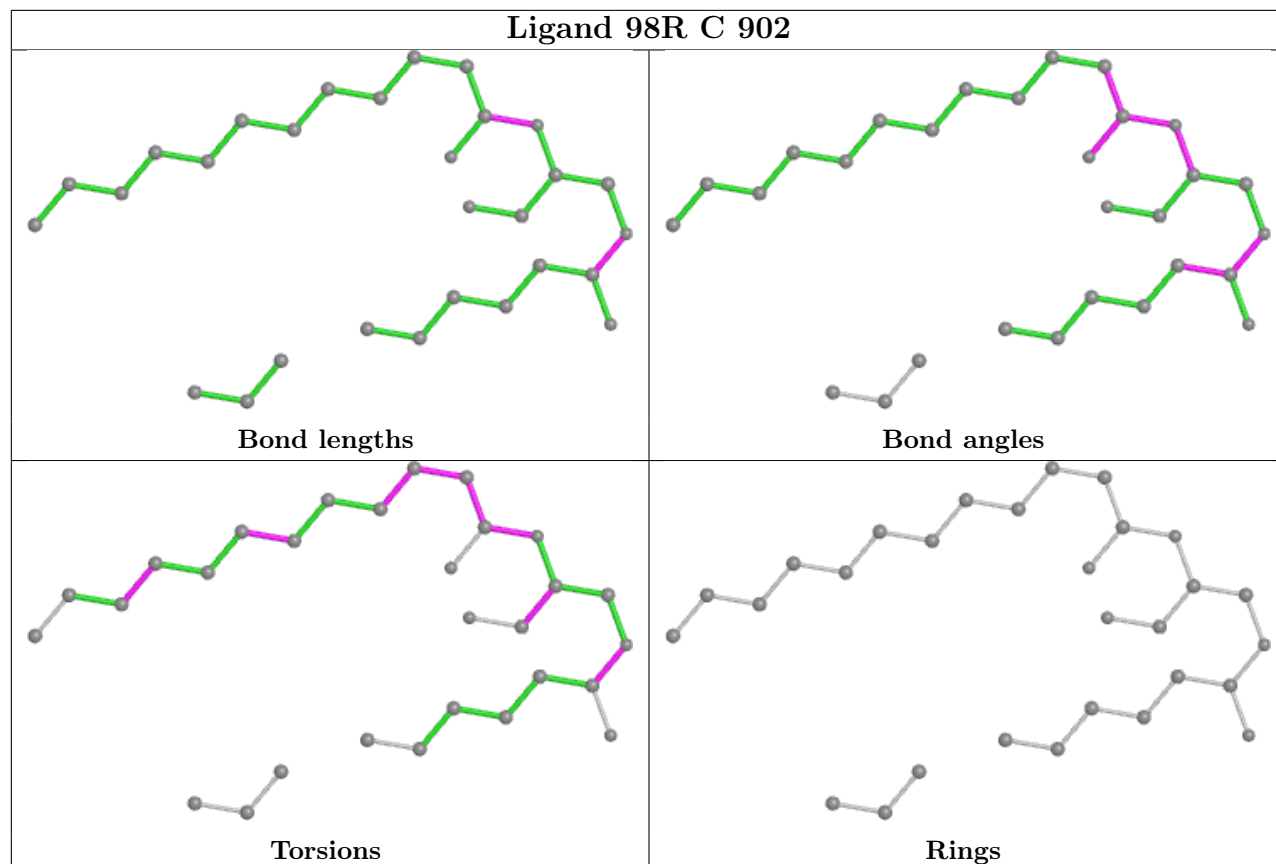
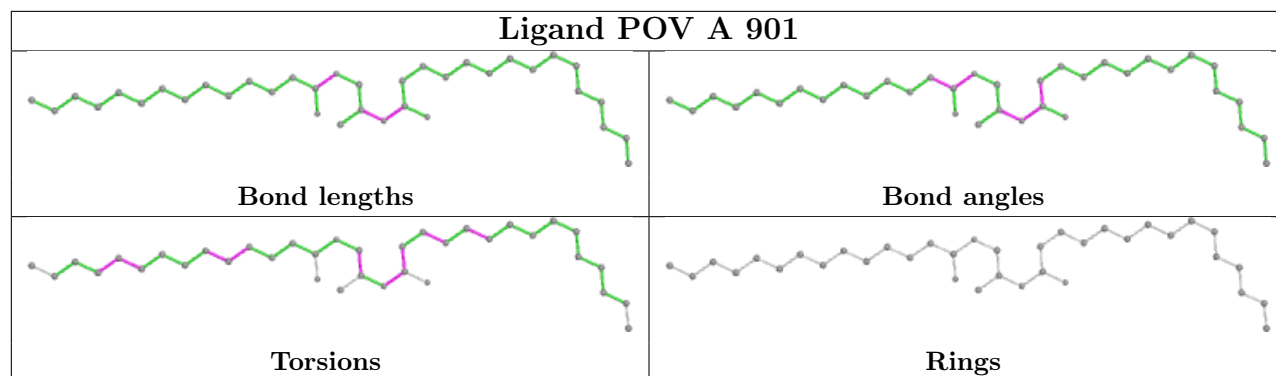
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	904	POV	2	0
2	D	901	Y01	3	0
4	C	901	POV	2	0
5	D	905	98R	5	0
5	A	902	98R	5	0
2	B	901	Y01	2	0
2	B	903	Y01	6	0
4	A	901	POV	2	0
5	C	902	98R	5	0
2	C	903	Y01	2	0
5	B	905	98R	5	0
2	D	903	Y01	7	0
2	A	903	Y01	2	0
4	D	904	POV	2	0
2	C	905	Y01	7	0
2	A	905	Y01	4	0

