



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 01:38 AM JST

PDB ID : 7DXF  
EMDB ID : EMD-30907  
Title : Structure of BTDM-bound human TRPC6 nanodisc at 2.9 angstrom in high calcium state  
Authors : Chen, L.; Guo, W.  
Deposited on : 2021-01-18  
Resolution : 2.90 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

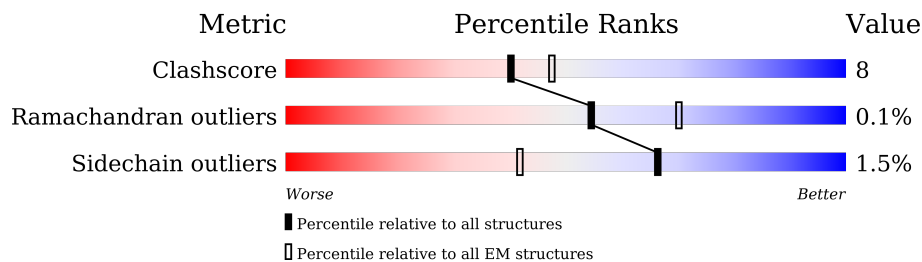
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	931	
1	B	931	
1	C	931	
1	D	931	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 22940 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.

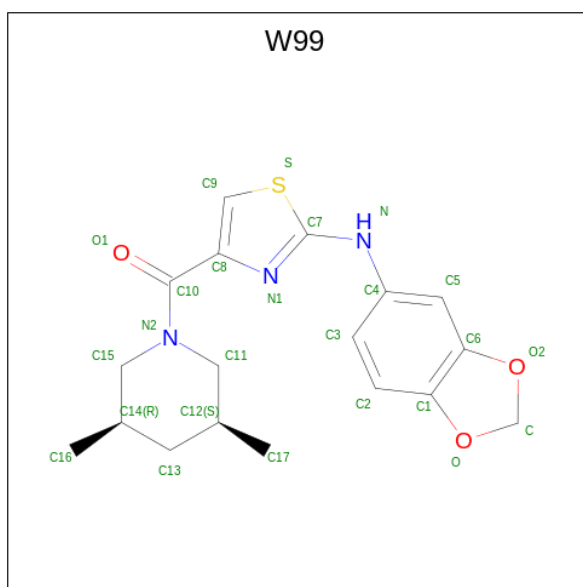
- Molecule 1 is a protein called Short transient receptor potential channel 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	685	5514	3582	905	991	36	0	0
1	B	685	5514	3582	905	991	36	0	0
1	C	685	5514	3582	905	991	36	0	0
1	D	685	5514	3582	905	991	36	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

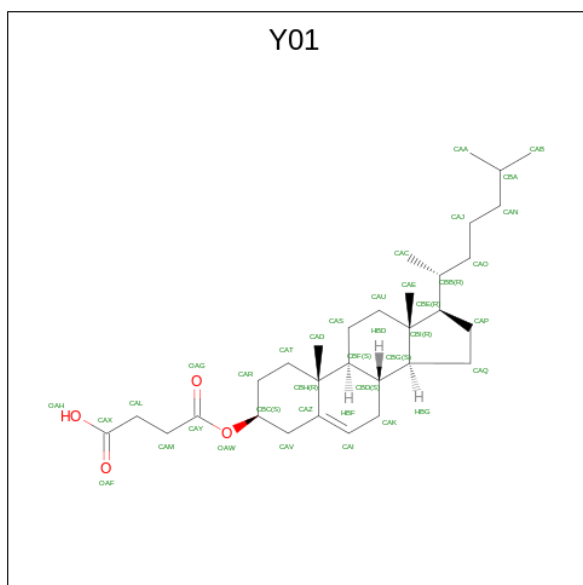
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	A	1	1	1	0
2	B	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

- Molecule 3 is [2-(1,3-benzodioxol-5-ylamino)-1,3-thiazol-4-yl]-[(3R,5S)-3,5-dimethylpiperidin-1-yl]methanone (three-letter code: W99) (formula: C<sub>18</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
3	A	1	Total	C	N	O	S	0
			25	18	3	3	1	
3	B	1	Total	C	N	O	S	0
			25	18	3	3	1	
3	C	1	Total	C	N	O	S	0
			25	18	3	3	1	
3	D	1	Total	C	N	O	S	0
			25	18	3	3	1	

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).

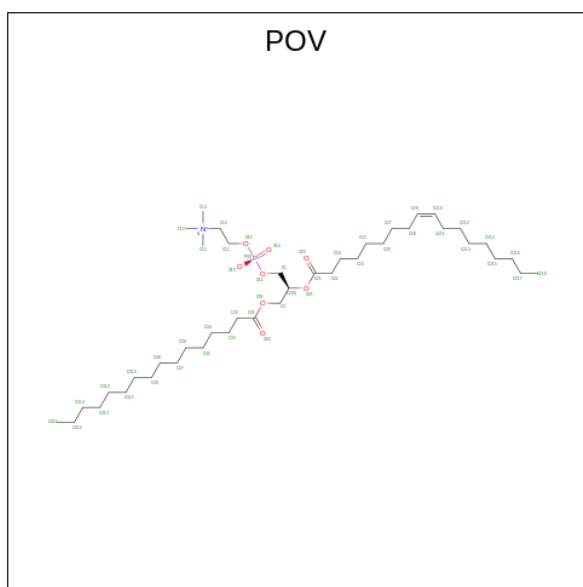


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			105	93	12	
4	A	1	Total	C	O	0
			105	93	12	
4	A	1	Total	C	O	0
			105	93	12	
4	B	1	Total	C	O	0
			105	93	12	
4	B	1	Total	C	O	0
			105	93	12	
4	B	1	Total	C	O	0
			105	93	12	
4	C	1	Total	C	O	0
			105	93	12	
4	C	1	Total	C	O	0
			105	93	12	
4	C	1	Total	C	O	0
			105	93	12	
4	D	1	Total	C	O	0
			105	93	12	
4	D	1	Total	C	O	0
			105	93	12	
4	D	1	Total	C	O	0
			105	93	12	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

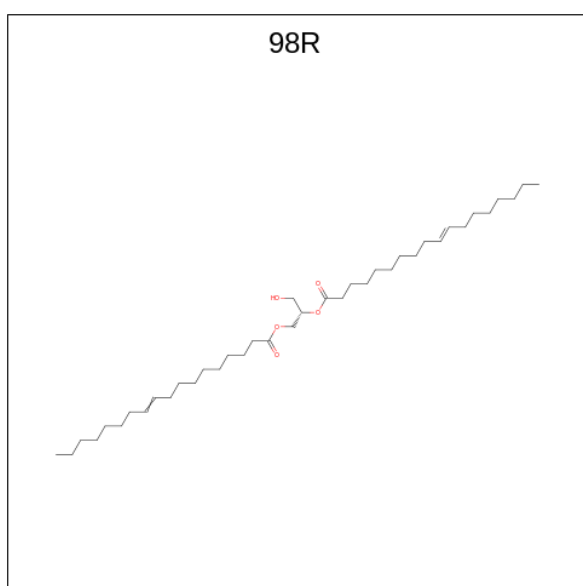
Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	Ca	0
			3	3	
5	B	3	Total	Ca	0
			3	3	
5	C	3	Total	Ca	0
			3	3	
5	D	3	Total	Ca	0
			3	3	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)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
			Total	C	N	O	P	
6	A	1	Total 46	C 36	N 1	O 8	P 1	0
6	B	1	Total 46	C 36	N 1	O 8	P 1	0
6	C	1	Total 46	C 36	N 1	O 8	P 1	0
6	D	1	Total 46	C 36	N 1	O 8	P 1	0

- Molecule 7 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>).

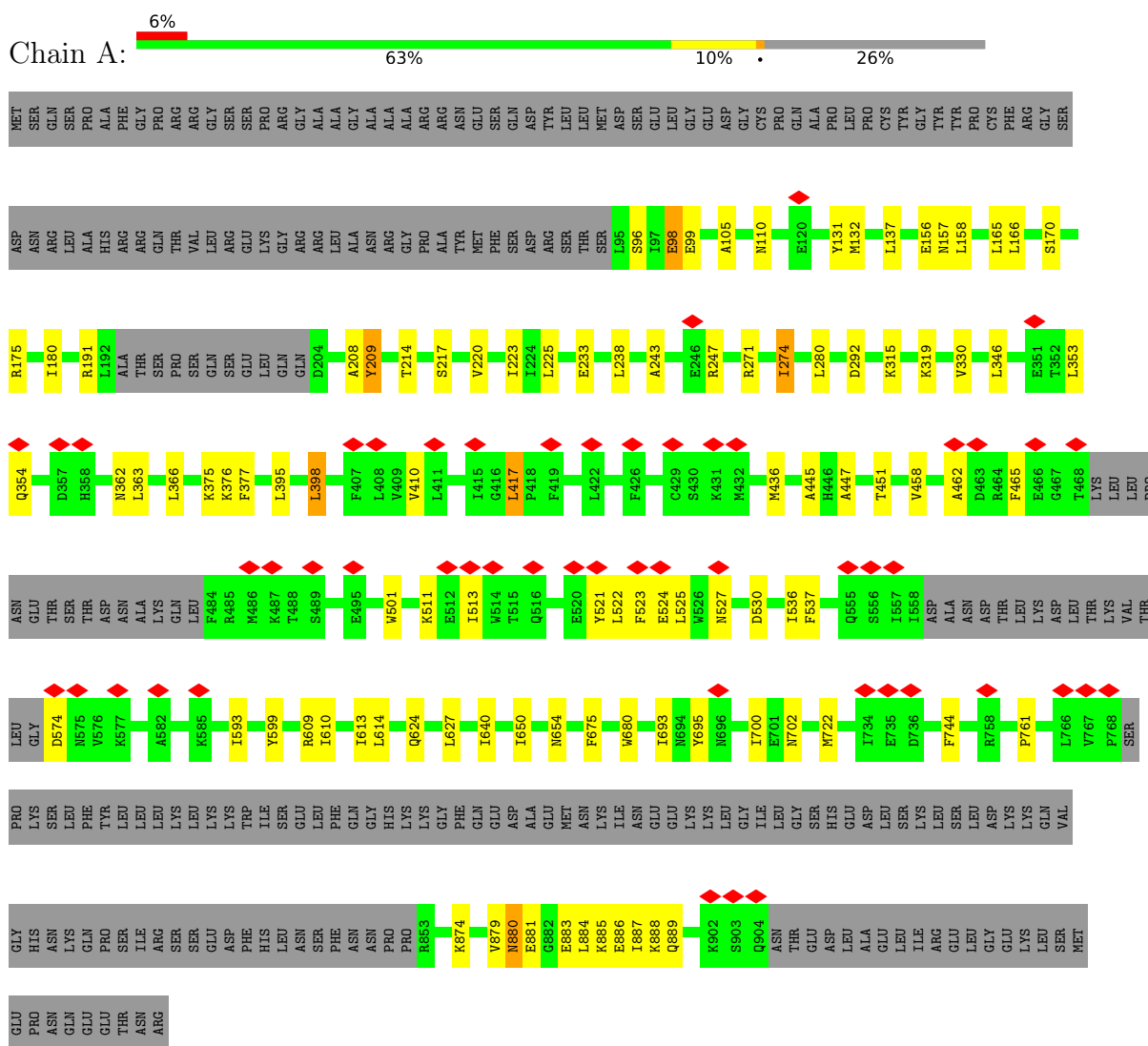


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 41	C 36	O 5	0
7	B	1	Total 41	C 36	O 5	0
7	C	1	Total 41	C 36	O 5	0
7	D	1	Total 41	C 36	O 5	0

### 3 Residue-property plots

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

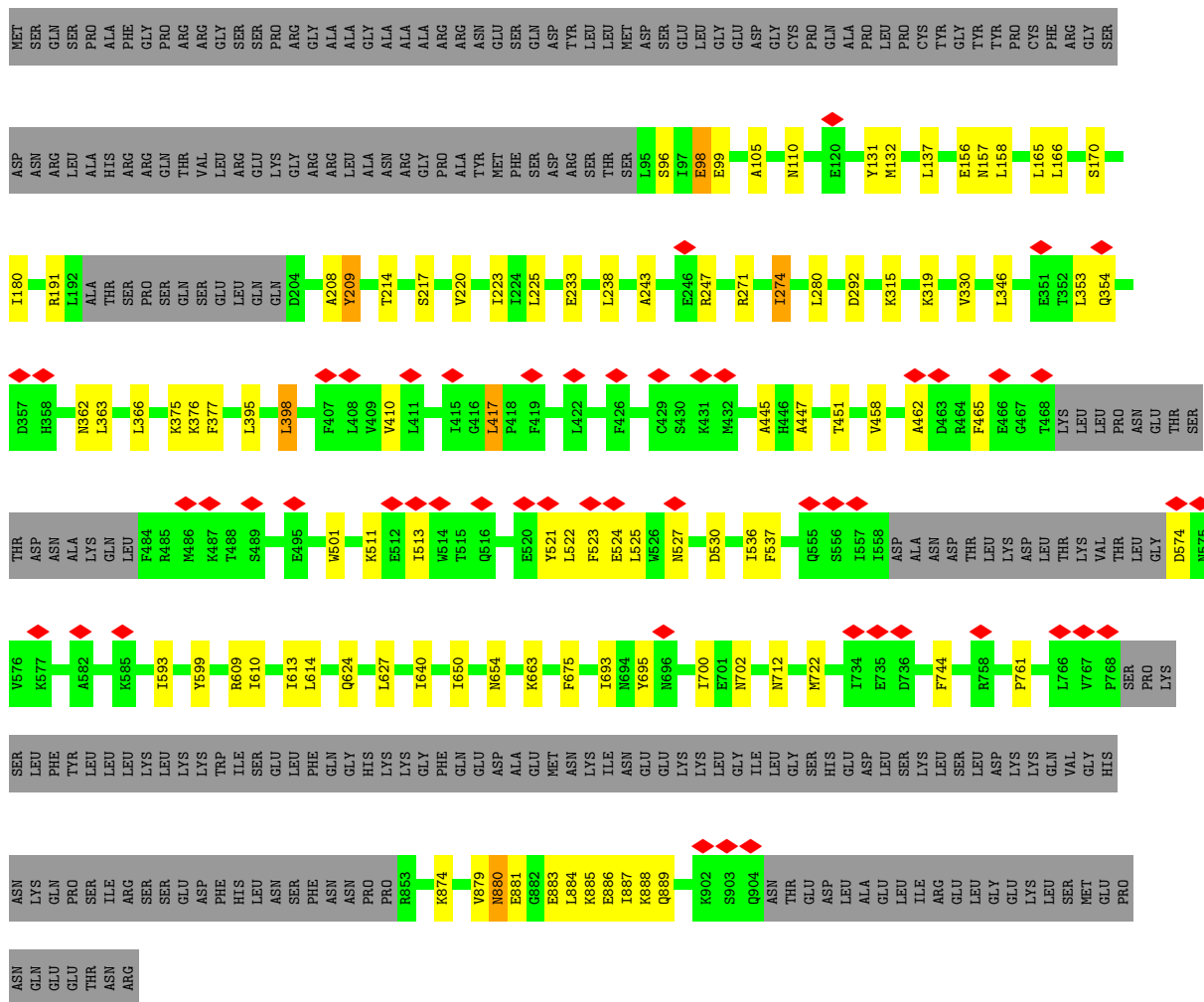
- Molecule 1: Short transient receptor potential channel 6



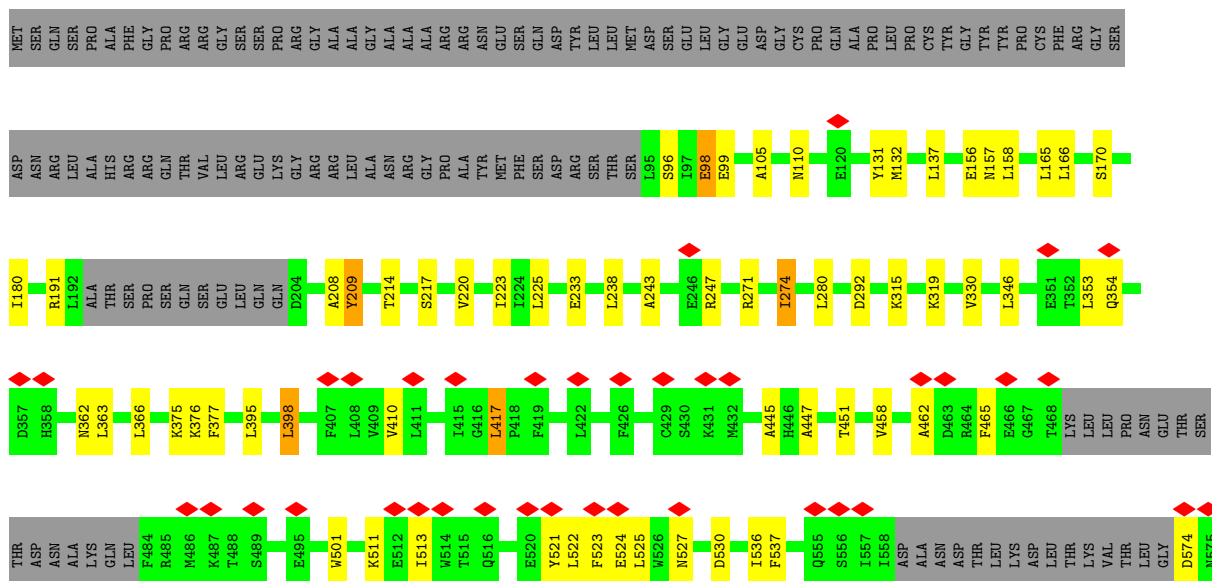
- Molecule 1: Short transient receptor potential channel 6







● Molecule 1: Short transient receptor potential channel 6





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95686	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	6.291	Depositor
Minimum map value	-2.815	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.194	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: CA, 98R, W99, POV, Y01, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/5636	0.38	0/7613
1	B	0.26	0/5636	0.38	0/7613
1	C	0.26	0/5636	0.38	0/7613
1	D	0.26	0/5636	0.38	0/7613
All	All	0.26	0/22544	0.38	0/30452

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	5514	0	5504	91	0
1	B	5514	0	5504	92	0
1	C	5514	0	5504	91	0
1	D	5514	0	5504	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	1	0
3	C	25	0	0	1	0
3	D	25	0	0	1	0
4	A	105	0	147	11	0
4	B	105	0	147	10	0
4	C	105	0	147	10	0
4	D	105	0	147	11	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
6	A	46	0	64	10	0
6	B	46	0	64	9	0
6	C	46	0	64	10	0
6	D	46	0	64	10	0
7	A	41	0	0	0	0
7	B	41	0	0	0	0
7	C	41	0	0	0	0
7	D	41	0	0	0	0
All	All	22940	0	22860	347	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 8.