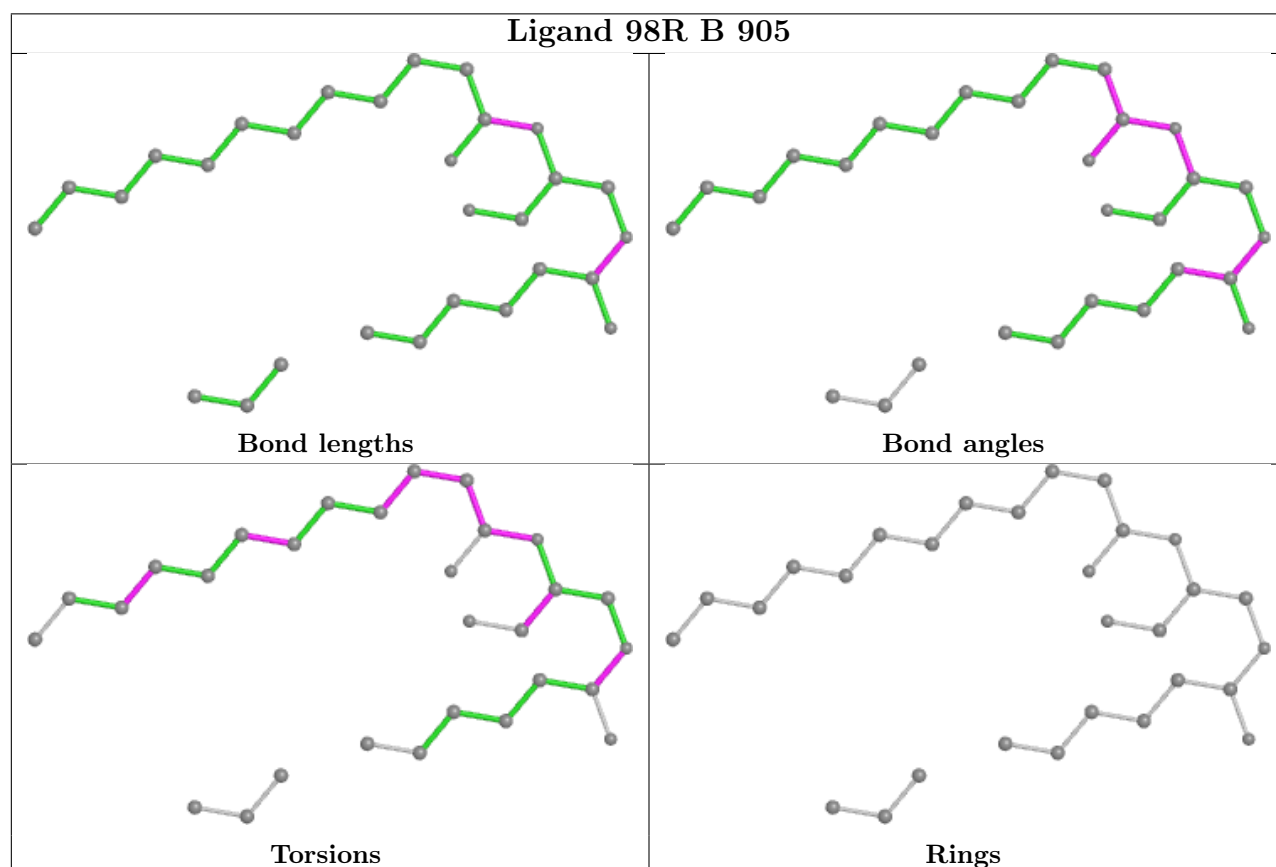
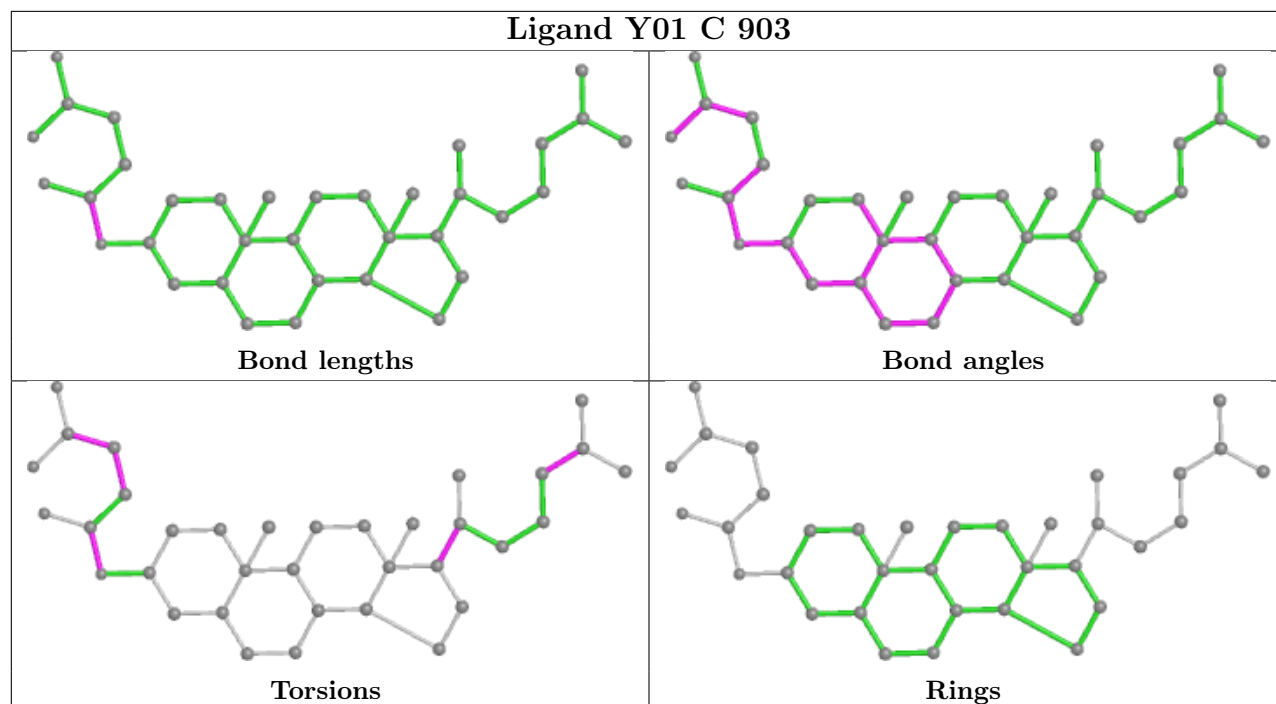
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

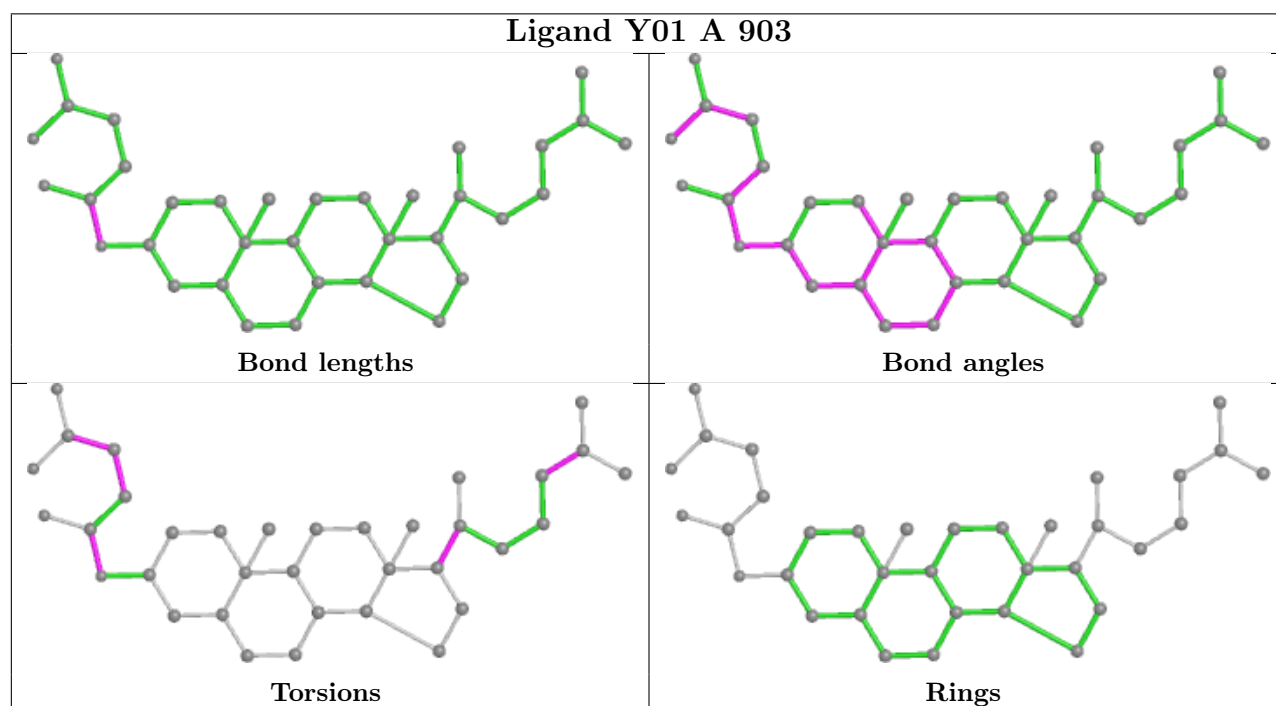
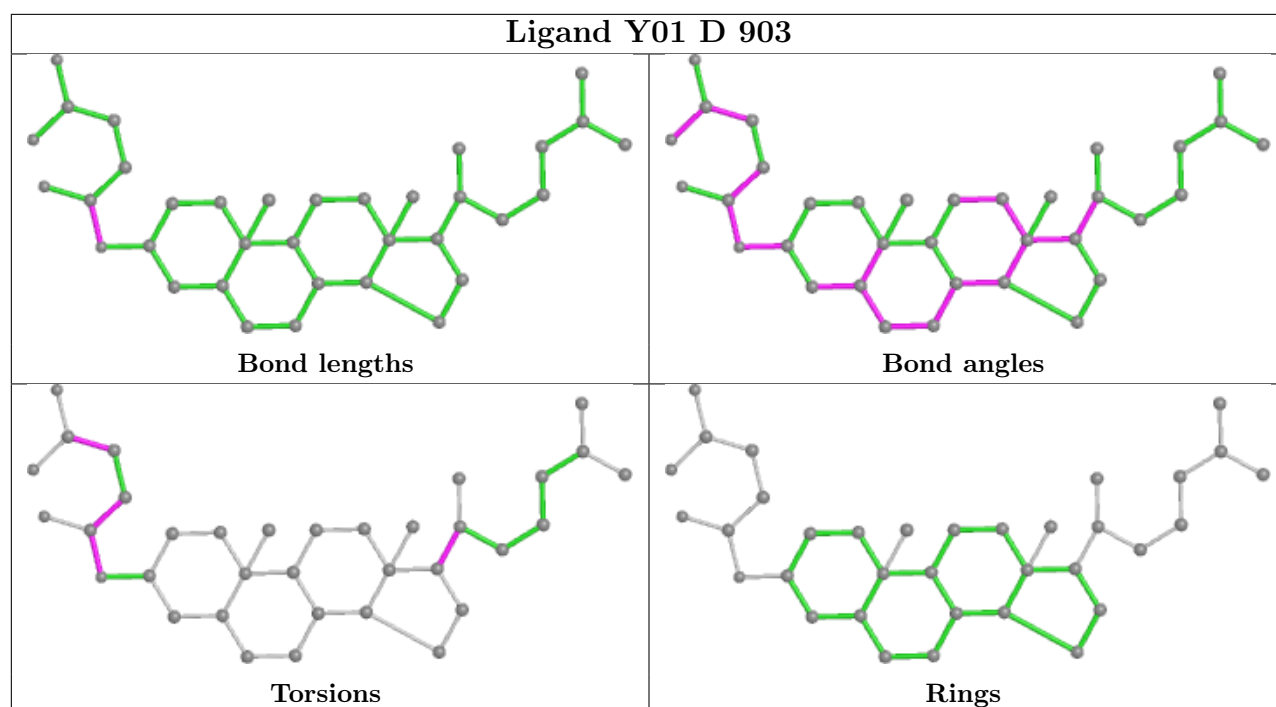