All (347) 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:B:881:GLU:HG2	1:C:883:GLU:OE2	1.27	1.34
1:A:881:GLU:HG2	1:B:883:GLU:OE2	1.27	1.32
1:A:883:GLU:OE2	1:D:881:GLU:HG2	1.27	1.26
1:C:881:GLU:HG2	1:D:883:GLU:OE2	1.27	1.24
1:B:888:LYS:HE3	1:C:886:GLU:OE2	1.41	1.20
1:A:888:LYS:HE3	1:B:886:GLU:OE2	1.41	1.19
1:A:886:GLU:OE2	1:D:888:LYS:HE3	1.41	1.16
1:C:888:LYS:HE3	1:D:886:GLU:OE2	1.41	1.16
1:A:888:LYS:CE	1:B:886:GLU:OE2	2.25	0.85
1:C:888:LYS:CE	1:D:886:GLU:OE2	2.25	0.85
1:A:886:GLU:OE2	1:D:888:LYS:CE	2.25	0.85
1:B:888:LYS:CE	1:C:886:GLU:OE2	2.25	0.83
1:A:881:GLU:CG	1:B:883:GLU:OE2	2.22	0.80
1:B:881:GLU:CG	1:C:883:GLU:OE2	2.22	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:GLU:CG	1:D:883:GLU:OE2	2.22	0.76
1:A:883:GLU:OE2	1:D:881:GLU:CG	2.22	0.75
1:A:702:ASN:HD21	6:B:1006:POV:H15A	1.58	0.69
1:D:522:LEU:O	1:D:524:GLU:N	2.26	0.69
1:A:354:GLN:O	1:A:362:ASN:ND2	2.27	0.68
1:D:511:LYS:HB3	1:D:511:LYS:NZ	2.08	0.68
1:A:511:LYS:HB3	1:A:511:LYS:NZ	2.08	0.68
1:B:511:LYS:NZ	1:B:511:LYS:HB3	2.08	0.68
1:C:511:LYS:NZ	1:C:511:LYS:HB3	2.08	0.68
1:B:525:LEU:HD12	1:B:525:LEU:O	1.94	0.68
1:C:702:ASN:HD21	6:D:1008:POV:H15A	1.58	0.68
1:A:525:LEU:HD12	1:A:525:LEU:O	1.94	0.68
1:B:702:ASN:HD21	6:C:1006:POV:H15A	1.58	0.68
1:C:354:GLN:O	1:C:362:ASN:ND2	2.27	0.68
6:A:1006:POV:H15A	1:D:702:ASN:HD21	1.58	0.67
1:B:522:LEU:O	1:B:524:GLU:N	2.26	0.67
1:D:354:GLN:O	1:D:362:ASN:ND2	2.27	0.67
1:A:522:LEU:O	1:A:524:GLU:N	2.26	0.67
1:D:525:LEU:HD12	1:D:525:LEU:O	1.94	0.67
1:C:525:LEU:HD12	1:C:525:LEU:O	1.94	0.66
1:B:354:GLN:O	1:B:362:ASN:ND2	2.27	0.66
1:C:522:LEU:O	1:C:524:GLU:N	2.26	0.66
1:D:521:TYR:O	1:D:527:ASN:ND2	2.28	0.65
1:B:521:TYR:O	1:B:527:ASN:ND2	2.28	0.64
1:A:521:TYR:O	1:A:527:ASN:ND2	2.28	0.64
1:C:96:SER:O	1:C:99:GLU:N	2.30	0.64
1:B:884:LEU:HD22	1:C:879:VAL:HG11	1.80	0.64
1:A:884:LEU:HD22	1:B:879:VAL:HG11	1.80	0.64
1:A:879:VAL:HG11	1:D:884:LEU:HD22	1.80	0.64
1:D:96:SER:O	1:D:99:GLU:N	2.30	0.64
1:A:363:LEU:HD22	1:A:366:LEU:HD12	1.79	0.64
1:B:880:ASN:ND2	1:B:883:GLU:HB2	2.13	0.63
1:C:880:ASN:ND2	1:C:883:GLU:HB2	2.13	0.63
1:D:363:LEU:HD22	1:D:366:LEU:HD12	1.79	0.63
1:A:880:ASN:ND2	1:A:883:GLU:HB2	2.13	0.63
1:C:521:TYR:O	1:C:527:ASN:ND2	2.28	0.63
1:D:137:LEU:HD22	1:D:158:LEU:HD21	1.80	0.63
1:C:884:LEU:HD22	1:D:879:VAL:HG11	1.80	0.63
1:B:137:LEU:HD22	1:B:158:LEU:HD21	1.80	0.63
1:B:363:LEU:HD22	1:B:366:LEU:HD12	1.79	0.63
1:D:880:ASN:ND2	1:D:883:GLU:HB2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD22	1:A:158:LEU:HD21	1.80	0.62
1:B:96:SER:O	1:B:99:GLU:N	2.30	0.62
1:C:363:LEU:HD22	1:C:366:LEU:HD12	1.79	0.62
1:A:96:SER:O	1:A:99:GLU:N	2.30	0.62
1:C:137:LEU:HD22	1:C:158:LEU:HD21	1.80	0.61
1:C:693:ILE:HG22	1:C:695:TYR:H	1.66	0.61
1:B:880:ASN:C	1:B:880:ASN:HD22	2.04	0.61
1:C:880:ASN:HD22	1:C:880:ASN:C	2.04	0.61
1:A:880:ASN:C	1:A:880:ASN:HD22	2.04	0.61
1:D:693:ILE:HG22	1:D:695:TYR:H	1.66	0.61
1:C:395:LEU:HD13	1:C:398:LEU:HD13	1.82	0.60
1:B:693:ILE:HG22	1:B:695:TYR:H	1.66	0.60
1:C:885:LYS:HZ2	1:C:889:GLN:HE21	1.50	0.60
1:D:395:LEU:HD13	1:D:398:LEU:HD13	1.82	0.60
1:B:395:LEU:HD13	1:B:398:LEU:HD13	1.82	0.60
1:A:693:ILE:HG22	1:A:695:TYR:H	1.66	0.60
4:B:1010:Y01:HAJ2	1:C:536:ILE:HD11	1.84	0.60
1:D:880:ASN:C	1:D:880:ASN:HD22	2.04	0.60
1:A:395:LEU:HD13	1:A:398:LEU:HD13	1.82	0.59
4:A:1010:Y01:HAJ2	1:B:536:ILE:HD11	1.84	0.59
1:A:536:ILE:HD11	4:D:1002:Y01:HAJ2	1.84	0.59
1:A:884:LEU:HD11	1:B:887:ILE:HD12	1.85	0.58
1:A:887:ILE:HD12	1:D:884:LEU:HD11	1.85	0.58
1:D:511:LYS:HB3	1:D:511:LYS:HZ3	1.68	0.58
1:A:613:ILE:HD12	4:A:1003:Y01:HAD3	1.86	0.58
1:B:613:ILE:HD12	4:B:1003:Y01:HAD3	1.86	0.58
4:C:1010:Y01:HAJ2	1:D:536:ILE:HD11	1.84	0.58
1:B:884:LEU:HD11	1:C:887:ILE:HD12	1.85	0.57
1:D:613:ILE:HD12	4:D:1005:Y01:HAD3	1.86	0.57
1:B:884:LEU:HD22	1:C:879:VAL:CG1	2.34	0.57
1:C:884:LEU:HD11	1:D:887:ILE:HD12	1.86	0.57
1:A:879:VAL:CG1	1:D:884:LEU:HD22	2.34	0.56
1:A:884:LEU:HD22	1:B:879:VAL:CG1	2.34	0.56
1:C:884:LEU:HD22	1:D:879:VAL:CG1	2.34	0.56
1:C:613:ILE:HD12	4:C:1003:Y01:HAD3	1.86	0.56
1:D:885:LYS:NZ	1:D:889:GLN:HE21	2.04	0.56
1:A:610:ILE:HD11	4:A:1003:Y01:HAP1	1.89	0.55
1:B:610:ILE:HD11	4:B:1003:Y01:HAP1	1.89	0.55
1:C:885:LYS:NZ	1:C:889:GLN:HE21	2.04	0.55
1:A:885:LYS:NZ	1:A:889:GLN:HE21	2.04	0.55
1:B:885:LYS:NZ	1:B:889:GLN:HE21	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:VAL:HG21	1:C:376:LYS:HB3	1.89	0.55
1:A:885:LYS:HZ2	1:A:889:GLN:HE21	1.55	0.55
1:A:330:VAL:HG21	1:A:376:LYS:HB3	1.89	0.54
1:D:610:ILE:HD11	4:D:1005:Y01:HAP1	1.89	0.54
1:A:675:PHE:CE1	6:A:1006:POV:H28	2.43	0.54
1:D:330:VAL:HG21	1:D:376:LYS:HB3	1.89	0.54
1:C:610:ILE:HD11	4:C:1003:Y01:HAP1	1.89	0.54
1:D:675:PHE:CE1	6:D:1008:POV:H28	2.43	0.54
1:B:330:VAL:HG21	1:B:376:LYS:HB3	1.89	0.53
1:B:675:PHE:CE1	6:B:1006:POV:H28	2.43	0.53
1:C:223:ILE:HB	1:C:243:ALA:HB1	1.91	0.53
1:D:223:ILE:HB	1:D:243:ALA:HB1	1.91	0.53
6:B:1006:POV:H35	1:C:465:PHE:HE1	1.73	0.53
6:C:1006:POV:H35	1:D:465:PHE:HE1	1.73	0.53
1:A:223:ILE:HB	1:A:243:ALA:HB1	1.91	0.53
1:C:675:PHE:CE1	6:C:1006:POV:H28	2.43	0.53
1:A:465:PHE:HE1	6:D:1008:POV:H35	1.74	0.53
1:A:627:LEU:HD22	1:D:722:MET:HB3	1.91	0.53
1:D:451:THR:HG22	4:D:1005:Y01:HAE2	1.91	0.53
1:A:650:ILE:HD13	1:B:458:VAL:HG22	1.91	0.53
1:B:722:MET:HB3	1:C:627:LEU:HD22	1.91	0.53
1:A:451:THR:HG22	4:A:1003:Y01:HAE2	1.91	0.52
1:B:447:ALA:O	1:B:451:THR:HG23	2.09	0.52
1:C:447:ALA:O	1:C:451:THR:HG23	2.09	0.52
1:C:722:MET:HB3	1:D:627:LEU:HD22	1.91	0.52
1:A:346:LEU:HD23	1:A:377:PHE:CZ	2.45	0.52
1:B:511:LYS:NZ	1:B:511:LYS:CB	2.73	0.52
1:C:346:LEU:HD23	1:C:377:PHE:CZ	2.45	0.52
1:B:346:LEU:HD23	1:B:377:PHE:CZ	2.45	0.52
1:B:650:ILE:HD13	1:C:458:VAL:HG22	1.92	0.52
1:B:885:LYS:HZ2	1:B:889:GLN:HE21	1.56	0.52
1:A:447:ALA:O	1:A:451:THR:HG23	2.09	0.52
1:A:722:MET:HB3	1:B:627:LEU:HD22	1.91	0.52
1:C:650:ILE:HD13	1:D:458:VAL:HG22	1.92	0.52
6:A:1006:POV:O22	6:A:1006:POV:H1A	2.09	0.52
1:D:511:LYS:NZ	1:D:511:LYS:CB	2.73	0.52
1:A:458:VAL:HG22	1:D:650:ILE:HD13	1.92	0.52
1:A:511:LYS:NZ	1:A:511:LYS:CB	2.73	0.52
1:B:223:ILE:HB	1:B:243:ALA:HB1	1.90	0.52
1:C:451:THR:HG22	4:C:1003:Y01:HAE2	1.91	0.52
1:B:702:ASN:ND2	6:C:1006:POV:H15A	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ARG:HA	1:B:280:LEU:HD11	1.92	0.51
1:B:451:THR:HG22	4:B:1003:Y01:HAE2	1.91	0.51
1:C:511:LYS:NZ	1:C:511:LYS:CB	2.73	0.51
6:A:1006:POV:H15A	1:D:702:ASN:ND2	2.25	0.51
6:C:1006:POV:O22	6:C:1006:POV:H1A	2.09	0.51
1:D:346:LEU:HD23	1:D:377:PHE:CZ	2.45	0.51
6:D:1008:POV:H1A	6:D:1008:POV:O22	2.09	0.51
6:A:1006:POV:H35	1:B:465:PHE:HE1	1.73	0.51
1:A:247:ARG:HA	1:A:280:LEU:HD11	1.92	0.51
1:D:447:ALA:O	1:D:451:THR:HG23	2.10	0.51
4:C:1010:Y01:OAG	6:D:1008:POV:H15	2.11	0.51
1:B:410:VAL:HG21	4:B:1003:Y01:HAT2	1.93	0.51
1:C:410:VAL:HG21	4:C:1003:Y01:HAT2	1.93	0.51
1:D:247:ARG:HA	1:D:280:LEU:HD11	1.92	0.51
1:B:462:ALA:HA	1:B:465:PHE:CD2	2.47	0.50
6:B:1006:POV:H1A	6:B:1006:POV:O22	2.09	0.50
1:C:247:ARG:HA	1:C:280:LEU:HD11	1.92	0.50
1:A:410:VAL:HG21	4:A:1003:Y01:HAT2	1.93	0.50
1:A:702:ASN:ND2	6:B:1006:POV:H15A	2.25	0.50
1:B:208:ALA:HA	1:B:214:THR:HG22	1.94	0.50
1:D:885:LYS:HZ2	1:D:889:GLN:HE21	1.59	0.50
1:A:462:ALA:HA	1:A:465:PHE:CD2	2.47	0.50
1:D:410:VAL:HG21	4:D:1005:Y01:HAT2	1.93	0.50
6:A:1006:POV:H15	4:D:1002:Y01:OAG	2.11	0.50
4:B:1010:Y01:OAG	6:C:1006:POV:H15	2.11	0.50
1:C:462:ALA:HA	1:C:465:PHE:CD2	2.47	0.49
6:A:1006:POV:H13	4:D:1002:Y01:OAG	2.12	0.49
1:C:217:SER:HB3	1:C:220:VAL:HG23	1.94	0.49
1:D:217:SER:HB3	1:D:220:VAL:HG23	1.94	0.49
1:D:462:ALA:HA	1:D:465:PHE:CD2	2.47	0.49
4:A:1010:Y01:OAG	6:B:1006:POV:H15	2.11	0.49
1:A:208:ALA:HA	1:A:214:THR:HG22	1.94	0.49
4:C:1010:Y01:OAG	6:D:1008:POV:H13	2.12	0.49
1:B:217:SER:HB3	1:B:220:VAL:HG23	1.94	0.49
1:C:208:ALA:HA	1:C:214:THR:HG22	1.94	0.49
4:A:1010:Y01:OAG	6:B:1006:POV:H13	2.12	0.49
1:D:292:ASP:N	1:D:292:ASP:OD1	2.46	0.49
1:A:217:SER:HB3	1:A:220:VAL:HG23	1.94	0.49
4:B:1010:Y01:OAG	6:C:1006:POV:H13	2.12	0.49
1:C:292:ASP:OD1	1:C:292:ASP:N	2.46	0.49
1:D:208:ALA:HA	1:D:214:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ASN:ND2	6:D:1008:POV:H15A	2.25	0.48
1:B:292:ASP:OD1	1:B:292:ASP:N	2.46	0.47
4:C:1007:Y01:HAP1	4:C:1007:Y01:HAO1	1.63	0.47
1:B:511:LYS:HB3	1:B:511:LYS:HZ3	1.76	0.47
1:D:417:LEU:HD11	1:D:761:PRO:HG2	1.97	0.47
1:A:417:LEU:HD11	1:A:761:PRO:HG2	1.97	0.47
1:B:417:LEU:HD11	1:B:761:PRO:HG2	1.96	0.47
1:C:417:LEU:HD11	1:C:761:PRO:HG2	1.97	0.47
1:D:513:ILE:HG13	1:D:521:TYR:CD1	2.49	0.47
1:A:156:GLU:HG2	1:A:157:ASN:H	1.80	0.47
1:A:513:ILE:HG13	1:A:521:TYR:CD1	2.49	0.47
1:B:131:TYR:CZ	1:B:132:MET:HG2	2.49	0.47
1:B:156:GLU:HG2	1:B:157:ASN:H	1.80	0.47
1:C:156:GLU:HG2	1:C:157:ASN:H	1.80	0.47
1:D:156:GLU:HG2	1:D:157:ASN:H	1.80	0.47
4:D:1009:Y01:HAP1	4:D:1009:Y01:HAO1	1.63	0.47
1:B:513:ILE:HG13	1:B:521:TYR:CD1	2.49	0.47
1:C:131:TYR:CZ	1:C:132:MET:HG2	2.49	0.47
1:C:513:ILE:HG13	1:C:521:TYR:CD1	2.49	0.47
1:C:511:LYS:HB3	1:C:511:LYS:HZ2	1.78	0.47
1:A:131:TYR:CZ	1:A:132:MET:HG2	2.50	0.46
4:C:1007:Y01:HAE2	4:C:1007:Y01:HBB	1.58	0.46
1:A:131:TYR:OH	1:B:233:GLU:HG2	2.16	0.46
1:C:675:PHE:HE1	6:C:1006:POV:H28	1.81	0.46
1:A:292:ASP:OD1	1:A:292:ASP:N	2.46	0.46
1:C:191:ARG:HD2	1:C:238:LEU:HD22	1.98	0.46
1:D:131:TYR:CZ	1:D:132:MET:HG2	2.50	0.46
1:A:191:ARG:HD2	1:A:238:LEU:HD22	1.98	0.46
1:A:511:LYS:HB3	1:A:511:LYS:HZ1	1.78	0.46
1:D:191:ARG:HD2	1:D:238:LEU:HD22	1.98	0.46
1:B:191:ARG:HD2	1:B:238:LEU:HD22	1.98	0.46
1:C:375:LYS:HD3	1:C:744:PHE:CG	2.51	0.46
1:B:375:LYS:HD3	1:B:744:PHE:CG	2.51	0.46
1:D:375:LYS:HD3	1:D:744:PHE:CG	2.51	0.46
1:B:131:TYR:OH	1:C:233:GLU:HG2	2.16	0.45
1:C:376:LYS:HE3	1:C:376:LYS:HB2	1.80	0.45
1:A:375:LYS:HD3	1:A:744:PHE:CG	2.51	0.45
6:D:1008:POV:H28	6:D:1008:POV:H25	1.78	0.45
1:A:233:GLU:HG2	1:D:131:TYR:OH	2.16	0.45
1:B:640:ILE:HG23	3:C:1002:W99:C9	2.47	0.45
4:B:1007:Y01:HBB	4:B:1007:Y01:HAE2	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ASN:HD22	1:C:599:TYR:HE1	1.65	0.45
3:A:1002:W99:C9	1:D:640:ILE:HG23	2.47	0.45
1:B:530:ASP:OD2	1:B:609:ARG:NH1	2.50	0.45
1:C:640:ILE:HG23	3:D:1004:W99:C9	2.47	0.45
1:A:599:TYR:HE1	1:D:654:ASN:HD22	1.65	0.45
1:D:525:LEU:HD12	1:D:525:LEU:C	2.37	0.45
4:D:1009:Y01:HAE2	4:D:1009:Y01:HBB	1.58	0.45
1:C:654:ASN:HD22	1:D:599:TYR:HE1	1.65	0.45
1:A:530:ASP:OD2	1:A:609:ARG:NH1	2.50	0.45
1:A:640:ILE:HG23	3:B:1002:W99:C9	2.47	0.45
1:C:525:LEU:HD12	1:C:525:LEU:C	2.37	0.45
1:A:525:LEU:HD12	1:A:525:LEU:C	2.37	0.45
1:C:131:TYR:OH	1:D:233:GLU:HG2	2.16	0.45
1:A:654:ASN:HD22	1:B:599:TYR:HE1	1.65	0.44
6:B:1006:POV:H11A	6:B:1006:POV:H13B	1.46	0.44
1:D:530:ASP:OD2	1:D:609:ARG:NH1	2.50	0.44
1:D:663:LYS:HE2	1:D:663:LYS:HB3	1.88	0.44
1:D:675:PHE:HE1	6:D:1008:POV:H28	1.81	0.44
1:C:530:ASP:OD2	1:C:609:ARG:NH1	2.50	0.44
1:C:880:ASN:HD21	1:C:883:GLU:HB2	1.83	0.44
1:A:675:PHE:HE1	6:A:1006:POV:H28	1.81	0.44
1:D:209:TYR:H	1:D:209:TYR:HD2	1.65	0.44
1:B:525:LEU:HD12	1:B:525:LEU:C	2.37	0.44
6:C:1006:POV:H28	6:C:1006:POV:H25	1.78	0.44
6:A:1006:POV:H28	6:A:1006:POV:H25	1.78	0.44
4:D:1005:Y01:HAJ2	4:D:1005:Y01:HBE	1.86	0.44
4:C:1003:Y01:HAJ2	4:C:1003:Y01:HBE	1.87	0.44
1:B:209:TYR:H	1:B:209:TYR:HD2	1.65	0.44
1:D:880:ASN:HD21	1:D:883:GLU:HB2	1.82	0.43
6:D:1008:POV:H11A	6:D:1008:POV:H13B	1.46	0.43
4:A:1007:Y01:HAO1	4:A:1007:Y01:HAP1	1.63	0.43
1:A:700:ILE:HG13	1:B:593:ILE:HG23	2.00	0.43
1:B:513:ILE:HG13	1:B:521:TYR:CG	2.54	0.43
1:C:700:ILE:HG13	1:D:593:ILE:HG23	2.00	0.43
1:A:436:MET:HB2	1:A:436:MET:HE2	1.90	0.43
1:C:417:LEU:HD21	1:C:761:PRO:HG2	2.01	0.43
1:A:271:ARG:HA	1:A:274:ILE:HG22	2.01	0.43
1:A:593:ILE:HG23	1:D:700:ILE:HG13	2.00	0.43
1:B:675:PHE:HE1	6:B:1006:POV:H28	1.81	0.43
6:C:1006:POV:H11A	6:C:1006:POV:H13B	1.46	0.43
1:D:513:ILE:HG13	1:D:521:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1003:Y01:HAJ2	4:A:1003:Y01:HBE	1.87	0.43
1:C:105:ALA:HB1	1:C:110:ASN:HB3	2.01	0.43
1:A:209:TYR:H	1:A:209:TYR:HD2	1.65	0.43
1:B:663:LYS:HE2	1:B:663:LYS:HB3	1.88	0.43
4:B:1007:Y01:HAO1	4:B:1007:Y01:HAP1	1.63	0.43
1:A:513:ILE:HG13	1:A:521:TYR:CG	2.54	0.43
1:D:529:LEU:HD12	1:D:529:LEU:HA	1.90	0.43
1:C:209:TYR:H	1:C:209:TYR:HD2	1.65	0.42
1:C:513:ILE:HG13	1:C:521:TYR:CG	2.54	0.42
1:D:417:LEU:HD21	1:D:761:PRO:HG2	2.01	0.42
1:A:417:LEU:HD21	1:A:761:PRO:HG2	2.01	0.42
1:D:105:ALA:HB1	1:D:110:ASN:HB3	2.01	0.42
1:B:700:ILE:HG13	1:C:593:ILE:HG23	2.00	0.42
1:D:271:ARG:HA	1:D:274:ILE:HG22	2.01	0.42
1:A:886:GLU:O	1:A:886:GLU:HG2	2.18	0.42
1:A:170:SER:HB3	1:A:225:LEU:HD21	2.02	0.42
1:A:315:LYS:HG2	1:A:319:LYS:HE3	2.02	0.42
1:A:880:ASN:HD21	1:A:883:GLU:HB2	1.83	0.42
1:B:462:ALA:HA	1:B:465:PHE:HD2	1.84	0.42
1:D:886:GLU:O	1:D:886:GLU:HG2	2.18	0.42
1:D:462:ALA:HA	1:D:465:PHE:HD2	1.84	0.42
1:B:105:ALA:HB1	1:B:110:ASN:HB3	2.01	0.42
1:B:417:LEU:HD21	1:B:761:PRO:HG2	2.01	0.42
4:B:1010:Y01:HAD1	4:B:1010:Y01:HAR2	1.86	0.42
1:C:271:ARG:HA	1:C:274:ILE:HG22	2.01	0.42
1:B:315:LYS:HG2	1:B:319:LYS:HE3	2.02	0.42
1:B:445:ALA:HB1	1:B:761:PRO:HG3	2.02	0.42
1:B:170:SER:HB3	1:B:225:LEU:HD21	2.02	0.42
1:C:170:SER:HB3	1:C:225:LEU:HD21	2.02	0.42
1:B:880:ASN:HD21	1:B:883:GLU:HB2	1.82	0.41
1:C:96:SER:O	1:C:98:GLU:N	2.54	0.41
1:D:315:LYS:HG2	1:D:319:LYS:HE3	2.02	0.41
1:D:376:LYS:HE3	1:D:376:LYS:HB2	1.81	0.41
1:D:445:ALA:HB1	1:D:761:PRO:HG3	2.02	0.41
1:A:522:LEU:C	1:A:522:LEU:HD12	2.41	0.41
1:A:881:GLU:OE1	1:B:874:LYS:O	2.39	0.41
1:B:881:GLU:OE1	1:C:874:LYS:O	2.39	0.41
1:C:165:LEU:HB2	1:C:180:ILE:HG21	2.03	0.41
1:A:445:ALA:HB1	1:A:761:PRO:HG3	2.02	0.41
1:B:271:ARG:HA	1:B:274:ILE:HG22	2.01	0.41
1:C:522:LEU:O	1:C:522:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:ASP:N	1:C:574:ASP:OD1	2.53	0.41
1:D:880:ASN:ND2	1:D:880:ASN:C	2.73	0.41
1:A:522:LEU:O	1:A:522:LEU:HD12	2.21	0.41
1:B:376:LYS:HE3	1:B:376:LYS:HB2	1.80	0.41
1:A:105:ALA:HB1	1:A:110:ASN:HB3	2.01	0.41
1:A:353:LEU:HB3	1:A:362:ASN:ND2	2.36	0.41
1:C:353:LEU:HB3	1:C:362:ASN:ND2	2.36	0.41
1:C:445:ALA:HB1	1:C:761:PRO:HG3	2.02	0.41
1:D:165:LEU:HB2	1:D:180:ILE:HG21	2.03	0.41
1:D:353:LEU:HB3	1:D:362:ASN:ND2	2.36	0.41
4:A:1007:Y01:HBB	4:A:1007:Y01:HAE2	1.58	0.41
1:B:165:LEU:HB2	1:B:180:ILE:HG21	2.03	0.41
1:C:522:LEU:HD12	1:C:522:LEU:C	2.41	0.41
1:A:614:LEU:HB3	1:A:624:GLN:OE1	2.21	0.41
1:B:574:ASP:OD1	1:B:574:ASP:N	2.54	0.41
1:C:886:GLU:O	1:C:886:GLU:HG2	2.18	0.41
1:D:170:SER:HB3	1:D:225:LEU:HD21	2.02	0.41
1:A:96:SER:O	1:A:98:GLU:N	2.54	0.41
1:B:96:SER:O	1:B:98:GLU:N	2.54	0.41
1:B:353:LEU:HB3	1:B:362:ASN:ND2	2.36	0.41
1:C:881:GLU:OE1	1:D:874:LYS:O	2.39	0.41
1:D:522:LEU:O	1:D:522:LEU:HD12	2.21	0.41
1:D:522:LEU:C	1:D:522:LEU:HD12	2.41	0.41
1:D:574:ASP:OD1	1:D:574:ASP:N	2.53	0.41
1:A:165:LEU:HB2	1:A:180:ILE:HG21	2.03	0.41
1:A:462:ALA:HA	1:A:465:PHE:HD2	1.84	0.41
1:A:874:LYS:O	1:D:881:GLU:OE1	2.39	0.41
6:A:1006:POV:H13B	6:A:1006:POV:H11A	1.46	0.41
1:B:522:LEU:HD12	1:B:522:LEU:C	2.41	0.41
1:C:315:LYS:HG2	1:C:319:LYS:HE3	2.02	0.41
1:C:880:ASN:ND2	1:C:883:GLU:H	2.19	0.41
1:D:614:LEU:HB3	1:D:624:GLN:OE1	2.21	0.41
1:B:880:ASN:ND2	1:B:883:GLU:H	2.19	0.41
1:C:462:ALA:HA	1:C:465:PHE:HD2	1.84	0.41
1:C:663:LYS:HE2	1:C:663:LYS:HB3	1.88	0.41
1:A:175:ARG:HD2	1:D:108:TYR:CE1	2.57	0.40
1:A:680:TRP:HZ3	1:D:712:ASN:HD22	1.69	0.40
1:B:712:ASN:HD22	1:C:680:TRP:HZ3	1.69	0.40
1:D:96:SER:O	1:D:98:GLU:N	2.54	0.40
1:A:574:ASP:OD1	1:A:574:ASP:N	2.54	0.40
4:A:1007:Y01:HAD2	4:A:1007:Y01:HAS2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:LEU:HB3	1:B:624:GLN:OE1	2.21	0.40
1:B:880:ASN:ND2	1:B:880:ASN:C	2.73	0.40
1:D:880:ASN:ND2	1:D:883:GLU:H	2.19	0.40
4:D:1009:Y01:HAD2	4:D:1009:Y01:HAS2	1.84	0.40
1:B:522:LEU:O	1:B:522:LEU:HD12	2.21	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	675/931 (72%)	650 (96%)	24 (4%)	1 (0%)	51	82
1	B	675/931 (72%)	650 (96%)	24 (4%)	1 (0%)	51	82
1	C	675/931 (72%)	650 (96%)	24 (4%)	1 (0%)	51	82
1	D	675/931 (72%)	650 (96%)	24 (4%)	1 (0%)	51	82
All	All	2700/3724 (72%)	2600 (96%)	96 (4%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	PHE
1	B	523	PHE
1	C	523	PHE
1	D	523	PHE