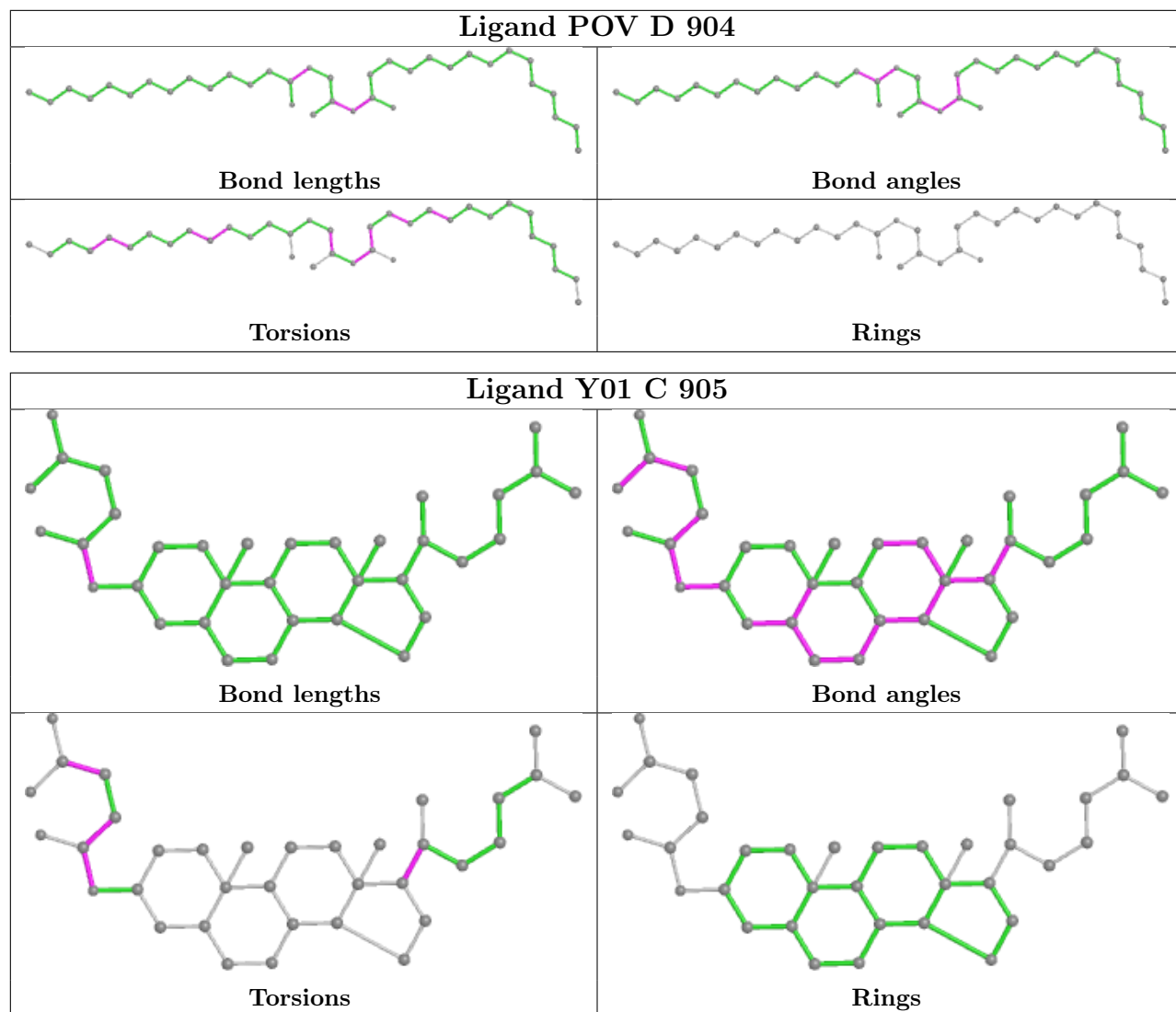




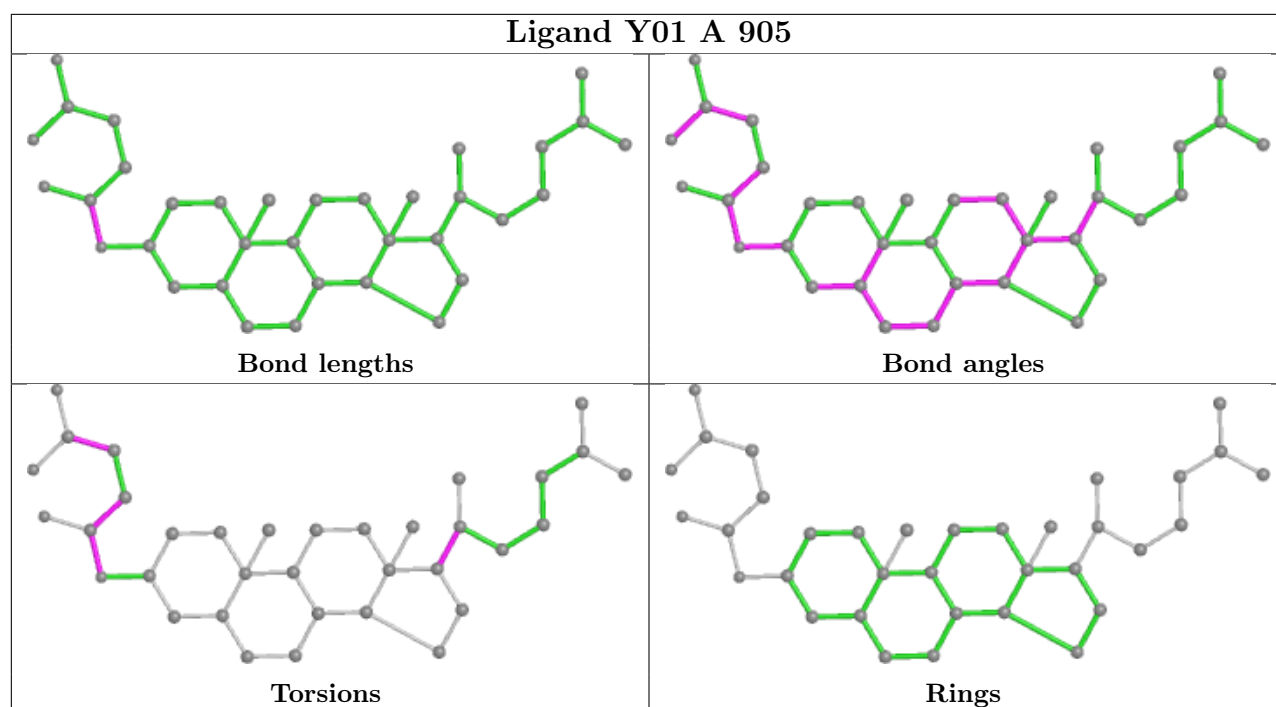












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

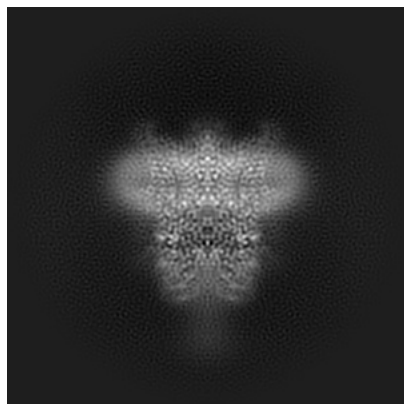
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30906. These allow visual inspection of the internal detail of the map and identification of artifacts.

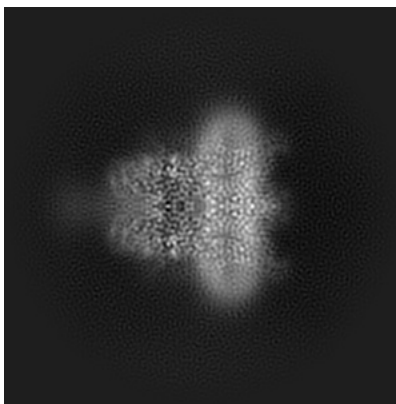
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

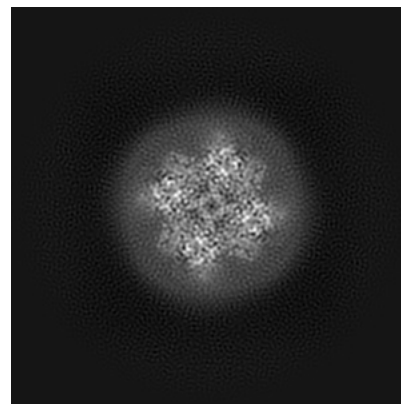
#### 6.1.1 Primary map



X

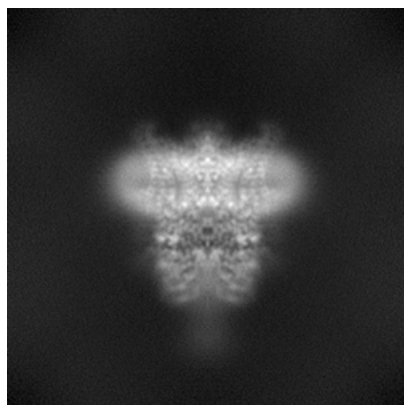


Y

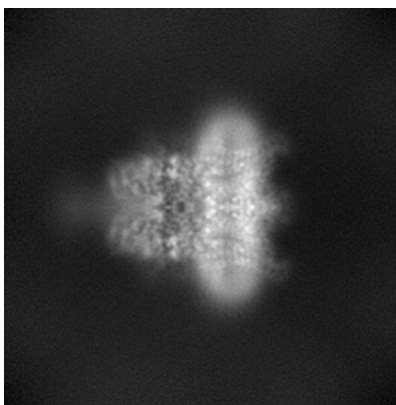


Z

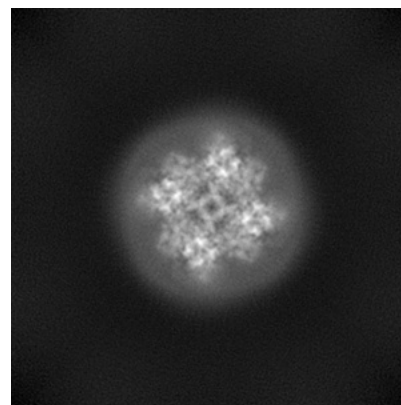
#### 6.1.2 Raw map



X



Y

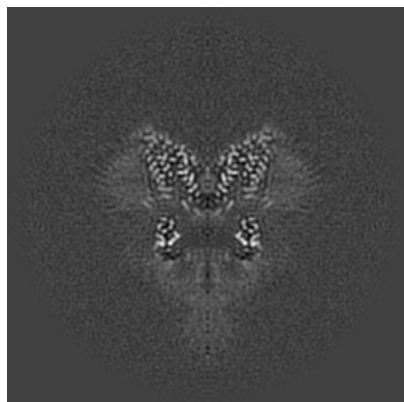


Z

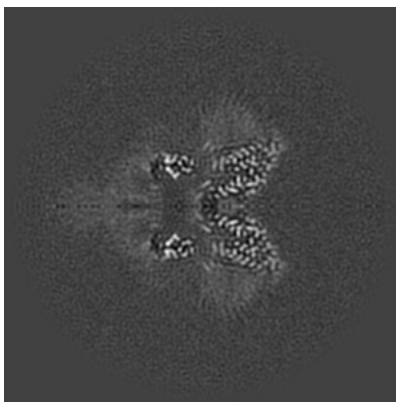
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

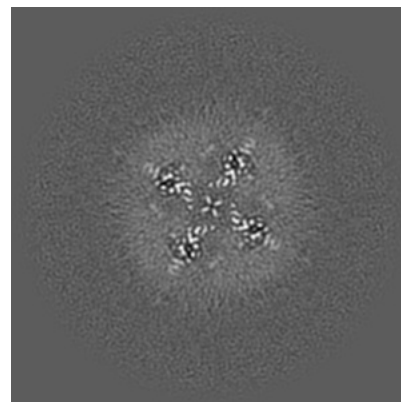
### 6.2.1 Primary map



X Index: 140

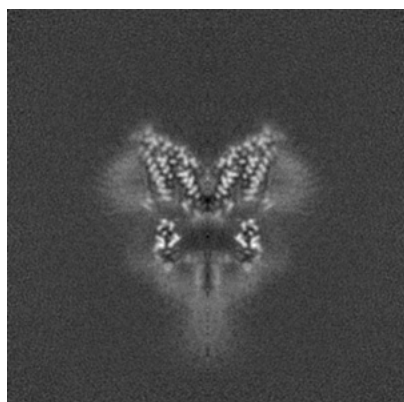


Y Index: 140

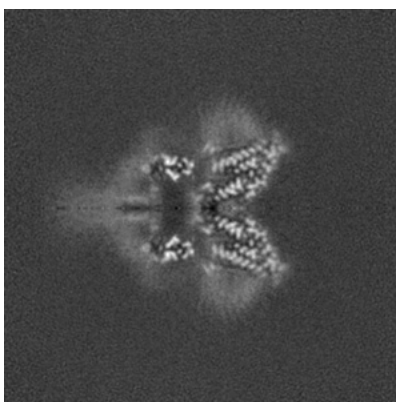


Z Index: 140

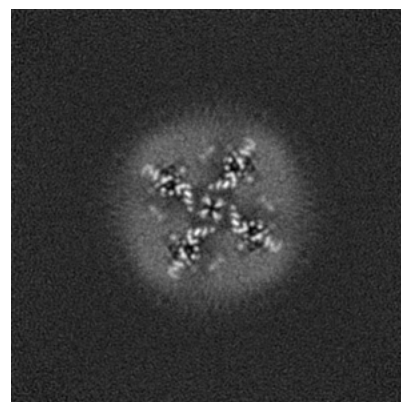
### 6.2.2 Raw map



X Index: 140



Y Index: 140

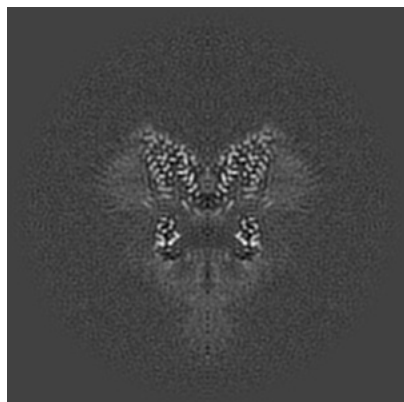


Z Index: 140

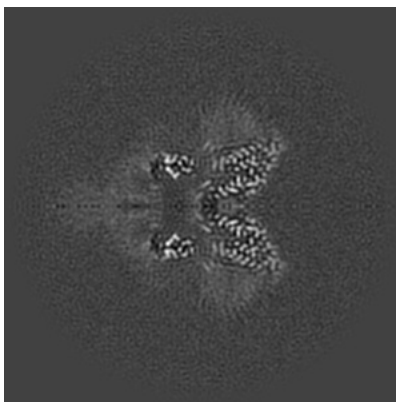
The images above show central slices of the map in three orthogonal directions.