### 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	591/813 (73%)	582 (98%)	9 (2%)	65	87
1	B	591/813 (73%)	582 (98%)	9 (2%)	65	87
1	C	591/813 (73%)	582 (98%)	9 (2%)	65	87
1	D	591/813 (73%)	582 (98%)	9 (2%)	65	87
All	All	2364/3252 (73%)	2328 (98%)	36 (2%)	66	87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	166	LEU
1	A	209	TYR
1	A	274	ILE
1	A	398	LEU
1	A	417	LEU
1	A	501	TRP
1	A	537	PHE
1	A	880	ASN
1	B	98	GLU
1	B	166	LEU
1	B	209	TYR
1	B	274	ILE
1	B	398	LEU
1	B	417	LEU
1	B	501	TRP
1	B	537	PHE
1	B	880	ASN
1	C	98	GLU
1	C	166	LEU
1	C	209	TYR
1	C	274	ILE
1	C	398	LEU
1	C	417	LEU
1	C	501	TRP
1	C	537	PHE
1	C	880	ASN
1	D	98	GLU
1	D	166	LEU
1	D	209	TYR

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Mol	Chain	Res	Type
1	D	274	ILE
1	D	398	LEU
1	D	417	LEU
1	D	501	TRP
1	D	537	PHE
1	D	880	ASN

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

Mol	Chain	Res	Type
1	A	702	ASN
1	A	880	ASN
1	A	889	GLN
1	B	702	ASN
1	B	880	ASN
1	B	889	GLN
1	C	702	ASN
1	C	880	ASN
1	C	889	GLN
1	D	702	ASN
1	D	880	ASN
1	D	889	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 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	Y01	B	1010	-	38,38,38	0.95	1 (2%)	57,57,57	1.35	7 (12%)
7	98R	D	1010	-	40,40,43	0.98	2 (5%)	42,42,45	1.13	2 (4%)
3	W99	B	1002	-	25,28,28	0.95	3 (12%)	30,40,40	1.49	5 (16%)
4	Y01	C	1007	-	38,38,38	0.97	1 (2%)	57,57,57	1.42	8 (14%)
6	POV	B	1006	-	45,45,51	0.98	2 (4%)	51,53,59	1.05	4 (7%)
3	W99	A	1002	-	25,28,28	0.94	3 (12%)	30,40,40	1.49	5 (16%)
6	POV	D	1008	-	45,45,51	0.97	2 (4%)	51,53,59	1.05	4 (7%)
4	Y01	C	1003	-	38,38,38	0.95	1 (2%)	57,57,57	1.37	9 (15%)
4	Y01	A	1003	-	38,38,38	0.95	1 (2%)	57,57,57	1.38	9 (15%)
3	W99	D	1004	-	25,28,28	0.95	3 (12%)	30,40,40	1.49	5 (16%)
7	98R	A	1008	-	40,40,43	0.97	2 (5%)	42,42,45	1.13	2 (4%)
4	Y01	B	1007	-	38,38,38	0.97	1 (2%)	57,57,57	1.42	7 (12%)
4	Y01	D	1009	-	38,38,38	0.97	1 (2%)	57,57,57	1.42	8 (14%)
6	POV	C	1006	-	45,45,51	0.98	2 (4%)	51,53,59	1.05	4 (7%)
4	Y01	B	1003	-	38,38,38	0.95	1 (2%)	57,57,57	1.38	9 (15%)
4	Y01	C	1010	-	38,38,38	0.95	1 (2%)	57,57,57	1.35	7 (12%)
4	Y01	A	1007	-	38,38,38	0.97	1 (2%)	57,57,57	1.42	7 (12%)
7	98R	B	1008	-	40,40,43	0.97	2 (5%)	42,42,45	1.13	2 (4%)
4	Y01	D	1005	-	38,38,38	0.95	1 (2%)	57,57,57	1.38	9 (15%)
6	POV	A	1006	-	45,45,51	0.97	2 (4%)	51,53,59	1.05	4 (7%)
4	Y01	A	1010	-	38,38,38	0.95	1 (2%)	57,57,57	1.35	7 (12%)
4	Y01	D	1002	-	38,38,38	0.95	1 (2%)	57,57,57	1.35	7 (12%)
7	98R	C	1008	-	40,40,43	0.98	2 (5%)	42,42,45	1.13	2 (4%)
3	W99	C	1002	-	25,28,28	0.94	3 (12%)	30,40,40	1.49	6 (20%)

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	Y01	B	1010	-	-	9/19/77/77	0/4/4/4
7	98R	D	1010	-	-	21/42/42/45	-
3	W99	B	1002	-	-	4/6/30/30	0/4/4/4
4	Y01	C	1007	-	-	6/19/77/77	0/4/4/4
6	POV	B	1006	-	-	21/49/49/55	-
3	W99	A	1002	-	-	4/6/30/30	0/4/4/4
6	POV	D	1008	-	-	21/49/49/55	-
4	Y01	C	1003	-	-	7/19/77/77	0/4/4/4
4	Y01	A	1003	-	-	7/19/77/77	0/4/4/4
3	W99	D	1004	-	-	4/6/30/30	0/4/4/4
7	98R	A	1008	-	-	21/42/42/45	-
4	Y01	B	1007	-	-	6/19/77/77	0/4/4/4
4	Y01	D	1009	-	-	6/19/77/77	0/4/4/4
6	POV	C	1006	-	-	21/49/49/55	-
4	Y01	B	1003	-	-	7/19/77/77	0/4/4/4
4	Y01	C	1010	-	-	9/19/77/77	0/4/4/4
4	Y01	A	1007	-	-	6/19/77/77	0/4/4/4
7	98R	B	1008	-	-	22/42/42/45	-
4	Y01	D	1005	-	-	7/19/77/77	0/4/4/4
6	POV	A	1006	-	-	21/49/49/55	-
4	Y01	A	1010	-	-	9/19/77/77	0/4/4/4
4	Y01	D	1002	-	-	9/19/77/77	0/4/4/4
7	98R	C	1008	-	-	22/42/42/45	-
3	W99	C	1002	-	-	4/6/30/30	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1008	98R	O3-C11	4.21	1.45	1.33
4	C	1007	Y01	OAW-CAY	4.19	1.46	1.34
7	D	1010	98R	O3-C11	4.19	1.45	1.33
4	B	1003	Y01	OAW-CAY	4.19	1.46	1.34
4	C	1003	Y01	OAW-CAY	4.19	1.46	1.34
4	D	1005	Y01	OAW-CAY	4.19	1.46	1.34
4	A	1007	Y01	OAW-CAY	4.18	1.46	1.34
4	B	1007	Y01	OAW-CAY	4.17	1.46	1.34
7	B	1008	98R	O3-C11	4.17	1.45	1.33
7	A	1008	98R	O3-C11	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1009	Y01	OAW-CAY	4.16	1.46	1.34
4	A	1003	Y01	OAW-CAY	4.16	1.46	1.34
4	C	1010	Y01	OAW-CAY	4.12	1.45	1.34
4	A	1010	Y01	OAW-CAY	4.12	1.45	1.34
4	B	1010	Y01	OAW-CAY	4.12	1.45	1.34
4	D	1002	Y01	OAW-CAY	4.12	1.45	1.34
6	B	1006	POV	O31-C31	4.09	1.45	1.33
6	C	1006	POV	O31-C31	4.09	1.45	1.33
6	D	1008	POV	O31-C31	4.06	1.45	1.33
6	A	1006	POV	O31-C31	4.06	1.45	1.33
7	A	1008	98R	O2-C31	3.91	1.45	1.34
7	B	1008	98R	O2-C31	3.91	1.45	1.34
7	C	1008	98R	O2-C31	3.91	1.45	1.34
7	D	1010	98R	O2-C31	3.91	1.45	1.34
6	A	1006	POV	O21-C21	3.90	1.45	1.34
6	B	1006	POV	O21-C21	3.90	1.45	1.34
6	C	1006	POV	O21-C21	3.90	1.45	1.34
6	D	1008	POV	O21-C21	3.90	1.45	1.34
3	A	1002	W99	C6-C1	2.55	1.45	1.39
3	B	1002	W99	C6-C1	2.55	1.45	1.39
3	C	1002	W99	C6-C1	2.55	1.45	1.39
3	D	1004	W99	C6-C1	2.55	1.45	1.39
3	B	1002	W99	C4-N	-2.24	1.35	1.40
3	A	1002	W99	C4-N	-2.22	1.35	1.40
3	D	1004	W99	C4-N	-2.20	1.35	1.40
3	C	1002	W99	C4-N	-2.19	1.35	1.40
3	D	1004	W99	C9-S	2.18	1.74	1.70
3	B	1002	W99	C9-S	2.17	1.74	1.70
3	A	1002	W99	C9-S	2.15	1.74	1.70
3	C	1002	W99	C9-S	2.15	1.74	1.70