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

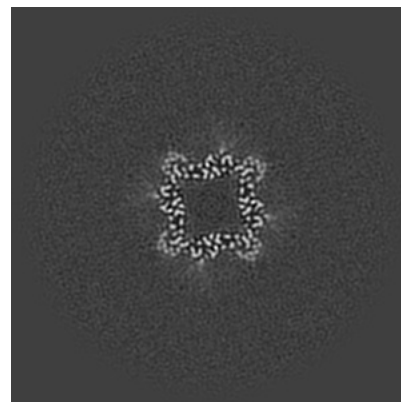
### 6.3.1 Primary map



X Index: 140

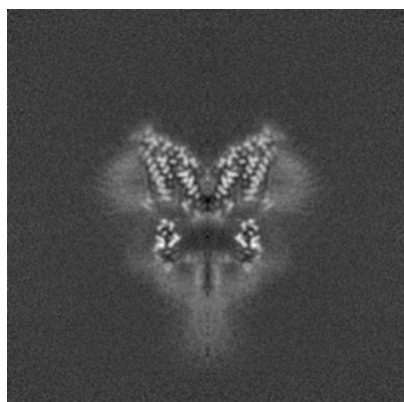


Y Index: 140

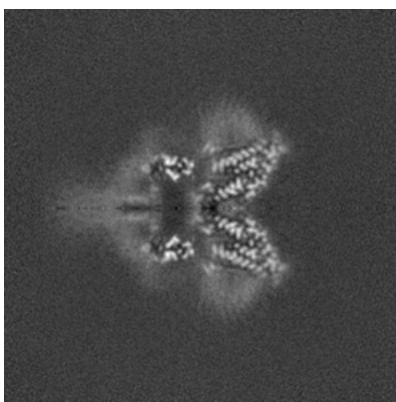


Z Index: 119

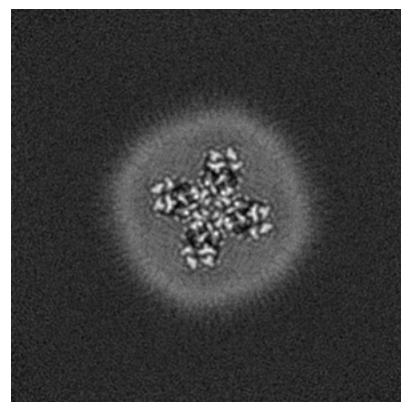
### 6.3.2 Raw map



X Index: 140



Y Index: 140

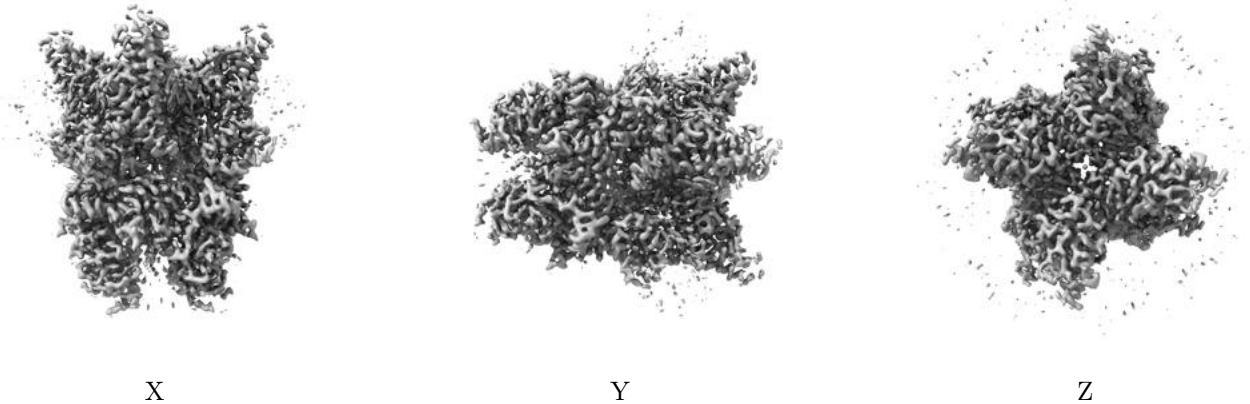


Z Index: 166

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

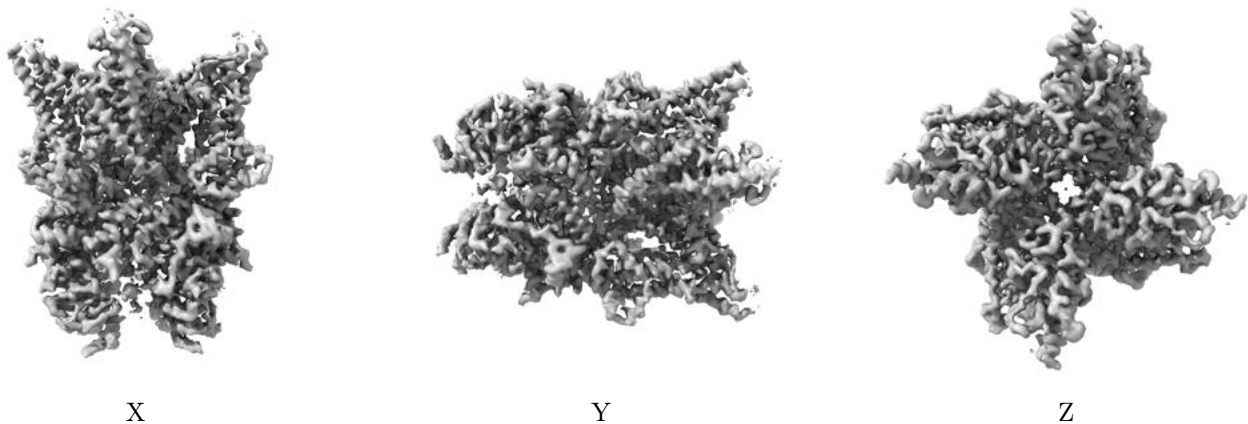
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