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1007	Y01	CBI-CBE-CBB	-4.29	112.77	119.49
4	D	1009	Y01	CBI-CBE-CBB	-4.29	112.77	119.49
4	C	1007	Y01	CBI-CBE-CBB	-4.27	112.80	119.49
4	A	1007	Y01	CBI-CBE-CBB	-4.27	112.80	119.49
4	A	1003	Y01	OAW-CAY-CAM	4.13	120.41	111.50
4	B	1003	Y01	OAW-CAY-CAM	4.13	120.40	111.50
4	C	1003	Y01	OAW-CAY-CAM	4.13	120.39	111.50
4	D	1005	Y01	OAW-CAY-CAM	4.13	120.39	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1008	98R	O2-C31-C32	4.11	120.35	111.50
7	C	1008	98R	O2-C31-C32	4.11	120.35	111.50
7	D	1010	98R	O2-C31-C32	4.11	120.35	111.50
7	B	1008	98R	O2-C31-C32	4.10	120.34	111.50
4	B	1007	Y01	OAW-CAY-CAM	3.93	119.97	111.50
4	D	1009	Y01	OAW-CAY-CAM	3.91	119.92	111.50
4	C	1010	Y01	OAW-CAY-CAM	3.90	119.90	111.50
4	A	1007	Y01	OAW-CAY-CAM	3.90	119.90	111.50
4	C	1007	Y01	OAW-CAY-CAM	3.89	119.88	111.50
4	A	1010	Y01	OAW-CAY-CAM	3.88	119.86	111.50
4	B	1010	Y01	OAW-CAY-CAM	3.88	119.86	111.50
4	D	1002	Y01	OAW-CAY-CAM	3.87	119.83	111.50
6	B	1006	POV	O21-C21-C22	3.83	119.76	111.50
6	A	1006	POV	O21-C21-C22	3.82	119.73	111.50
6	C	1006	POV	O21-C21-C22	3.82	119.72	111.50
6	D	1008	POV	O21-C21-C22	3.82	119.72	111.50
4	B	1010	Y01	CAV-CAZ-CBH	3.47	121.03	116.42
4	C	1010	Y01	CAV-CAZ-CBH	3.47	121.02	116.42
4	D	1002	Y01	CAV-CAZ-CBH	3.44	120.99	116.42
4	A	1010	Y01	CAV-CAZ-CBH	3.43	120.97	116.42
4	D	1005	Y01	CAK-CBD-CBF	3.33	113.75	109.71
4	A	1003	Y01	CAK-CBD-CBF	3.30	113.71	109.71
4	B	1003	Y01	CAK-CBD-CBF	3.30	113.71	109.71
4	C	1003	Y01	CAK-CBD-CBF	3.30	113.71	109.71
6	B	1006	POV	C2-O21-C21	-2.94	110.56	117.79
6	C	1006	POV	C2-O21-C21	-2.92	110.59	117.79
6	D	1008	POV	C2-O21-C21	-2.92	110.59	117.79
6	A	1006	POV	C2-O21-C21	-2.92	110.61	117.79
3	B	1002	W99	C8-C9-S	-2.90	108.23	111.79
3	D	1004	W99	C8-C9-S	-2.87	108.27	111.79
3	A	1002	W99	C8-C9-S	-2.84	108.30	111.79
3	C	1002	W99	C8-C9-S	-2.84	108.30	111.79
4	A	1007	Y01	CBG-CBI-CBE	2.84	103.44	100.07
4	B	1007	Y01	CBG-CBI-CBE	2.83	103.42	100.07
4	C	1007	Y01	CBG-CBI-CBE	2.83	103.42	100.07
4	D	1009	Y01	CBG-CBI-CBE	2.82	103.42	100.07
4	B	1007	Y01	CAV-CAZ-CBH	2.74	120.06	116.42
3	D	1004	W99	C-O-C1	2.73	108.89	105.34
3	A	1002	W99	C-O-C1	2.73	108.88	105.34
3	C	1002	W99	C-O-C1	2.73	108.88	105.34
3	B	1002	W99	C-O-C1	2.72	108.87	105.34
3	C	1002	W99	C4-N-C7	-2.70	122.55	129.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1007	Y01	CAV-CAZ-CBH	2.70	120.01	116.42
3	A	1002	W99	C4-N-C7	-2.70	122.55	129.39
4	D	1002	Y01	CBC-CAV-CAZ	2.70	115.71	111.52
4	A	1010	Y01	CBC-CAV-CAZ	2.69	115.70	111.52
4	A	1007	Y01	CAV-CAZ-CBH	2.69	120.00	116.42
7	A	1008	98R	O3-C11-C12	2.69	120.36	111.91
7	B	1008	98R	O3-C11-C12	2.69	120.36	111.91
4	D	1009	Y01	CAV-CAZ-CBH	2.69	120.00	116.42
3	D	1004	W99	C4-N-C7	-2.69	122.58	129.39
4	C	1010	Y01	CBC-CAV-CAZ	2.68	115.67	111.52
3	B	1002	W99	C4-N-C7	-2.68	122.61	129.39
7	C	1008	98R	O3-C11-C12	2.67	120.30	111.91
7	D	1010	98R	O3-C11-C12	2.67	120.29	111.91
4	B	1010	Y01	CBC-CAV-CAZ	2.67	115.66	111.52
3	D	1004	W99	C-O2-C6	2.65	108.78	105.34
3	A	1002	W99	C-O2-C6	2.64	108.77	105.34
3	C	1002	W99	C-O2-C6	2.64	108.77	105.34
3	B	1002	W99	C-O2-C6	2.62	108.74	105.34
4	B	1003	Y01	CBC-OAW-CAY	-2.46	111.73	117.79
4	C	1003	Y01	CBC-OAW-CAY	-2.44	111.77	117.79
4	D	1005	Y01	CBC-OAW-CAY	-2.44	111.77	117.79
4	A	1003	Y01	CBC-OAW-CAY	-2.44	111.80	117.79
3	A	1002	W99	C15-N2-C11	2.37	119.27	114.49
3	B	1002	W99	C15-N2-C11	2.37	119.27	114.49
3	D	1004	W99	C15-N2-C11	2.37	119.27	114.49
3	C	1002	W99	C15-N2-C11	2.36	119.26	114.49
4	A	1003	Y01	CBC-CAV-CAZ	-2.30	107.95	111.52
4	B	1003	Y01	CBC-CAV-CAZ	-2.30	107.95	111.52
4	C	1003	Y01	CBC-CAV-CAZ	-2.29	107.95	111.52
4	D	1005	Y01	CBC-CAV-CAZ	-2.29	107.95	111.52
4	A	1010	Y01	CAT-CBH-CBF	2.24	111.86	108.73
6	B	1006	POV	O31-C31-C32	2.22	118.89	111.91
6	C	1006	POV	O31-C31-C32	2.22	118.89	111.91
6	D	1008	POV	O31-C31-C32	2.22	118.88	111.91
6	A	1006	POV	O31-C31-C32	2.22	118.88	111.91
4	C	1010	Y01	CAT-CBH-CBF	2.22	111.83	108.73
4	D	1009	Y01	CAS-CAU-CBI	-2.21	108.99	112.78
4	D	1002	Y01	CAT-CBH-CBF	2.21	111.81	108.73
4	C	1007	Y01	CAS-CAU-CBI	-2.21	108.99	112.78
4	B	1010	Y01	CAT-CBH-CBF	2.20	111.80	108.73
4	A	1007	Y01	CAS-CAU-CBI	-2.19	109.02	112.78
4	B	1007	Y01	CAS-CAU-CBI	-2.19	109.03	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1007	Y01	CBD-CAK-CAI	-2.17	109.62	112.73
4	A	1003	Y01	CAV-CAZ-CBH	2.16	119.29	116.42
4	B	1003	Y01	CAV-CAZ-CBH	2.16	119.29	116.42
4	C	1003	Y01	CAV-CAZ-CBH	2.16	119.29	116.42
4	D	1005	Y01	CAV-CAZ-CBH	2.16	119.29	116.42
4	C	1007	Y01	CBD-CAK-CAI	-2.16	109.63	112.73
4	A	1007	Y01	CBD-CAK-CAI	-2.13	109.67	112.73
4	D	1009	Y01	CBD-CAK-CAI	-2.12	109.68	112.73
4	D	1005	Y01	CAJ-CAO-CBB	-2.11	108.98	115.03
4	A	1003	Y01	CAJ-CAO-CBB	-2.10	109.00	115.03
4	C	1003	Y01	CAJ-CAO-CBB	-2.10	109.00	115.03
4	B	1003	Y01	CAJ-CAO-CBB	-2.10	109.01	115.03
4	D	1009	Y01	CAS-CBF-CBH	-2.08	110.33	113.08
4	C	1010	Y01	CAK-CBD-CBF	2.08	112.23	109.71
4	A	1007	Y01	CAS-CBF-CBH	-2.06	110.36	113.08
4	B	1010	Y01	CAK-CBD-CBF	2.06	112.21	109.71
4	B	1010	Y01	CBH-CAZ-CAI	-2.06	119.76	122.90
4	D	1002	Y01	CAK-CBD-CBF	2.05	112.20	109.71
4	A	1010	Y01	CBH-CAZ-CAI	-2.05	119.76	122.90
4	A	1003	Y01	OAH-CAX-CAL	2.05	120.60	114.03
4	C	1003	Y01	CAC-CBB-CBE	2.04	116.05	112.92
4	B	1003	Y01	OAH-CAX-CAL	2.04	120.60	114.03
4	C	1010	Y01	CBH-CAZ-CAI	-2.04	119.78	122.90
4	D	1002	Y01	CBH-CAZ-CAI	-2.04	119.78	122.90
4	D	1005	Y01	CAC-CBB-CBE	2.04	116.05	112.92
4	B	1003	Y01	CAC-CBB-CAO	-2.04	107.16	110.36
4	C	1003	Y01	OAH-CAX-CAL	2.04	120.58	114.03
4	D	1005	Y01	OAH-CAX-CAL	2.04	120.58	114.03
4	A	1010	Y01	CAK-CBD-CBF	2.04	112.18	109.71
4	A	1003	Y01	CAC-CBB-CBE	2.04	116.04	112.92
6	C	1006	POV	O21-C21-O22	-2.03	118.79	123.70
4	A	1003	Y01	CAC-CBB-CAO	-2.03	107.18	110.36
4	A	1010	Y01	OAH-CAX-CAL	2.03	120.55	114.03
4	C	1007	Y01	CAS-CBF-CBH	-2.03	110.41	113.08
6	A	1006	POV	O21-C21-O22	-2.03	118.80	123.70
4	C	1003	Y01	CAC-CBB-CAO	-2.02	107.19	110.36
6	B	1006	POV	O21-C21-O22	-2.02	118.81	123.70
6	D	1008	POV	O21-C21-O22	-2.02	118.81	123.70
3	C	1002	W99	C2-C3-C4	2.02	122.63	120.30
4	D	1005	Y01	CAC-CBB-CAO	-2.02	107.20	110.36
4	B	1010	Y01	OAH-CAX-CAL	2.02	120.52	114.03
4	B	1003	Y01	CAC-CBB-CBE	2.02	116.01	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	Y01	OAH-CAX-CAL	2.01	120.50	114.03
4	C	1010	Y01	OAH-CAX-CAL	2.01	120.49	114.03
4	D	1009	Y01	OAH-CAX-CAL	2.01	120.48	114.03
4	C	1007	Y01	OAH-CAX-CAL	2.01	120.48	114.03
4	B	1007	Y01	CAS-CBF-CBH	-2.00	110.44	113.08

There are no chirality outliers.

All (274) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	W99	C8-C10-N2-C15
3	B	1002	W99	C8-C10-N2-C15
3	C	1002	W99	C8-C10-N2-C15
3	D	1004	W99	C8-C10-N2-C15
4	A	1010	Y01	CAM-CAY-OAW-CBC
4	B	1010	Y01	CAM-CAY-OAW-CBC
4	C	1010	Y01	CAM-CAY-OAW-CBC
4	D	1002	Y01	CAM-CAY-OAW-CBC
6	A	1006	POV	C1-O11-P-O12
6	A	1006	POV	C1-O11-P-O14
6	A	1006	POV	C11-O12-P-O11
6	A	1006	POV	C11-O12-P-O14
6	A	1006	POV	O12-C11-C12-N
6	A	1006	POV	C22-C21-O21-C2
6	B	1006	POV	C1-O11-P-O12
6	B	1006	POV	C1-O11-P-O14
6	B	1006	POV	C11-O12-P-O11
6	B	1006	POV	C11-O12-P-O14
6	B	1006	POV	O12-C11-C12-N
6	B	1006	POV	C22-C21-O21-C2
6	C	1006	POV	C1-O11-P-O12
6	C	1006	POV	C1-O11-P-O14
6	C	1006	POV	C11-O12-P-O11
6	C	1006	POV	C11-O12-P-O14
6	C	1006	POV	O12-C11-C12-N
6	C	1006	POV	C22-C21-O21-C2
6	D	1008	POV	C1-O11-P-O12
6	D	1008	POV	C1-O11-P-O14
6	D	1008	POV	C11-O12-P-O11
6	D	1008	POV	C11-O12-P-O14
6	D	1008	POV	O12-C11-C12-N
6	D	1008	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
7	A	1008	98R	C32-C31-O2-C2
7	B	1008	98R	C32-C31-O2-C2
7	C	1008	98R	C32-C31-O2-C2
7	D	1010	98R	C32-C31-O2-C2
7	A	1008	98R	O11-C11-O3-C3
7	B	1008	98R	O11-C11-O3-C3
7	C	1008	98R	O11-C11-O3-C3
7	D	1010	98R	O11-C11-O3-C3
7	A	1008	98R	C12-C11-O3-C3
7	B	1008	98R	C12-C11-O3-C3
7	C	1008	98R	C12-C11-O3-C3
7	D	1010	98R	C12-C11-O3-C3
4	A	1007	Y01	CAO-CBB-CBE-CBI
4	B	1007	Y01	CAO-CBB-CBE-CBI
4	C	1007	Y01	CAO-CBB-CBE-CBI
4	D	1009	Y01	CAO-CBB-CBE-CBI
4	A	1010	Y01	OAG-CAY-OAW-CBC
4	B	1010	Y01	OAG-CAY-OAW-CBC
4	C	1010	Y01	OAG-CAY-OAW-CBC
4	D	1002	Y01	OAG-CAY-OAW-CBC
4	A	1007	Y01	CAC-CBB-CBE-CBI
4	B	1007	Y01	CAC-CBB-CBE-CBI
4	C	1007	Y01	CAC-CBB-CBE-CBI
4	D	1009	Y01	CAC-CBB-CBE-CBI
3	A	1002	W99	O1-C10-N2-C15
3	B	1002	W99	O1-C10-N2-C15
3	C	1002	W99	O1-C10-N2-C15
3	D	1004	W99	O1-C10-N2-C15
6	A	1006	POV	O22-C21-O21-C2
6	B	1006	POV	O22-C21-O21-C2
6	C	1006	POV	O22-C21-O21-C2
6	D	1008	POV	O22-C21-O21-C2
7	A	1008	98R	O31-C31-O2-C2
7	B	1008	98R	O31-C31-O2-C2
7	C	1008	98R	O31-C31-O2-C2
7	D	1010	98R	O31-C31-O2-C2
4	A	1010	Y01	CAJ-CAO-CBB-CAC
4	B	1010	Y01	CAJ-CAO-CBB-CAC
4	C	1010	Y01	CAJ-CAO-CBB-CAC
4	D	1002	Y01	CAJ-CAO-CBB-CAC
6	A	1006	POV	C32-C31-O31-C3
6	B	1006	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	C	1006	POV	C32-C31-O31-C3
6	D	1008	POV	C32-C31-O31-C3
4	A	1007	Y01	CAC-CBB-CBE-CAP
4	B	1007	Y01	CAC-CBB-CBE-CAP
4	C	1007	Y01	CAC-CBB-CBE-CAP
4	D	1009	Y01	CAC-CBB-CBE-CAP
3	A	1002	W99	O1-C10-N2-C11
3	B	1002	W99	O1-C10-N2-C11
3	C	1002	W99	O1-C10-N2-C11
3	D	1004	W99	O1-C10-N2-C11
6	A	1006	POV	O32-C31-O31-C3
6	B	1006	POV	O32-C31-O31-C3
6	C	1006	POV	O32-C31-O31-C3
6	D	1008	POV	O32-C31-O31-C3
3	A	1002	W99	C8-C10-N2-C11
3	B	1002	W99	C8-C10-N2-C11
3	C	1002	W99	C8-C10-N2-C11
3	D	1004	W99	C8-C10-N2-C11
6	A	1006	POV	C22-C23-C24-C25
6	B	1006	POV	C22-C23-C24-C25
6	C	1006	POV	C22-C23-C24-C25
6	D	1008	POV	C22-C23-C24-C25
4	A	1007	Y01	CAM-CAY-OAW-CBC
4	B	1007	Y01	CAM-CAY-OAW-CBC
4	C	1007	Y01	CAM-CAY-OAW-CBC
4	D	1009	Y01	CAM-CAY-OAW-CBC
4	A	1007	Y01	CAO-CBB-CBE-CAP
4	B	1007	Y01	CAO-CBB-CBE-CAP
4	C	1007	Y01	CAO-CBB-CBE-CAP
4	D	1009	Y01	CAO-CBB-CBE-CAP
4	A	1007	Y01	OAG-CAY-OAW-CBC
4	B	1007	Y01	OAG-CAY-OAW-CBC
4	C	1007	Y01	OAG-CAY-OAW-CBC
4	D	1009	Y01	OAG-CAY-OAW-CBC
7	A	1008	98R	C15-C16-C17-C18
7	B	1008	98R	C15-C16-C17-C18
7	C	1008	98R	C15-C16-C17-C18
7	D	1010	98R	C15-C16-C17-C18
7	A	1008	98R	C42-C43-C44-C45
7	B	1008	98R	C42-C43-C44-C45
7	C	1008	98R	C42-C43-C44-C45
7	D	1010	98R	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
4	A	1003	Y01	CAM-CAY-OAW-CBC
4	B	1003	Y01	CAM-CAY-OAW-CBC
4	C	1003	Y01	CAM-CAY-OAW-CBC
4	D	1005	Y01	CAM-CAY-OAW-CBC
4	A	1010	Y01	CAX-CAL-CAM-CAY
4	B	1010	Y01	CAX-CAL-CAM-CAY
4	C	1010	Y01	CAX-CAL-CAM-CAY
4	D	1002	Y01	CAX-CAL-CAM-CAY
4	A	1003	Y01	OAG-CAY-OAW-CBC
4	B	1003	Y01	OAG-CAY-OAW-CBC
4	C	1003	Y01	OAG-CAY-OAW-CBC
4	D	1005	Y01	OAG-CAY-OAW-CBC
6	B	1006	POV	C24-C25-C26-C27
6	C	1006	POV	C24-C25-C26-C27
6	D	1008	POV	C24-C25-C26-C27
6	A	1006	POV	C24-C25-C26-C27
4	A	1003	Y01	CAN-CAJ-CAO-CBB
4	B	1003	Y01	CAN-CAJ-CAO-CBB
4	C	1003	Y01	CAN-CAJ-CAO-CBB
4	D	1005	Y01	CAN-CAJ-CAO-CBB
7	C	1008	98R	C14-C15-C16-C17
7	A	1008	98R	C14-C15-C16-C17
7	B	1008	98R	C14-C15-C16-C17
7	D	1010	98R	C14-C15-C16-C17
6	A	1006	POV	C35-C36-C37-C38
6	B	1006	POV	C35-C36-C37-C38
6	C	1006	POV	C35-C36-C37-C38
6	D	1008	POV	C35-C36-C37-C38
7	A	1008	98R	C36-C37-C38-C39
7	B	1008	98R	C36-C37-C38-C39
7	C	1008	98R	C36-C37-C38-C39
7	D	1010	98R	C36-C37-C38-C39
6	A	1006	POV	C36-C37-C38-C39
6	D	1008	POV	C36-C37-C38-C39
6	B	1006	POV	C36-C37-C38-C39
6	C	1006	POV	C36-C37-C38-C39
7	C	1008	98R	C16-C17-C18-C19
7	D	1010	98R	C16-C17-C18-C19
7	B	1008	98R	C16-C17-C18-C19
7	A	1008	98R	C16-C17-C18-C19
6	D	1008	POV	C25-C26-C27-C28
6	B	1006	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	C	1006	POV	C25-C26-C27-C28
6	A	1006	POV	C25-C26-C27-C28
7	B	1008	98R	C13-C14-C15-C16
7	A	1008	98R	C13-C14-C15-C16
7	C	1008	98R	C13-C14-C15-C16
7	D	1010	98R	C13-C14-C15-C16
7	A	1008	98R	C22-C23-C24-C25
7	B	1008	98R	C22-C23-C24-C25
7	C	1008	98R	C22-C23-C24-C25
7	D	1010	98R	C22-C23-C24-C25
6	A	1006	POV	C1-C2-O21-C21
6	B	1006	POV	C1-C2-O21-C21
6	C	1006	POV	C1-C2-O21-C21
6	D	1008	POV	C1-C2-O21-C21
6	A	1006	POV	C1-C2-C3-O31
6	B	1006	POV	C1-C2-C3-O31
6	C	1006	POV	C1-C2-C3-O31
6	D	1008	POV	C1-C2-C3-O31
6	A	1006	POV	O21-C2-C3-O31
6	B	1006	POV	O21-C2-C3-O31
6	C	1006	POV	O21-C2-C3-O31
6	D	1008	POV	O21-C2-C3-O31
6	B	1006	POV	C34-C35-C36-C37
6	C	1006	POV	C34-C35-C36-C37
6	D	1008	POV	C34-C35-C36-C37
6	A	1006	POV	C34-C35-C36-C37
7	A	1008	98R	C35-C36-C37-C38
7	B	1008	98R	C35-C36-C37-C38
7	C	1008	98R	C35-C36-C37-C38
7	D	1010	98R	C35-C36-C37-C38
6	A	1006	POV	C33-C34-C35-C36
6	B	1006	POV	C33-C34-C35-C36
6	C	1006	POV	C33-C34-C35-C36
7	A	1008	98R	C33-C34-C35-C36
7	B	1008	98R	C33-C34-C35-C36
7	C	1008	98R	C33-C34-C35-C36
7	D	1010	98R	C33-C34-C35-C36
6	D	1008	POV	C33-C34-C35-C36
7	A	1008	98R	C18-C19-C20-C21
7	B	1008	98R	C18-C19-C20-C21
7	C	1008	98R	C18-C19-C20-C21
7	D	1010	98R	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
4	A	1010	Y01	CAM-CAL-CAX-OAH
4	B	1010	Y01	CAM-CAL-CAX-OAH
4	D	1002	Y01	CAM-CAL-CAX-OAH
4	C	1010	Y01	CAM-CAL-CAX-OAH
4	A	1010	Y01	CAM-CAL-CAX-OAF
4	B	1010	Y01	CAM-CAL-CAX-OAF
4	D	1002	Y01	CAM-CAL-CAX-OAF
4	A	1010	Y01	CAO-CAJ-CAN-CBA
4	B	1010	Y01	CAO-CAJ-CAN-CBA
4	C	1010	Y01	CAO-CAJ-CAN-CBA
4	D	1002	Y01	CAO-CAJ-CAN-CBA
4	C	1010	Y01	CAM-CAL-CAX-OAF
7	B	1008	98R	C32-C33-C34-C35
7	C	1008	98R	C32-C33-C34-C35
7	D	1010	98R	C32-C33-C34-C35
7	A	1008	98R	C32-C33-C34-C35
7	A	1008	98R	C40-C41-C42-C43
7	B	1008	98R	C40-C41-C42-C43
7	C	1008	98R	C40-C41-C42-C43
7	D	1010	98R	C40-C41-C42-C43
4	B	1003	Y01	CAM-CAL-CAX-OAH
4	A	1003	Y01	CAM-CAL-CAX-OAH
4	C	1003	Y01	CAM-CAL-CAX-OAH
4	D	1005	Y01	CAM-CAL-CAX-OAH
7	A	1008	98R	O3-C11-C12-C13
7	C	1008	98R	O3-C11-C12-C13
7	D	1010	98R	O3-C11-C12-C13
7	A	1008	98R	C38-C39-C40-C41
7	B	1008	98R	C38-C39-C40-C41
7	C	1008	98R	C38-C39-C40-C41
7	D	1010	98R	C38-C39-C40-C41
4	A	1003	Y01	CAM-CAL-CAX-OAF
4	B	1003	Y01	CAM-CAL-CAX-OAF
4	C	1003	Y01	CAM-CAL-CAX-OAF
7	B	1008	98R	C12-C13-C14-C15
7	D	1010	98R	C12-C13-C14-C15
4	D	1005	Y01	CAM-CAL-CAX-OAF
4	A	1003	Y01	CAL-CAM-CAY-OAW
4	C	1003	Y01	CAL-CAM-CAY-OAW
4	D	1005	Y01	CAL-CAM-CAY-OAW
7	B	1008	98R	O3-C11-C12-C13
7	A	1008	98R	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	C	1008	98R	C12-C13-C14-C15
4	B	1003	Y01	CAL-CAM-CAY-OAW
4	A	1010	Y01	CAJ-CAN-CBA-CAB
4	B	1010	Y01	CAJ-CAN-CBA-CAB
4	C	1010	Y01	CAJ-CAN-CBA-CAB
4	D	1002	Y01	CAJ-CAN-CBA-CAB
4	A	1003	Y01	CAL-CAM-CAY-OAG
4	B	1003	Y01	CAL-CAM-CAY-OAG
4	C	1003	Y01	CAL-CAM-CAY-OAG
4	D	1005	Y01	CAL-CAM-CAY-OAG
7	A	1008	98R	O11-C11-C12-C13
7	C	1008	98R	O11-C11-C12-C13
7	D	1010	98R	O11-C11-C12-C13
7	B	1008	98R	O11-C11-C12-C13
6	A	1006	POV	C27-C28-C29-C210
6	A	1006	POV	C11-C12-N-C13
6	B	1006	POV	C11-C12-N-C13
6	C	1006	POV	C11-C12-N-C13
6	D	1008	POV	C11-C12-N-C13
6	B	1006	POV	C27-C28-C29-C210
6	C	1006	POV	C27-C28-C29-C210
6	D	1008	POV	C27-C28-C29-C210
4	A	1010	Y01	CAL-CAM-CAY-OAW
4	B	1010	Y01	CAL-CAM-CAY-OAW
4	C	1010	Y01	CAL-CAM-CAY-OAW
4	D	1002	Y01	CAL-CAM-CAY-OAW
7	A	1008	98R	O2-C31-C32-C33
7	B	1008	98R	O2-C31-C32-C33
7	C	1008	98R	O2-C31-C32-C33
7	D	1010	98R	O2-C31-C32-C33
7	B	1008	98R	O31-C31-C32-C33
7	C	1008	98R	O31-C31-C32-C33

There are no ring outliers.