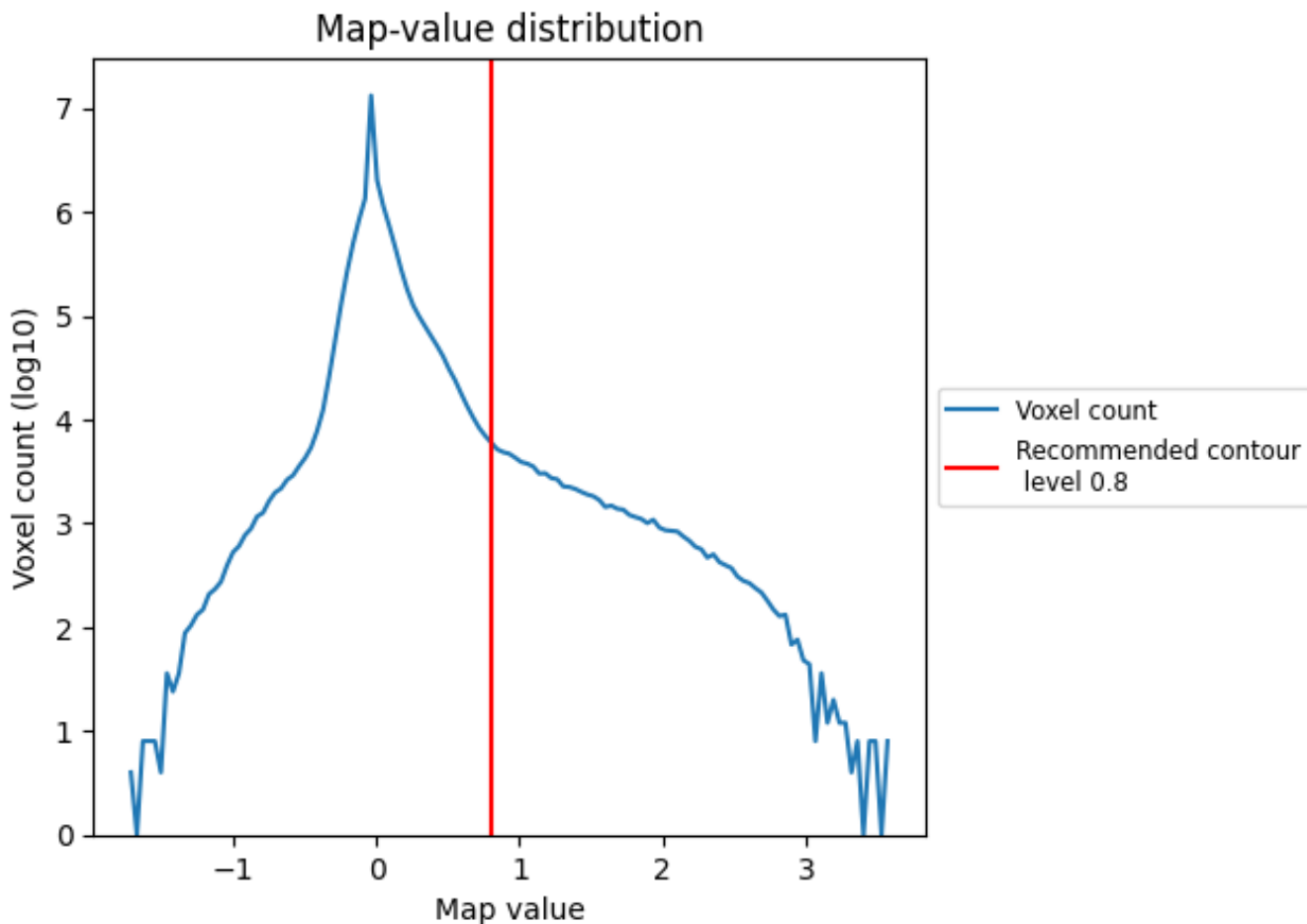
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

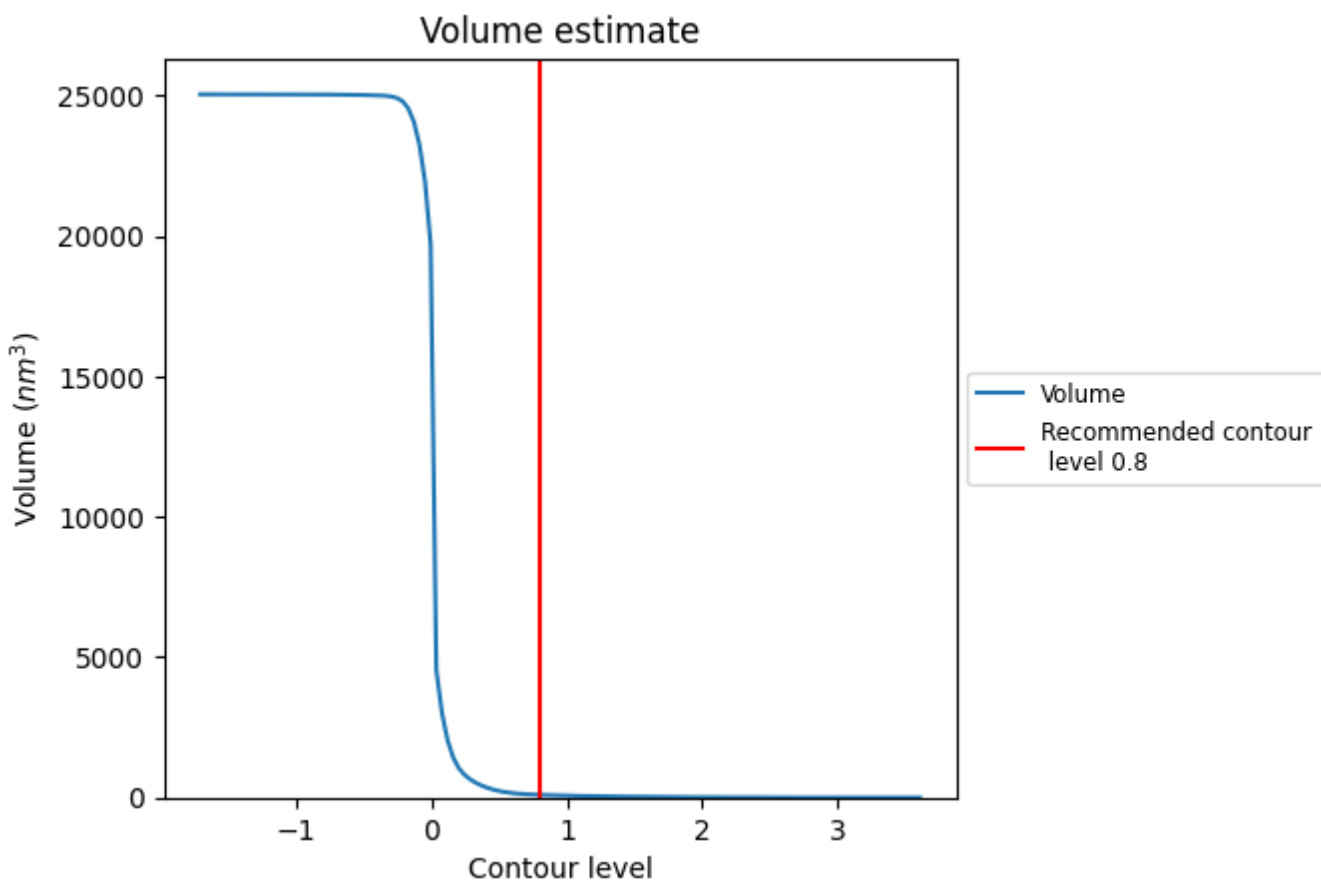
This section contains the results of statistical analysis of the map.