20 monomers are involved in 77 short contacts:

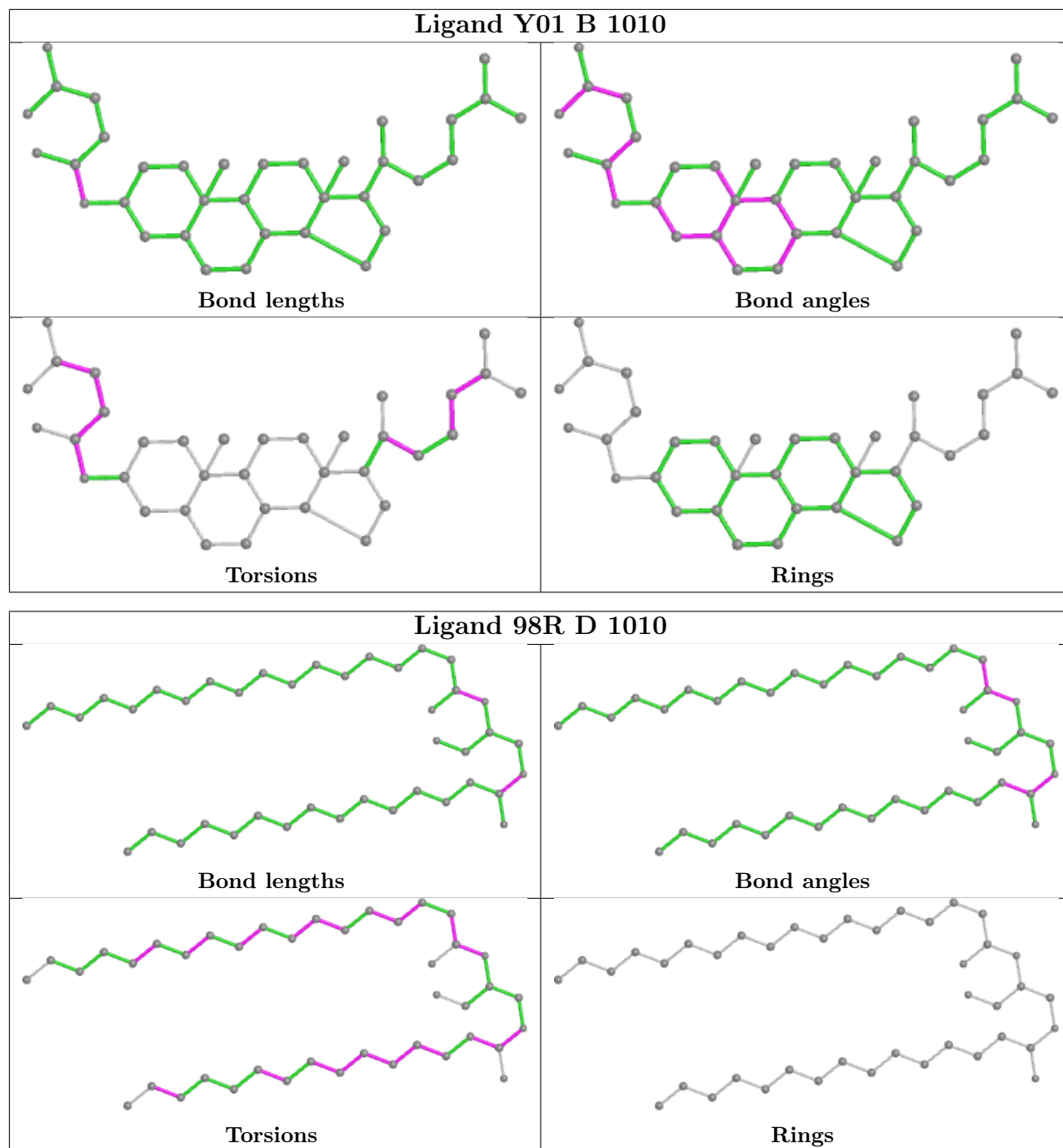
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1010	Y01	4	0
3	B	1002	W99	1	0
4	C	1007	Y01	2	0
6	B	1006	POV	9	0
3	A	1002	W99	1	0

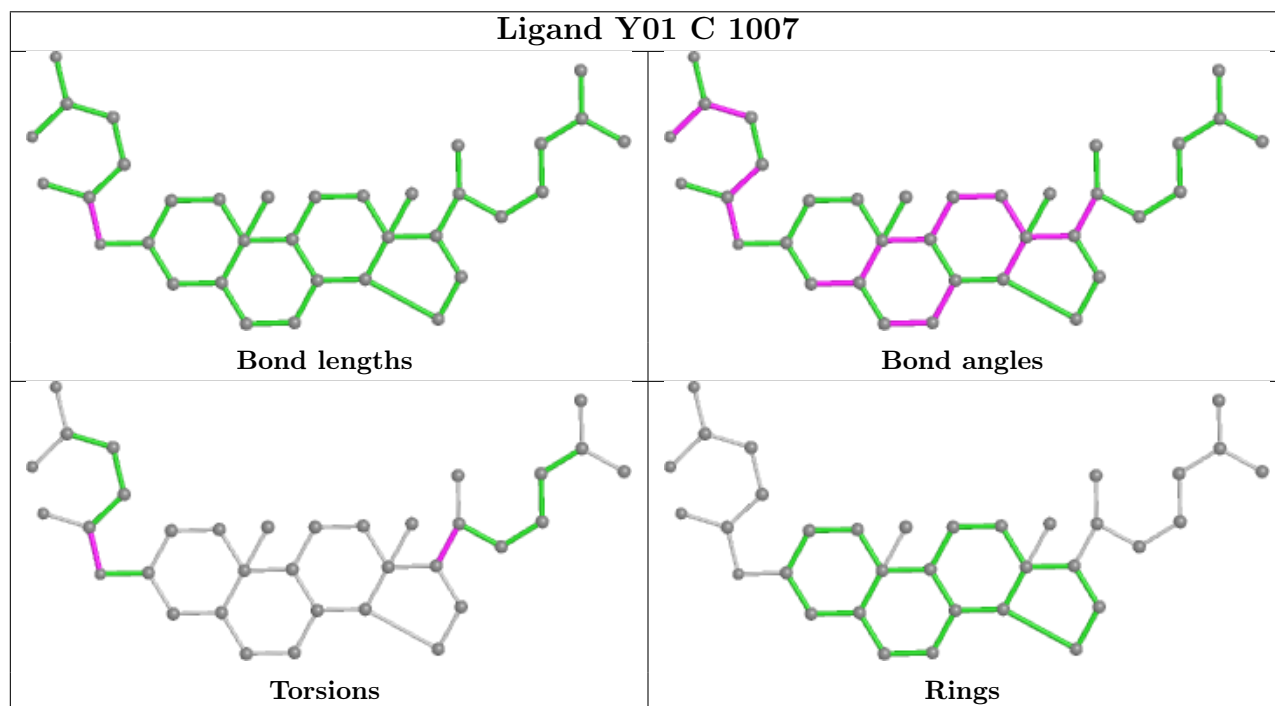
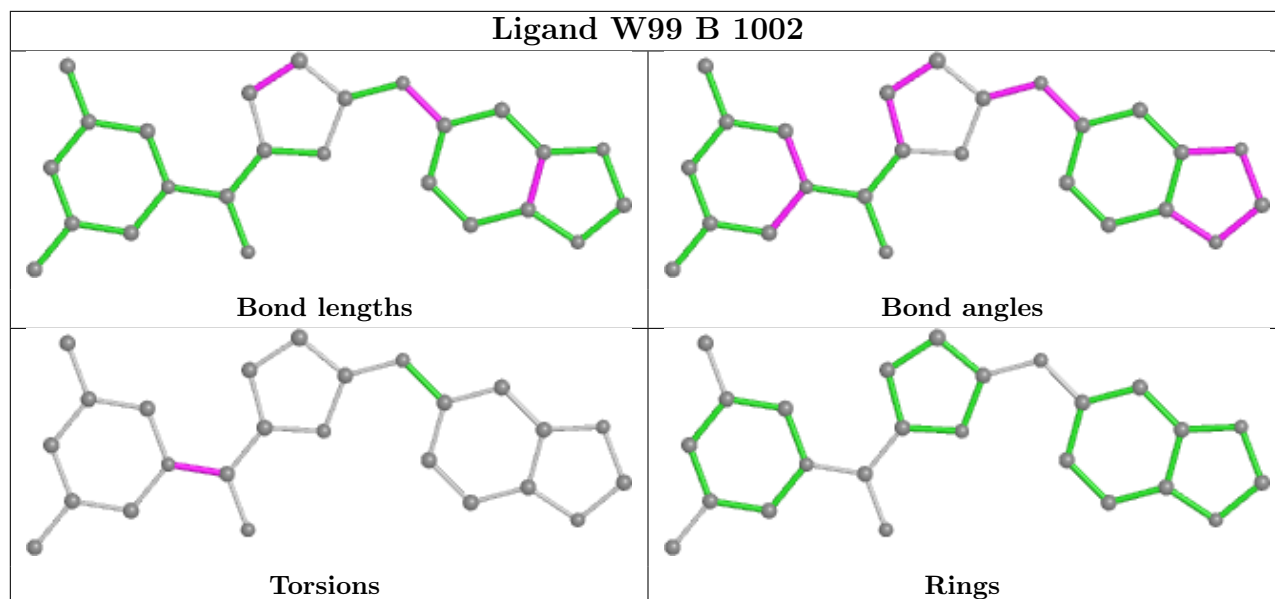
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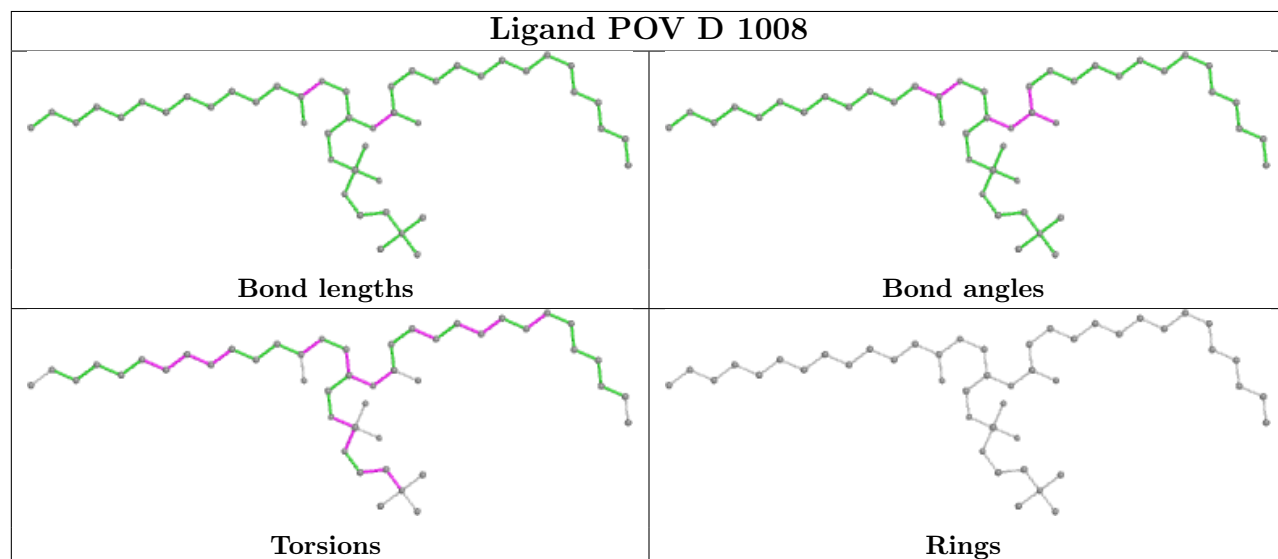
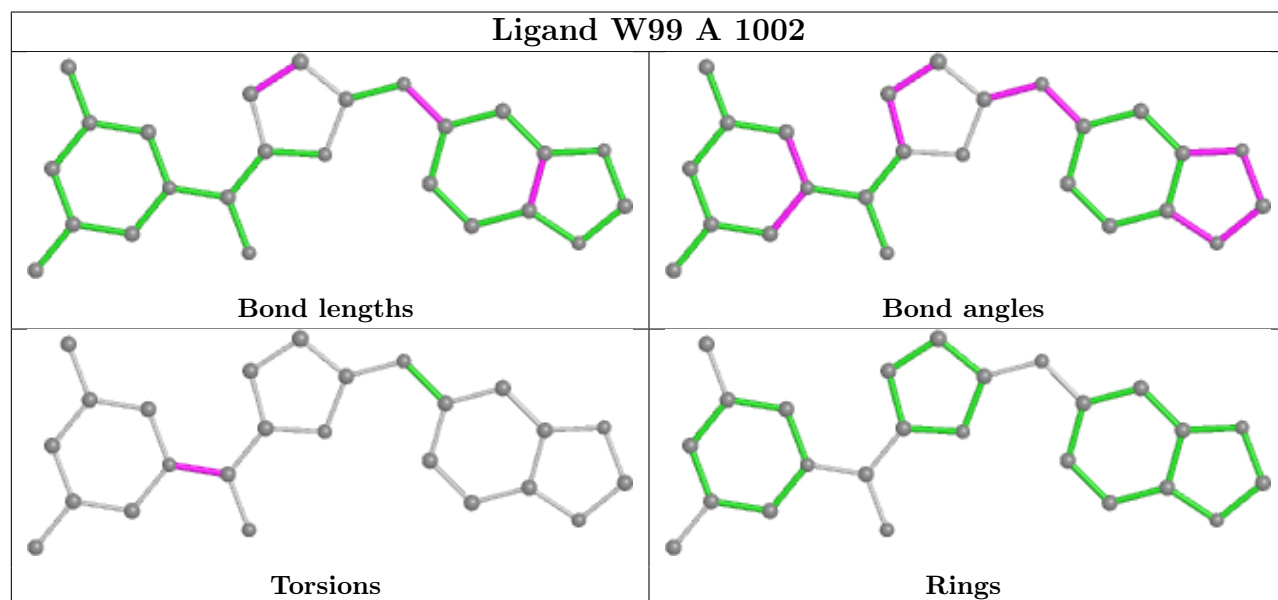
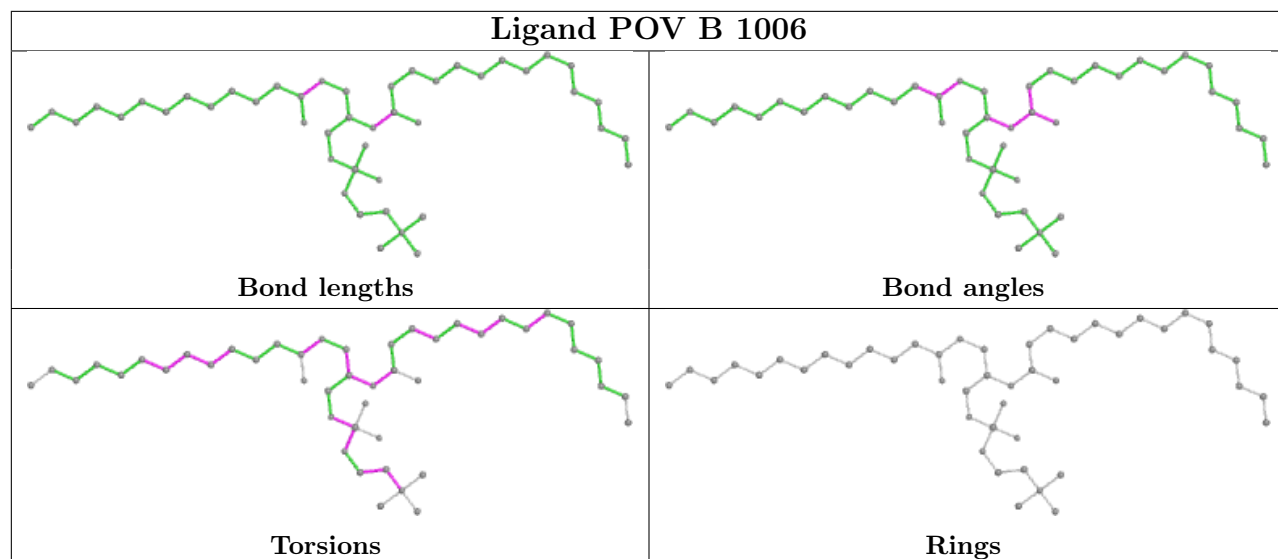
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1008	POV	10	0
4	C	1003	Y01	5	0
4	A	1003	Y01	5	0
3	D	1004	W99	1	0
4	B	1007	Y01	2	0
4	D	1009	Y01	3	0
6	C	1006	POV	10	0
4	B	1003	Y01	4	0
4	C	1010	Y01	3	0
4	A	1007	Y01	3	0
4	D	1005	Y01	5	0
6	A	1006	POV	10	0
4	A	1010	Y01	3	0
4	D	1002	Y01	3	0
3	C	1002	W99	1	0

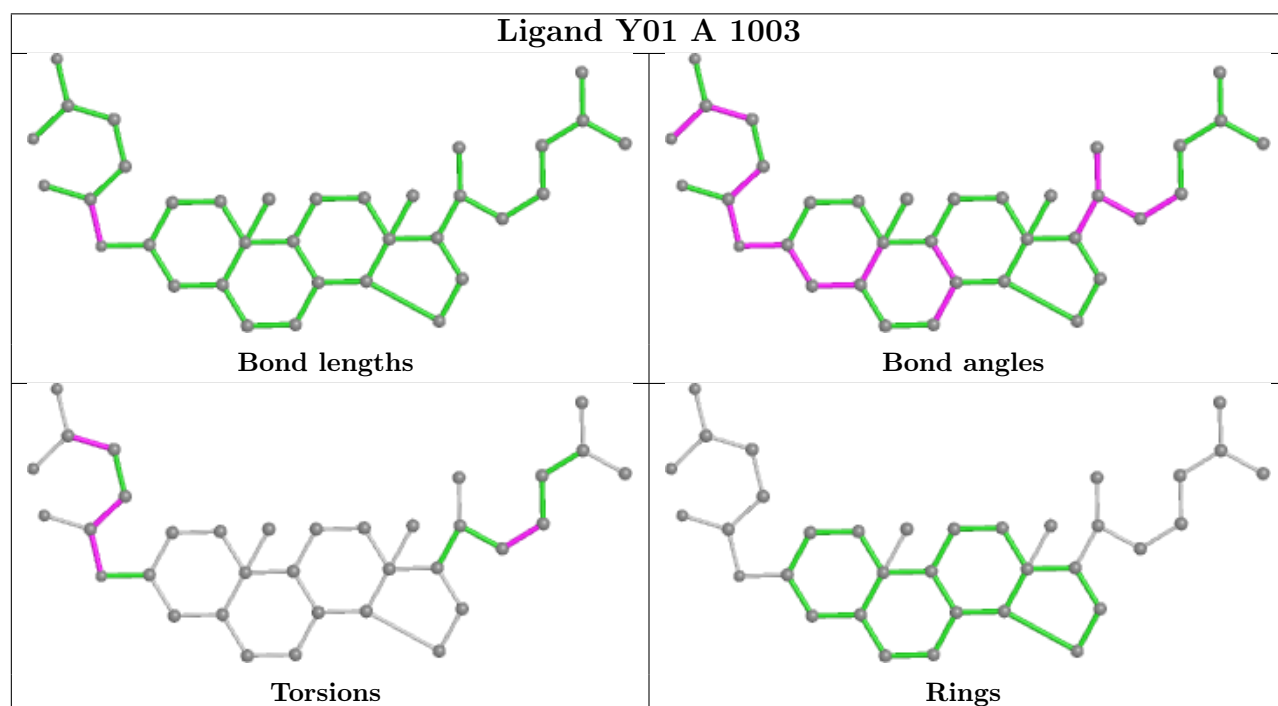
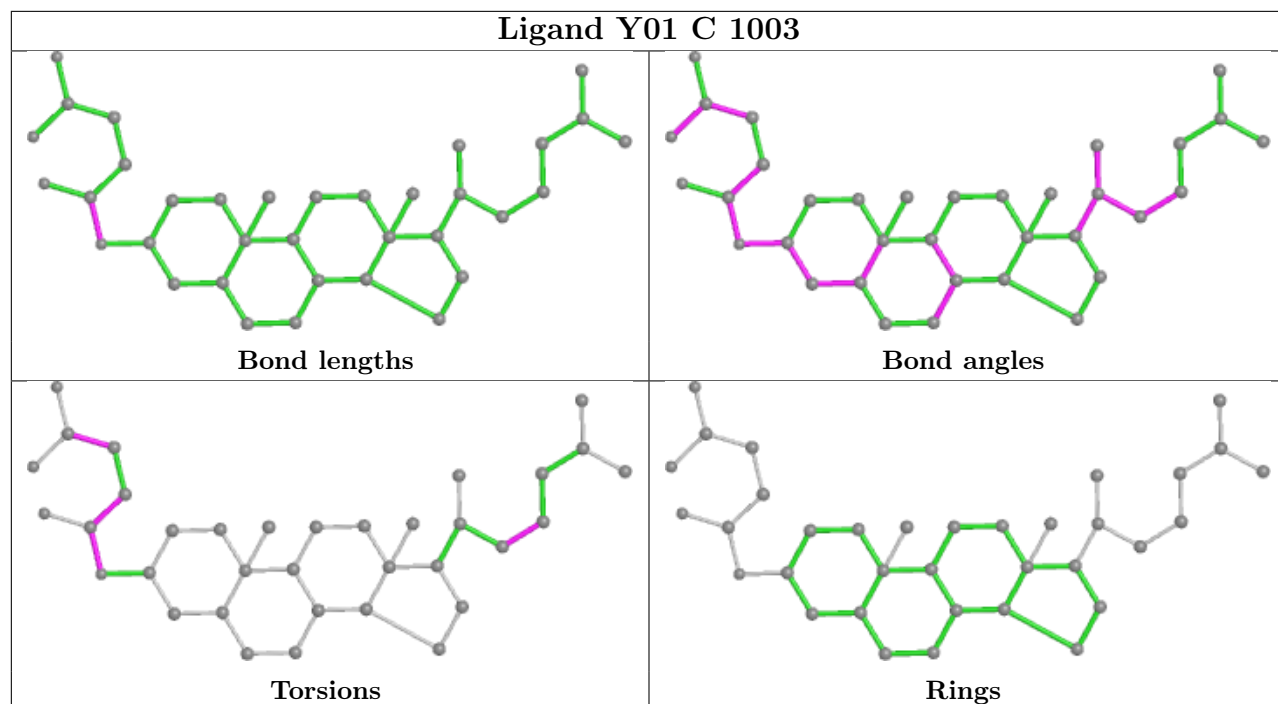
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

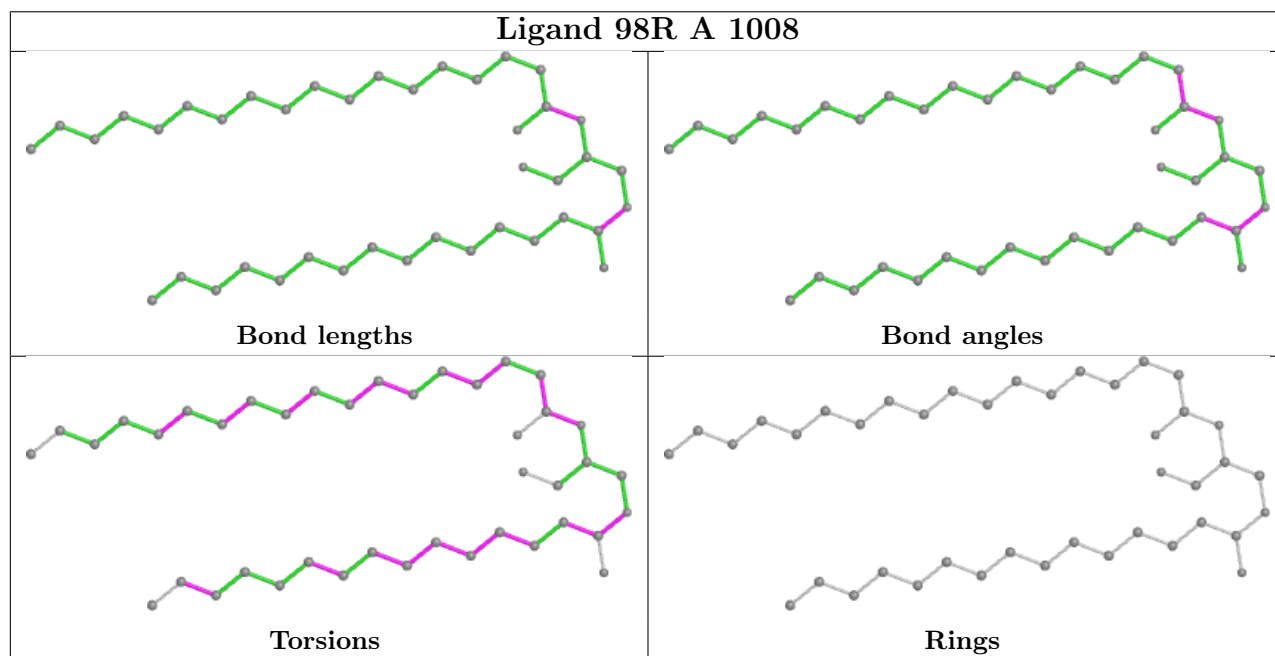
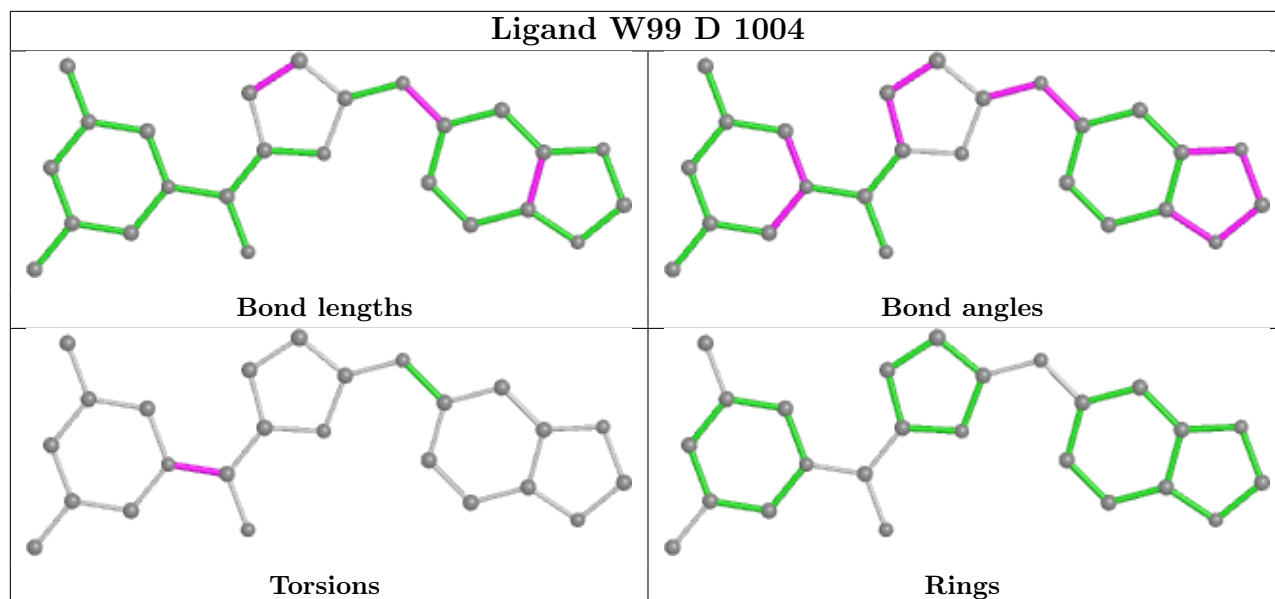


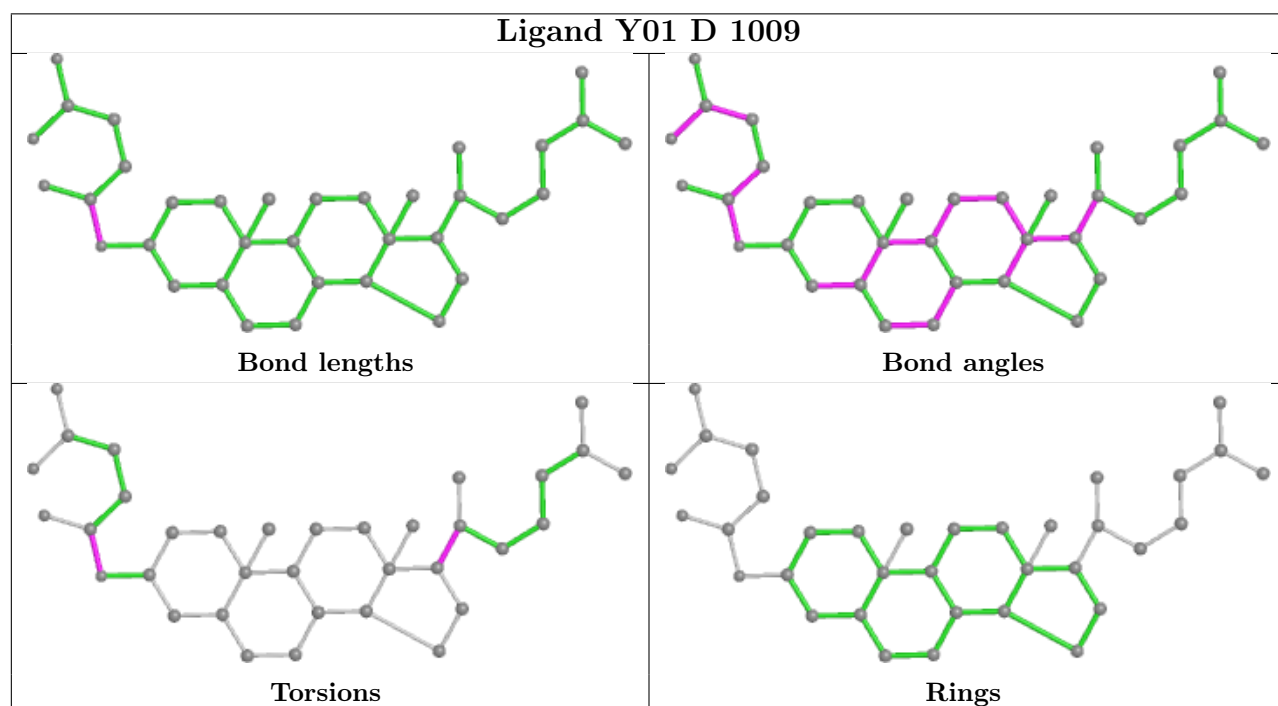
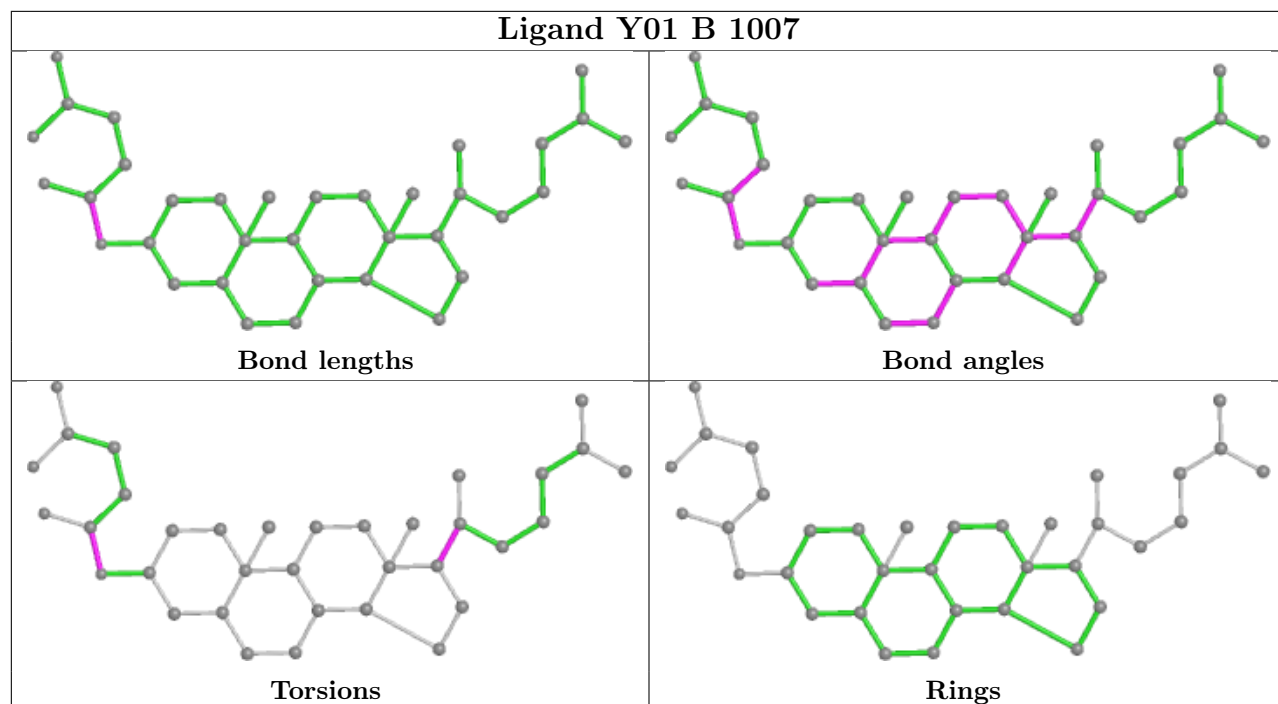


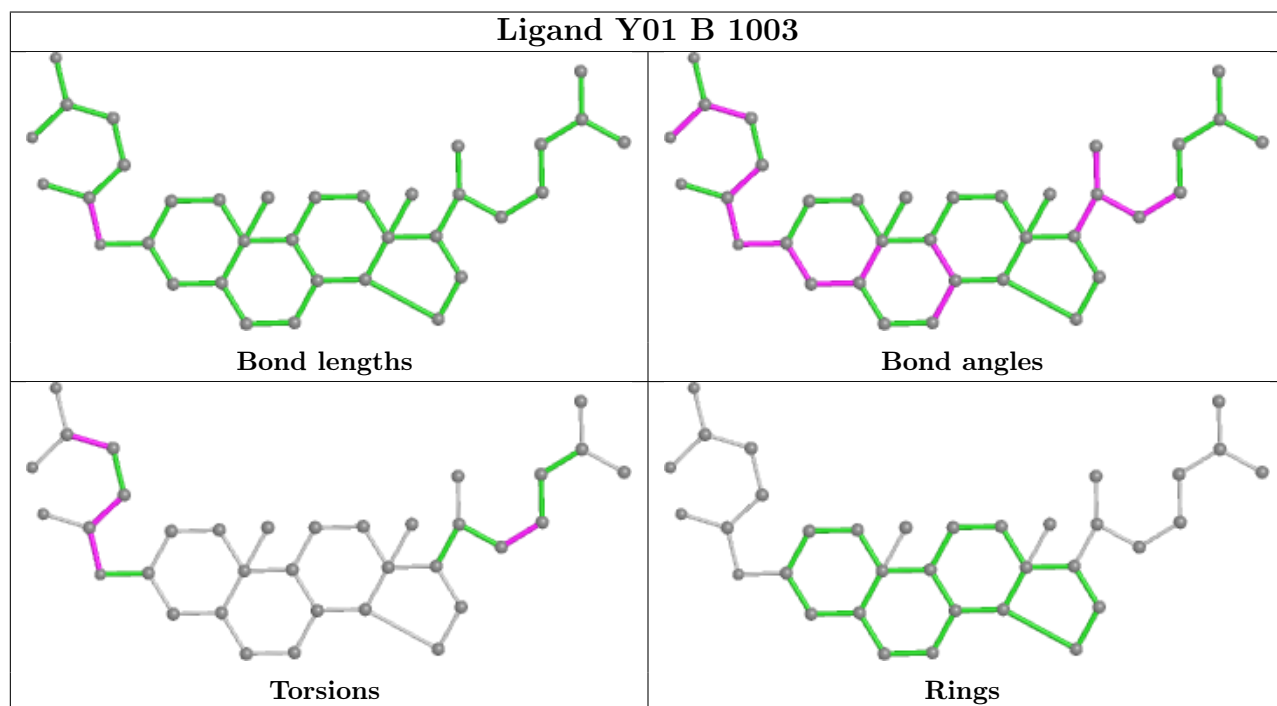
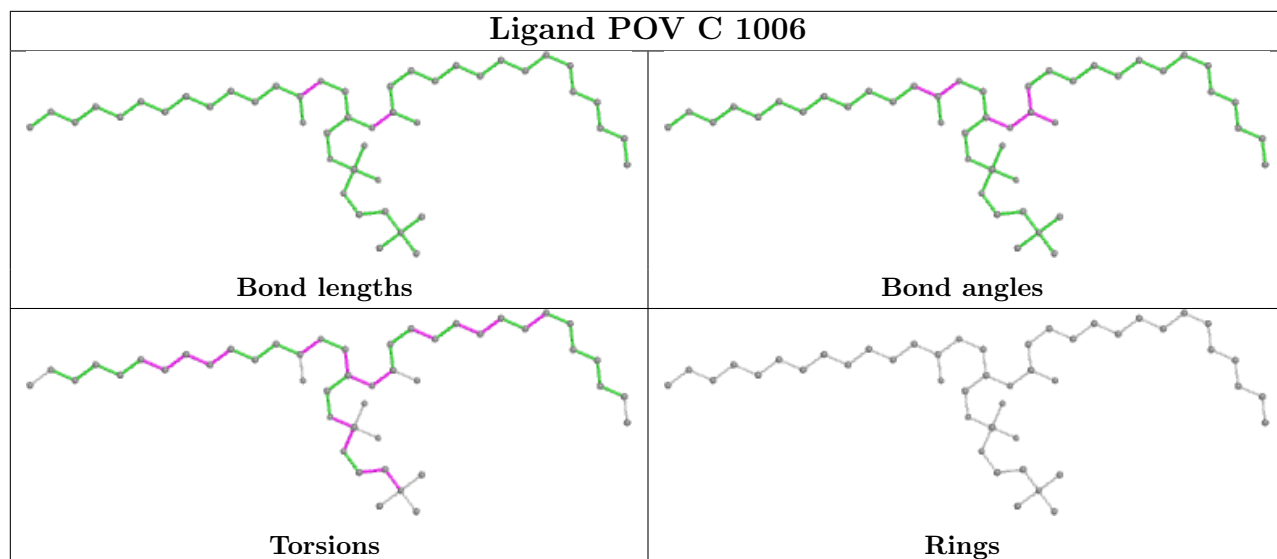