### 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.

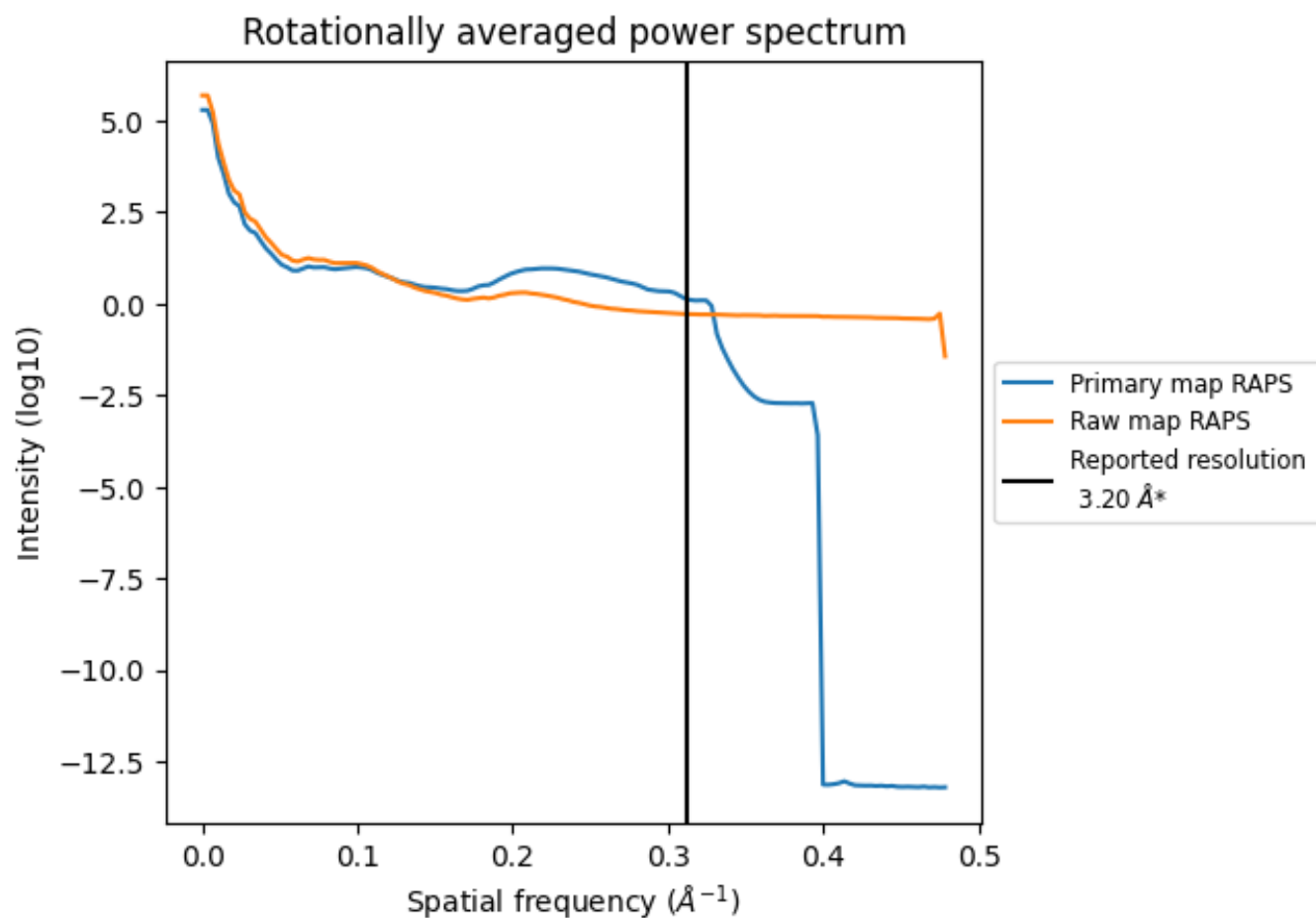
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm<sup>3</sup>; this corresponds to an approximate mass of 87 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i



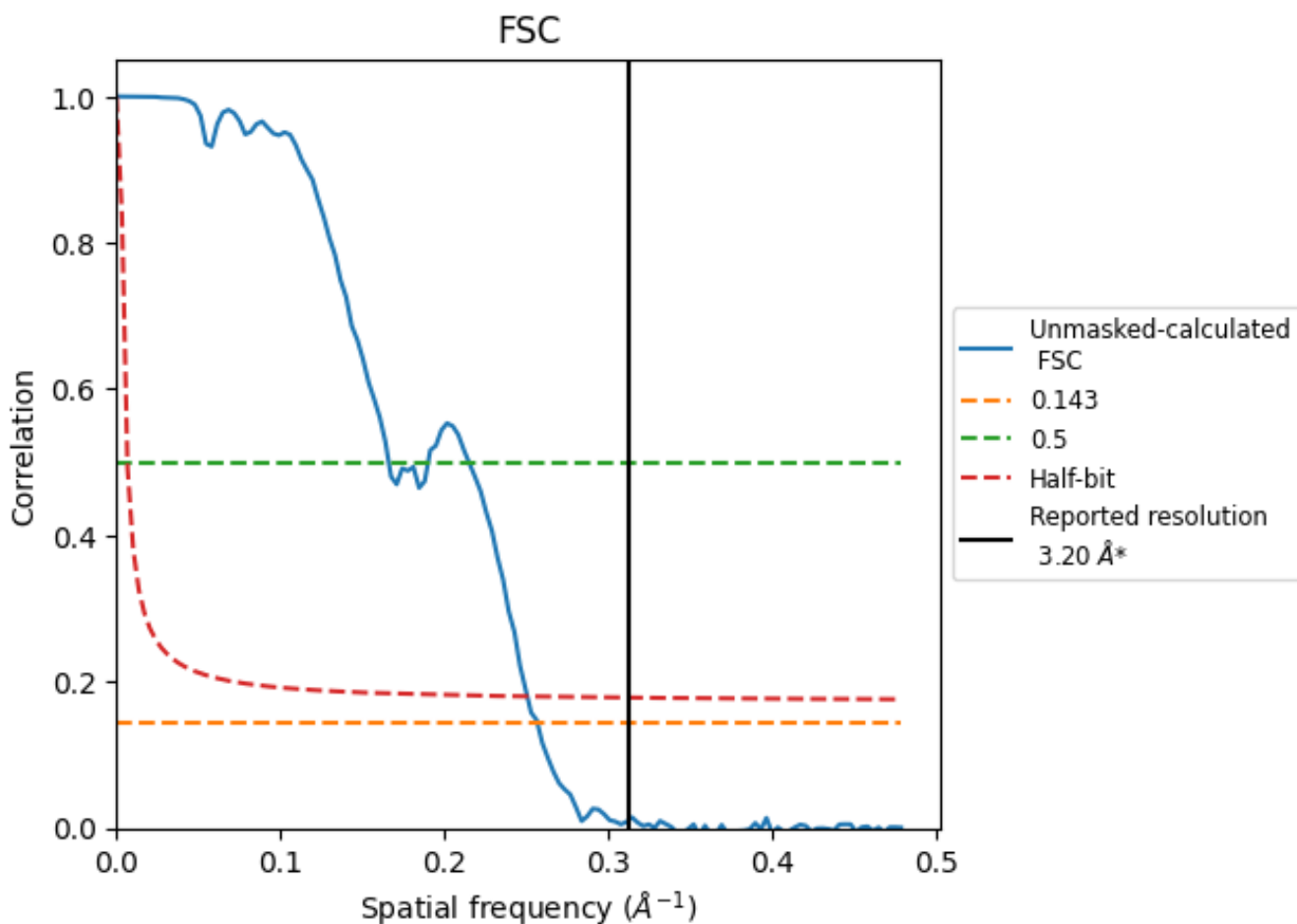
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 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](#)

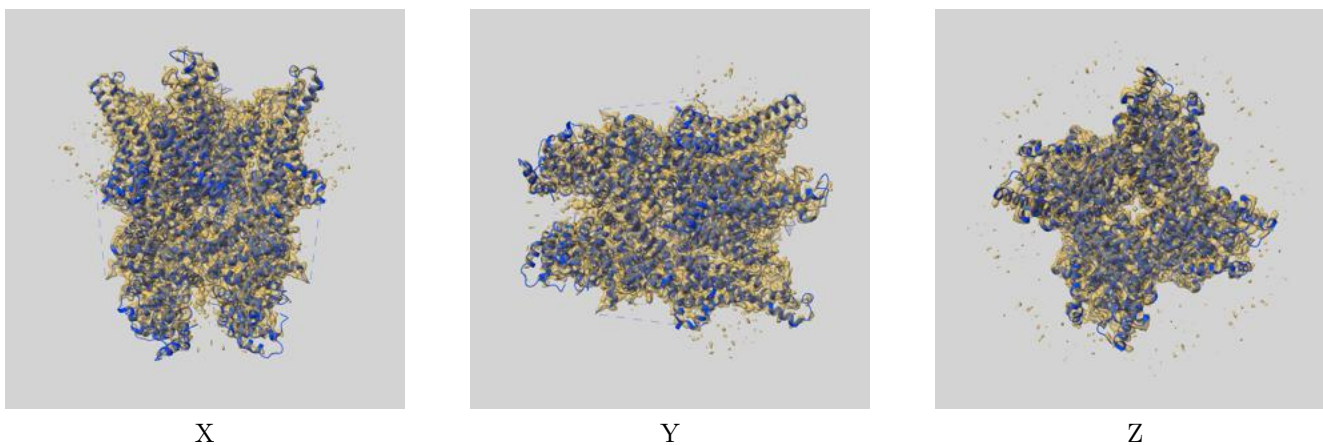
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.02	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.2 by more than 10 %