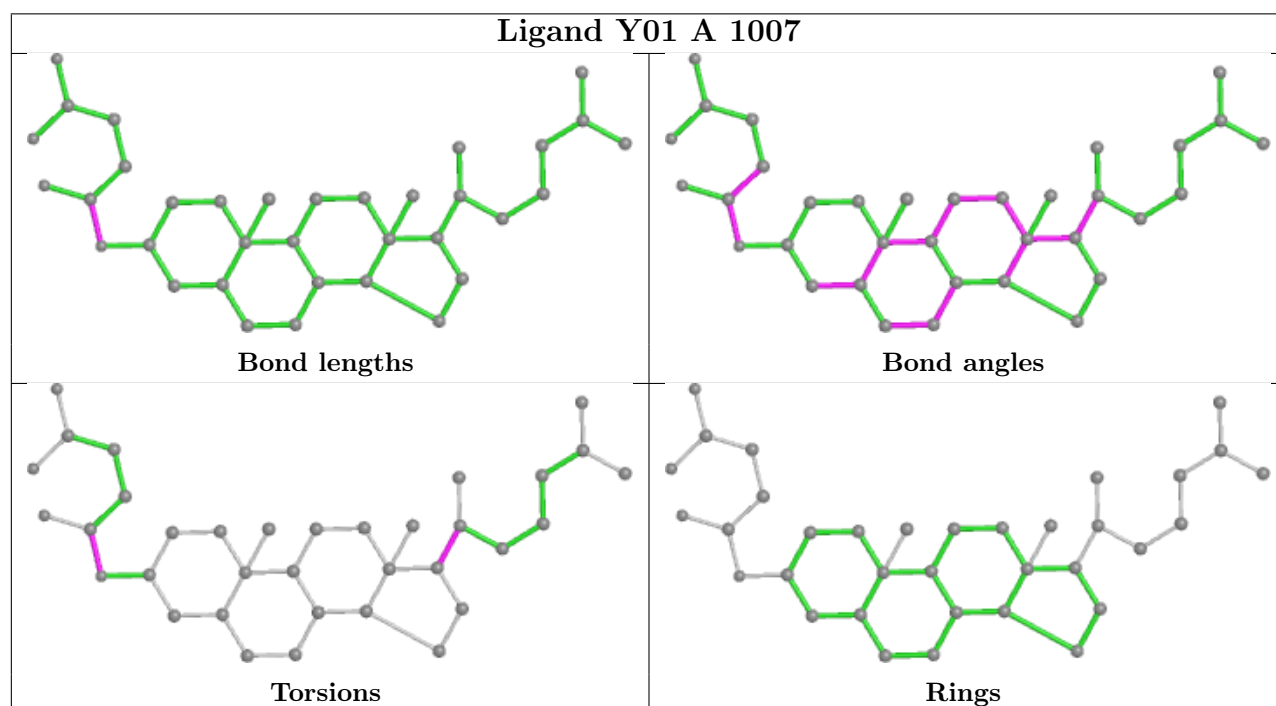
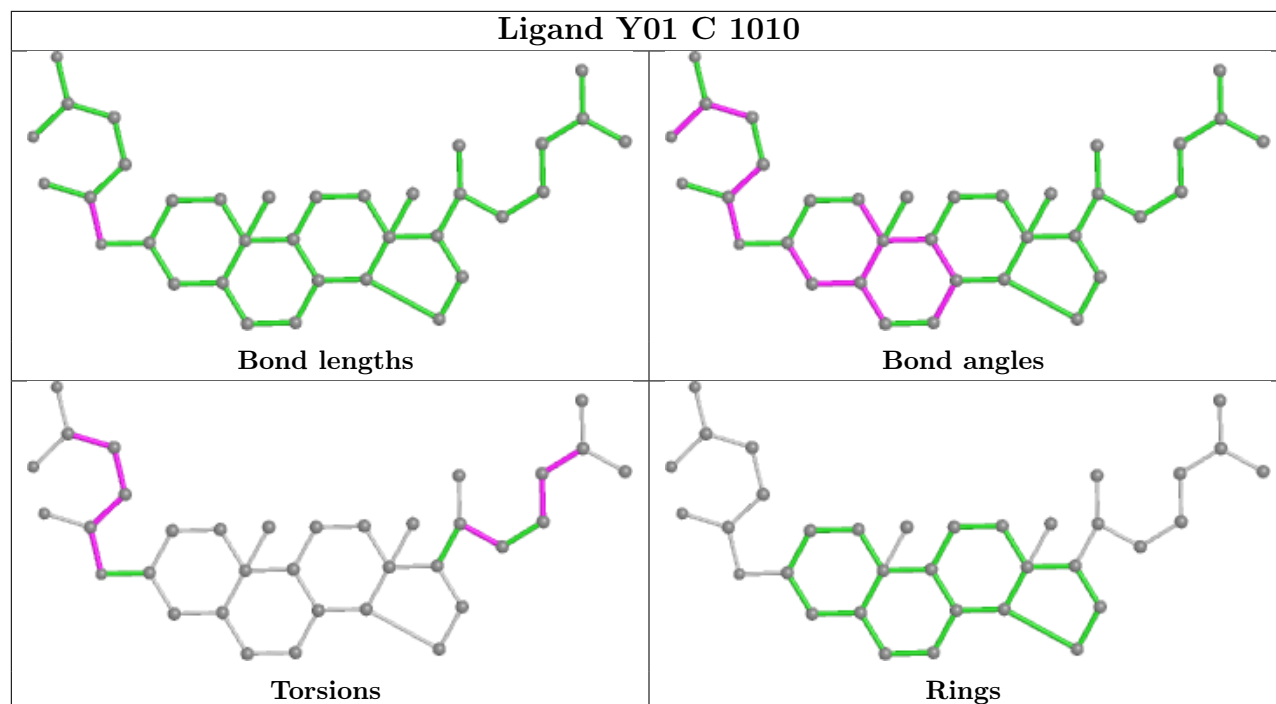


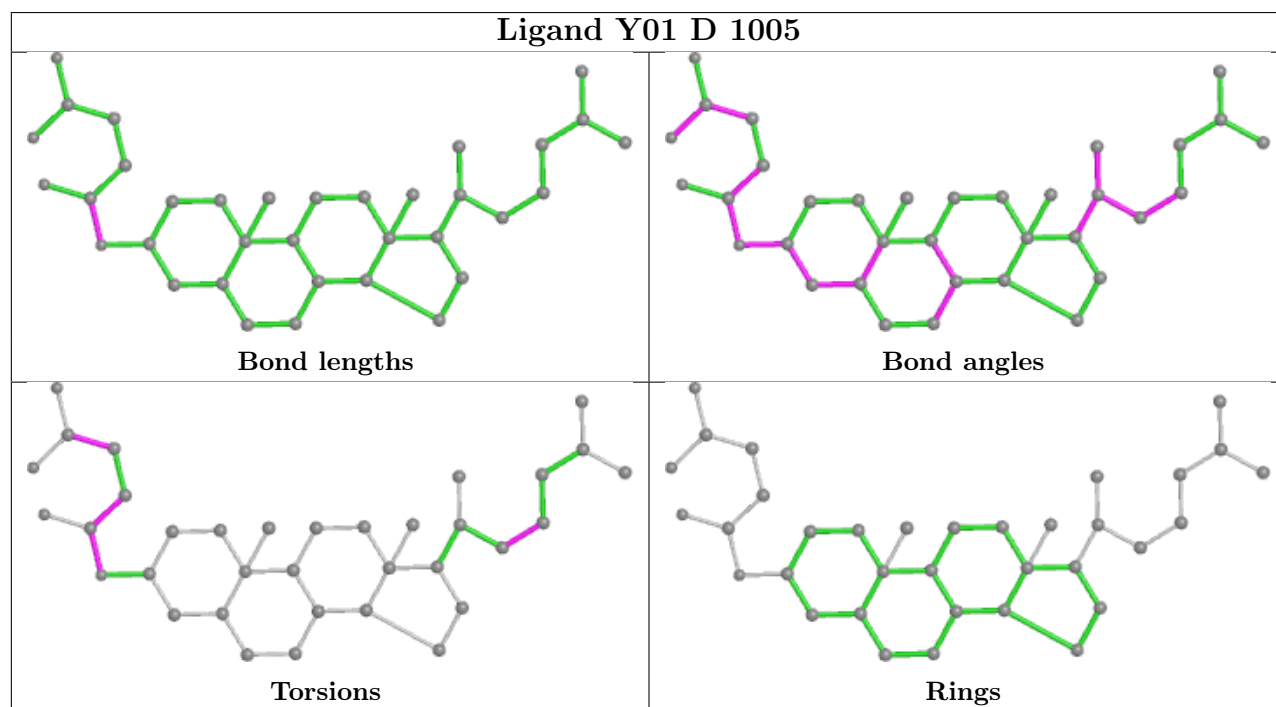
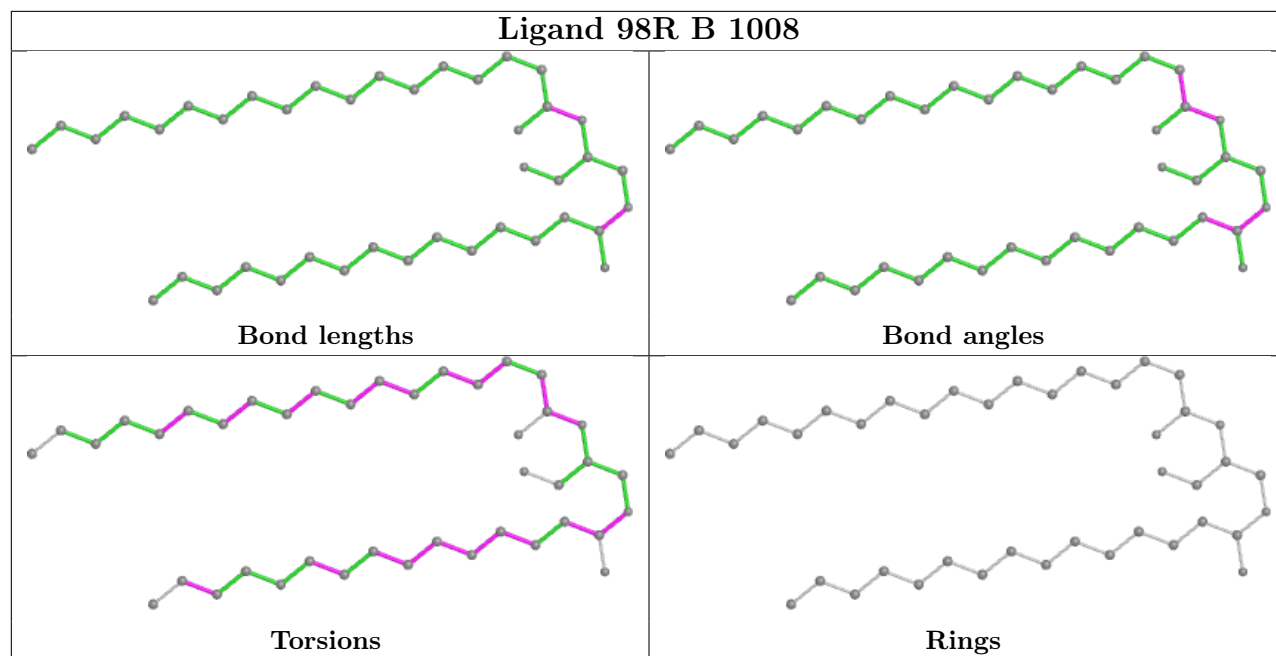


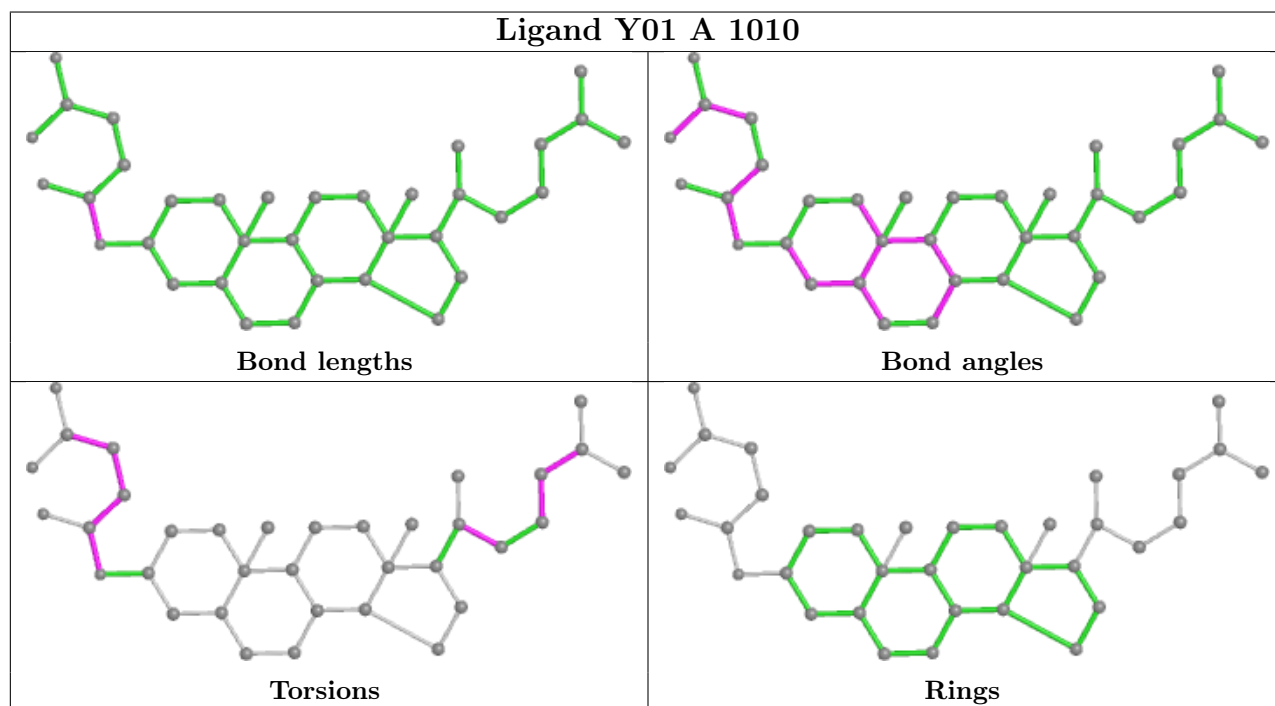
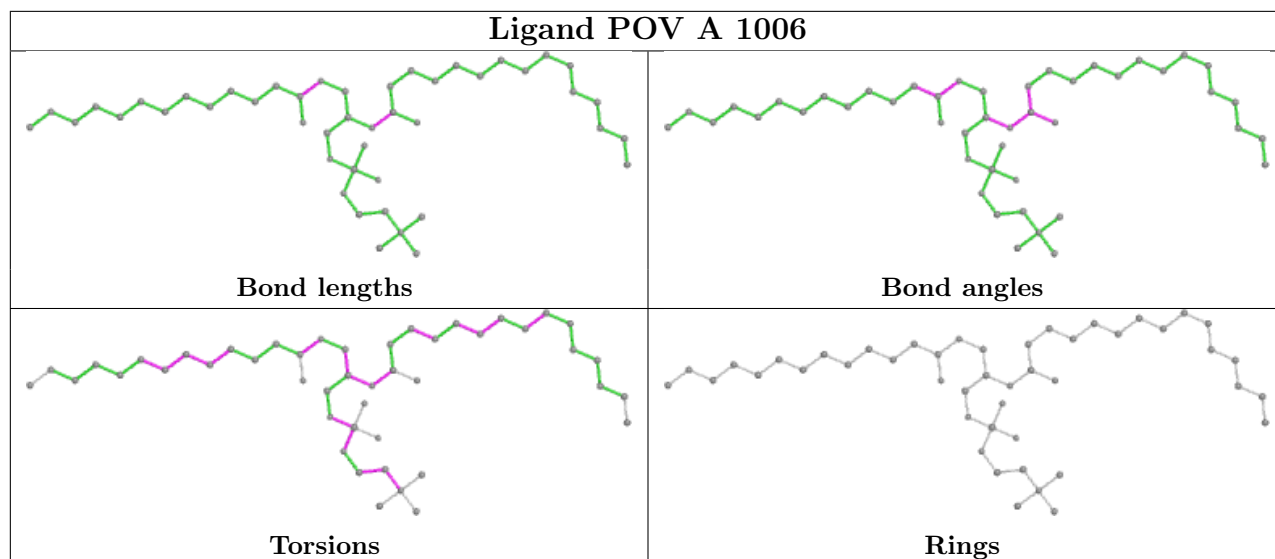




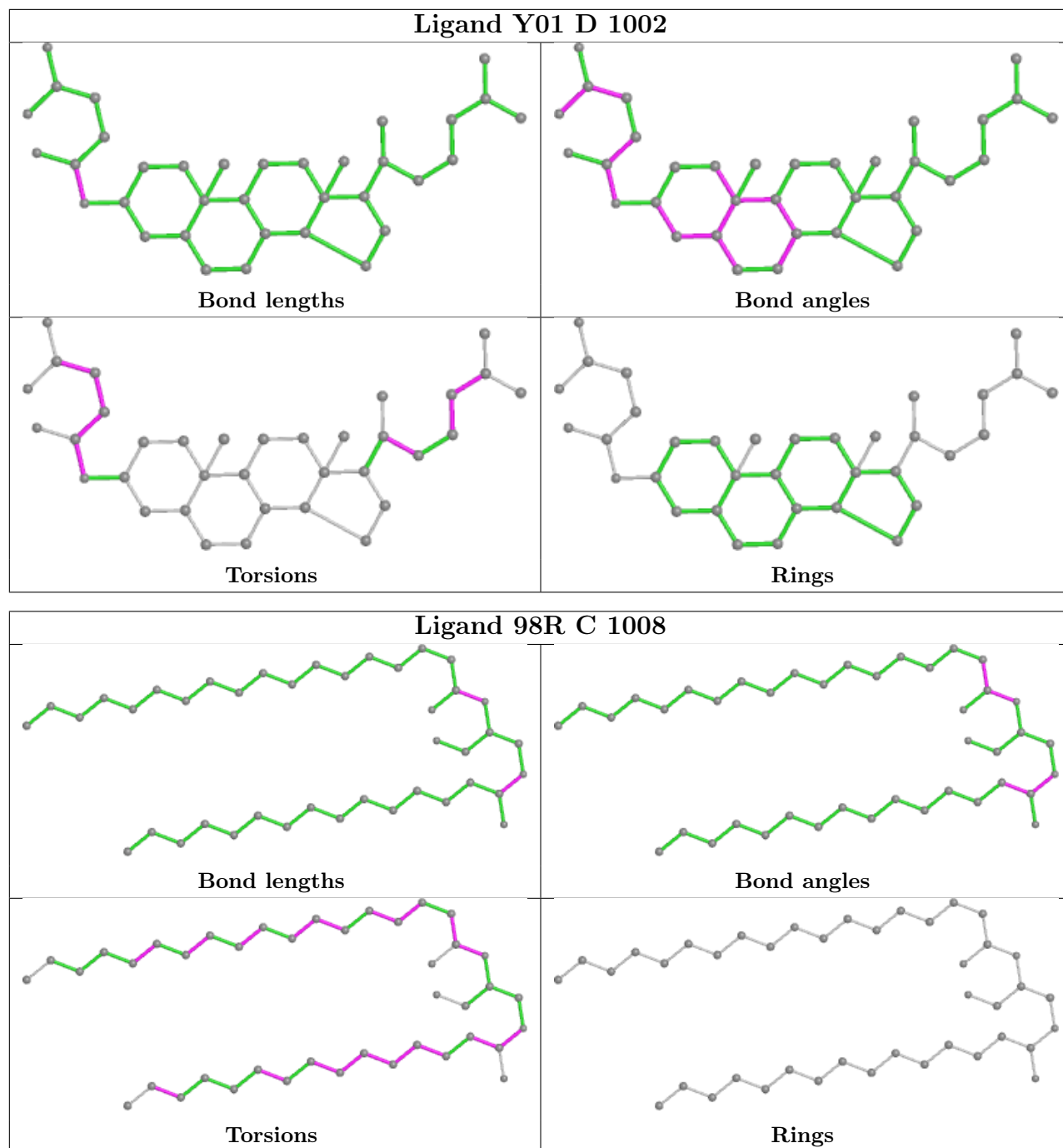


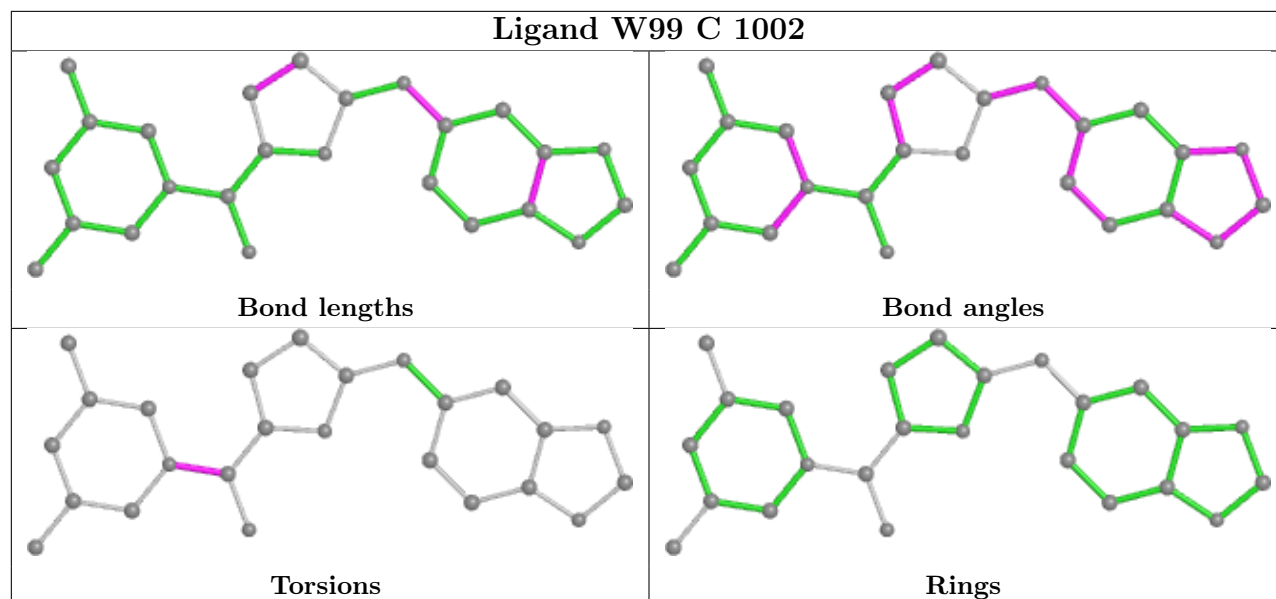












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

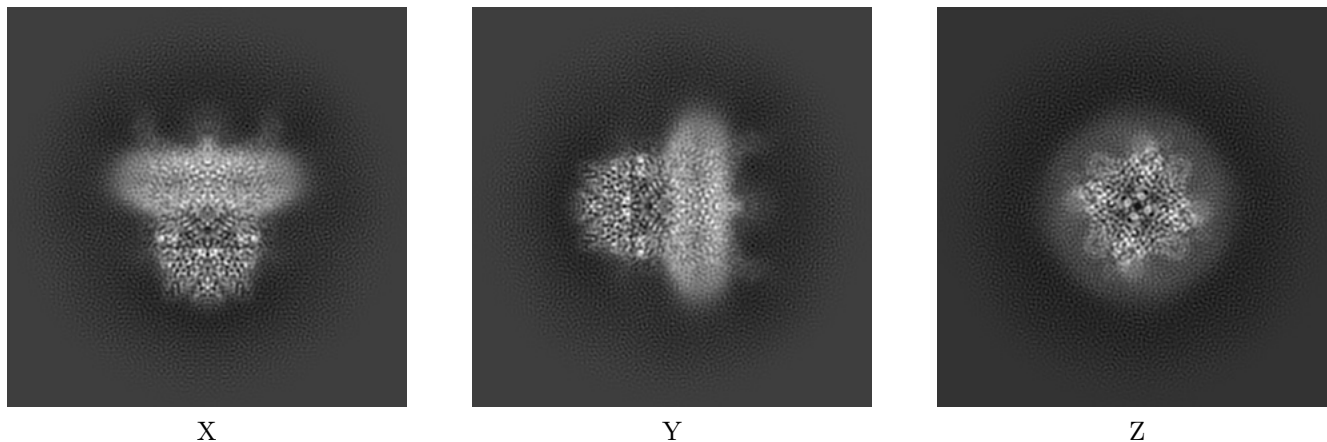
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30907. These allow visual inspection of the internal detail of the map and identification of artifacts.