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

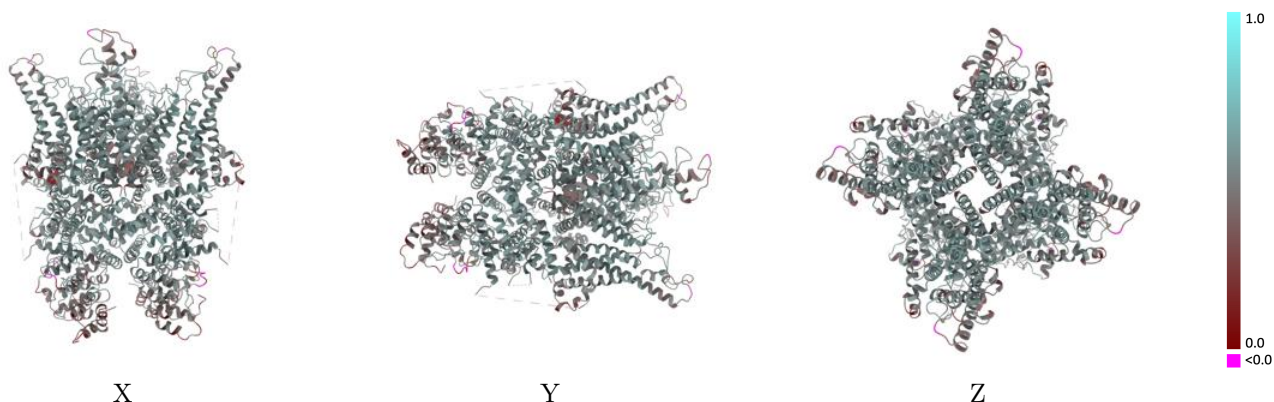
This section contains information regarding the fit between EMDB map EMD-30906 and PDB model 7DXE. Per-residue inclusion information can be found in section 3 on page 6.

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



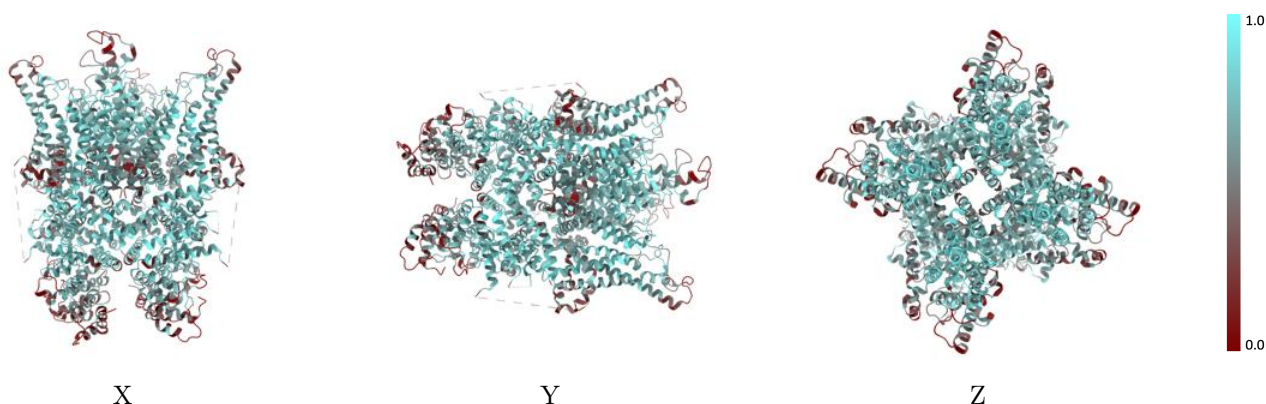
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



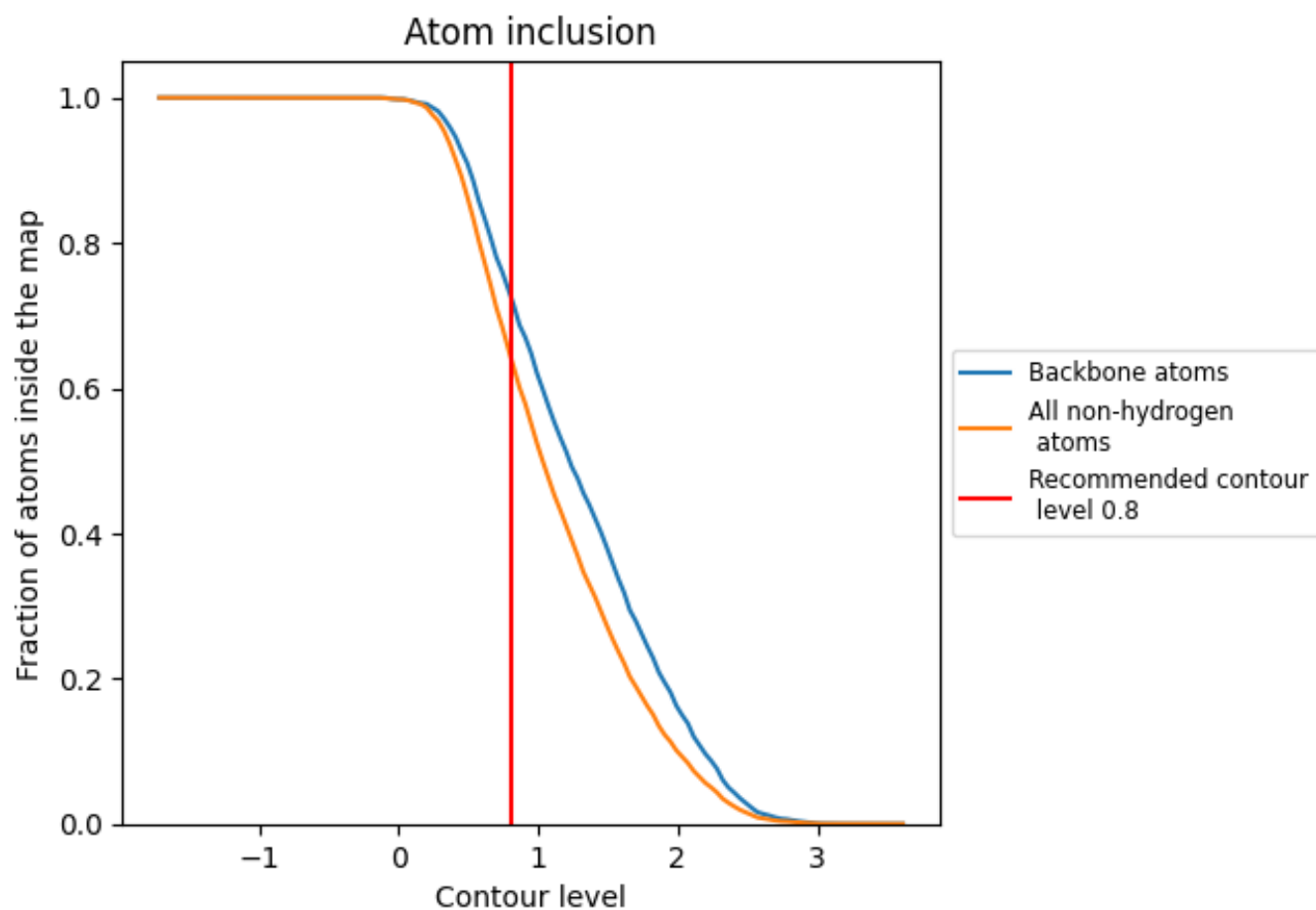
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6442	 0.5100
A	 0.6431	 0.5100
B	 0.6444	 0.5110
C	 0.6448	 0.5090
D	 0.6442	 0.5110