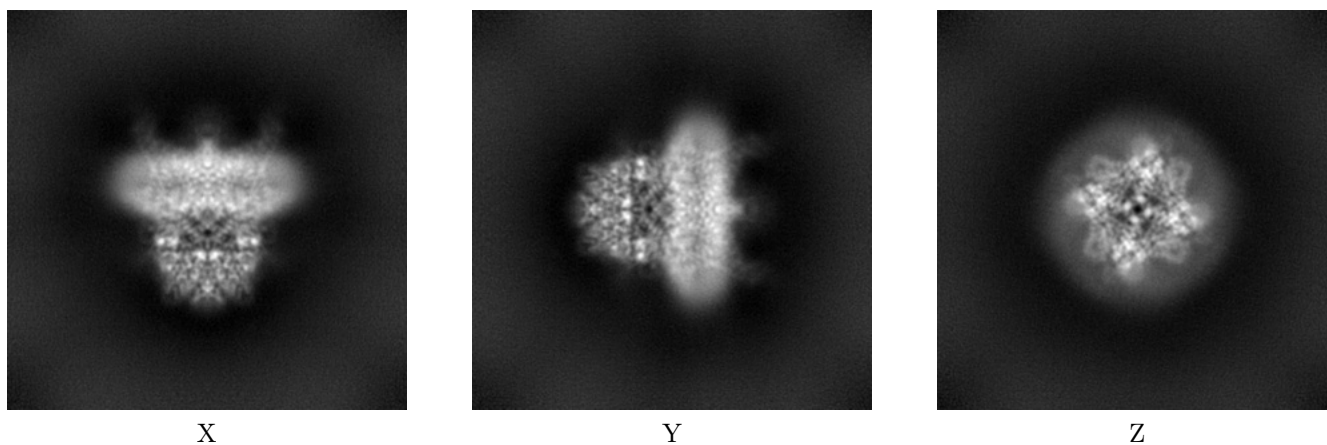
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



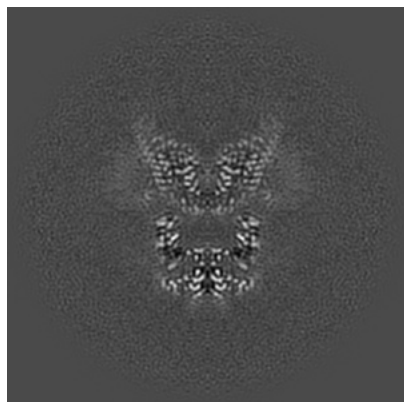
#### 6.1.2 Raw map



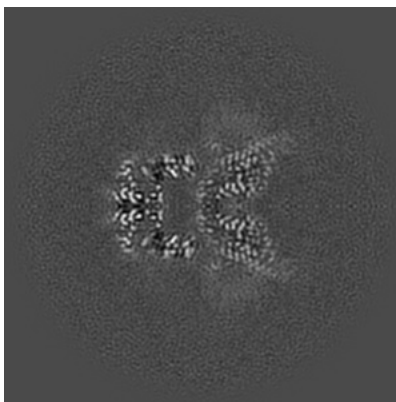
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

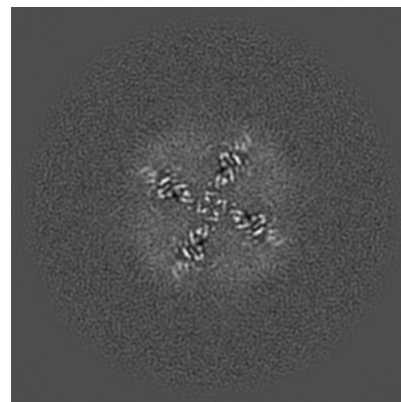
### 6.2.1 Primary map



X Index: 140

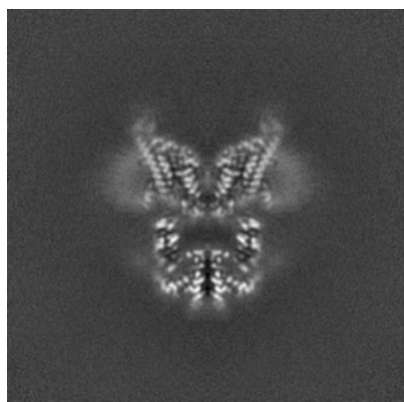


Y Index: 140

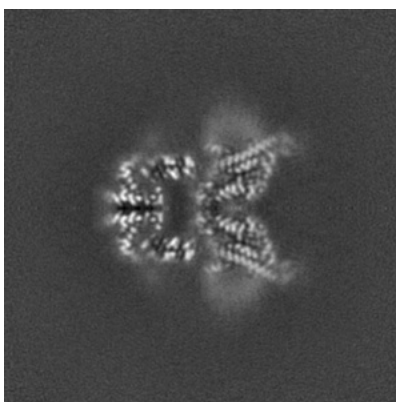


Z Index: 140

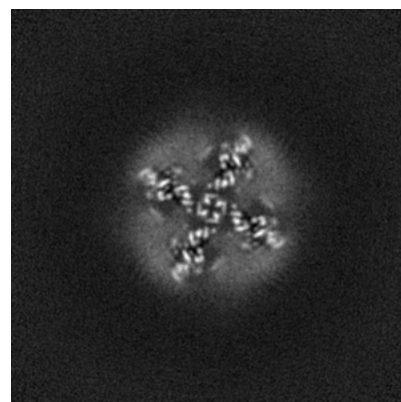
### 6.2.2 Raw map



X Index: 140



Y Index: 140

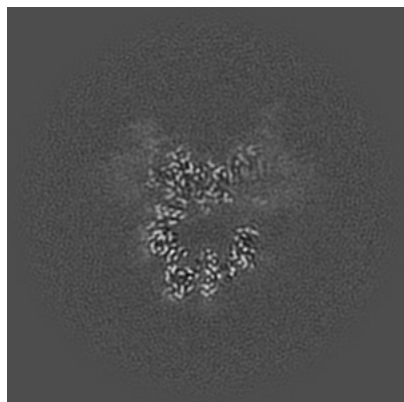


Z Index: 140

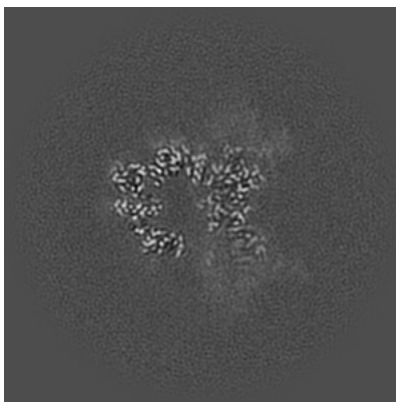
The images above show central slices of the map in three orthogonal directions.

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

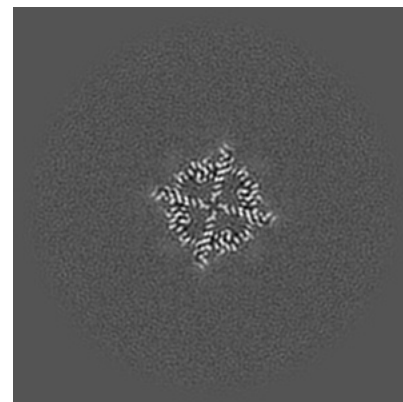
### 6.3.1 Primary map



X Index: 133

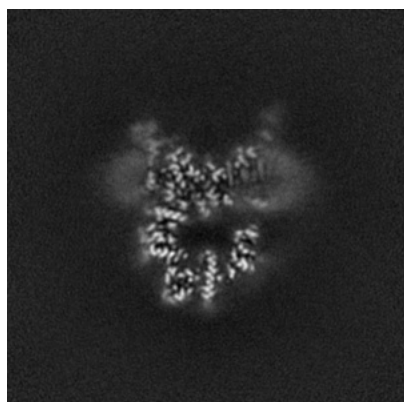


Y Index: 133

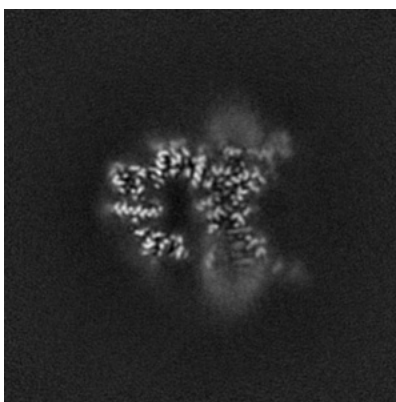


Z Index: 109

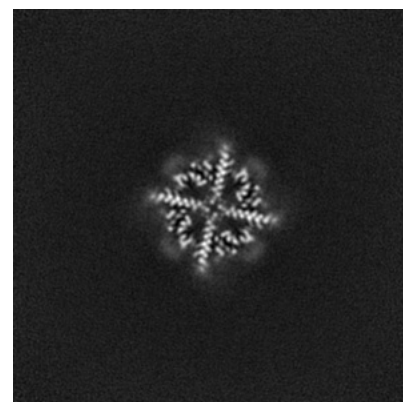
### 6.3.2 Raw map



X Index: 133



Y Index: 133

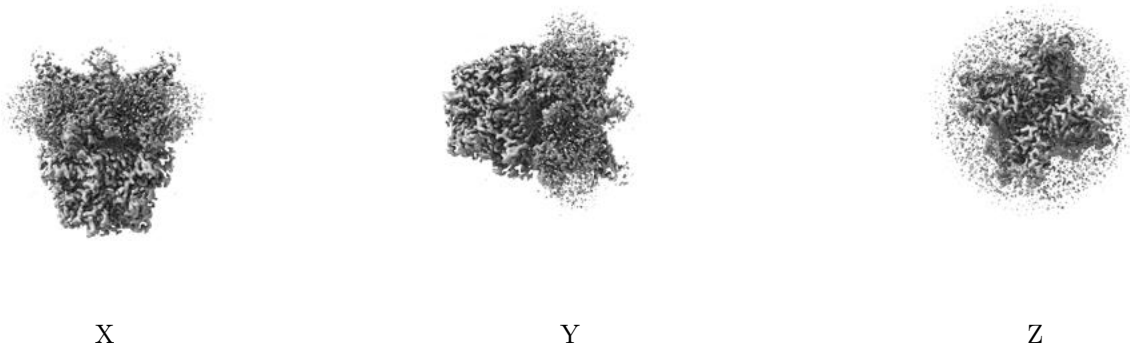


Z Index: 108

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.

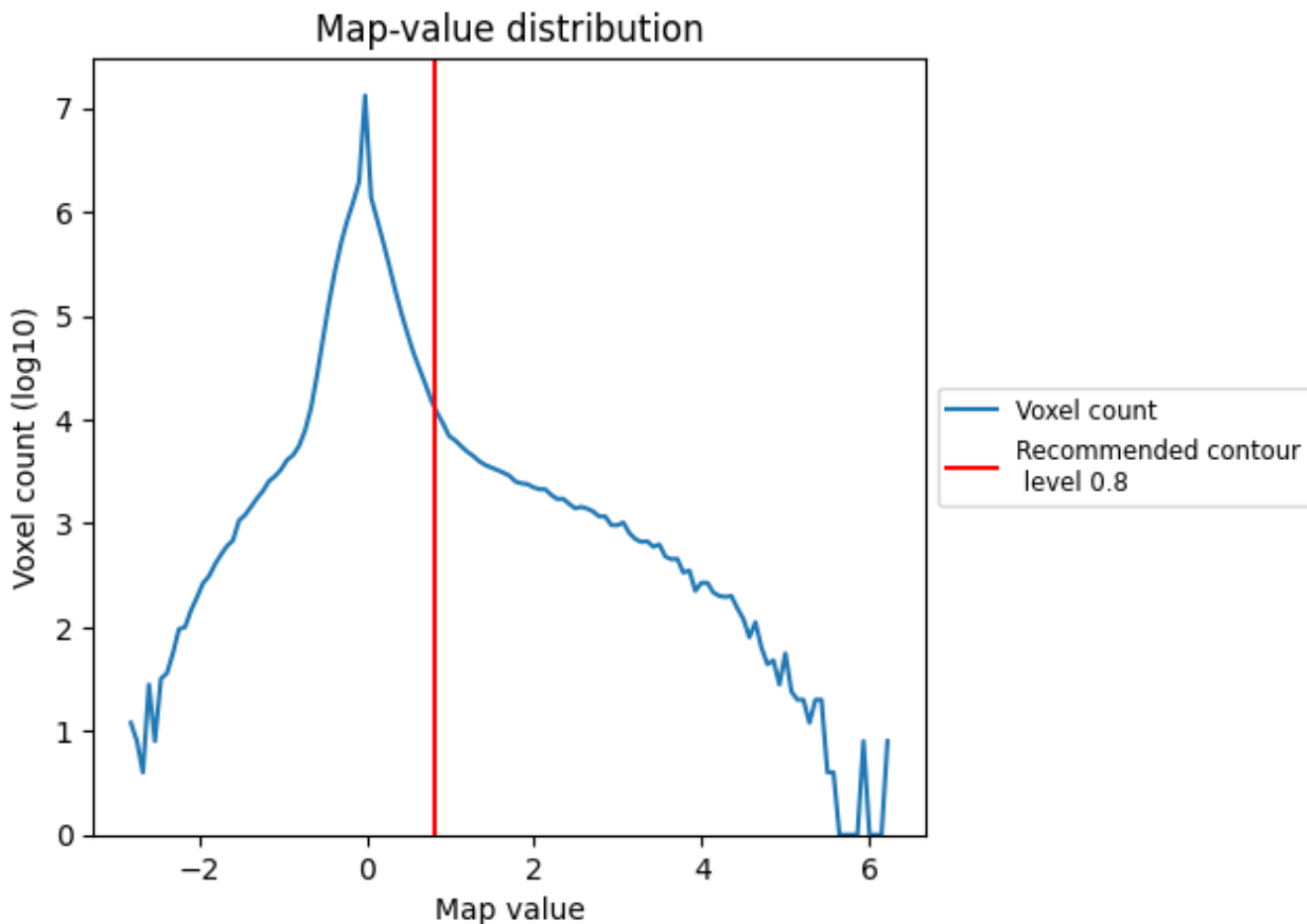
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

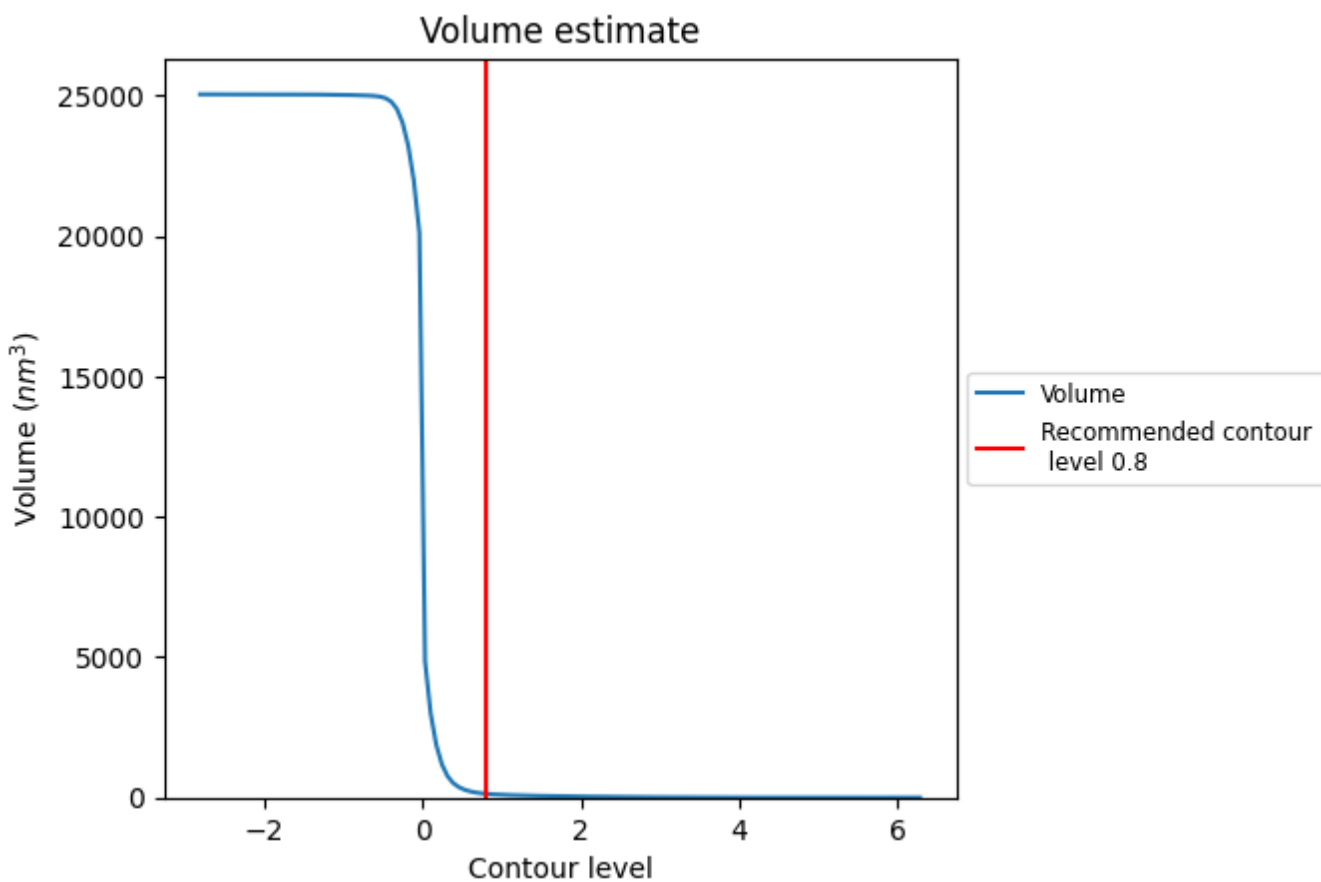
This section contains the results of statistical analysis of the map.

### 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](#)

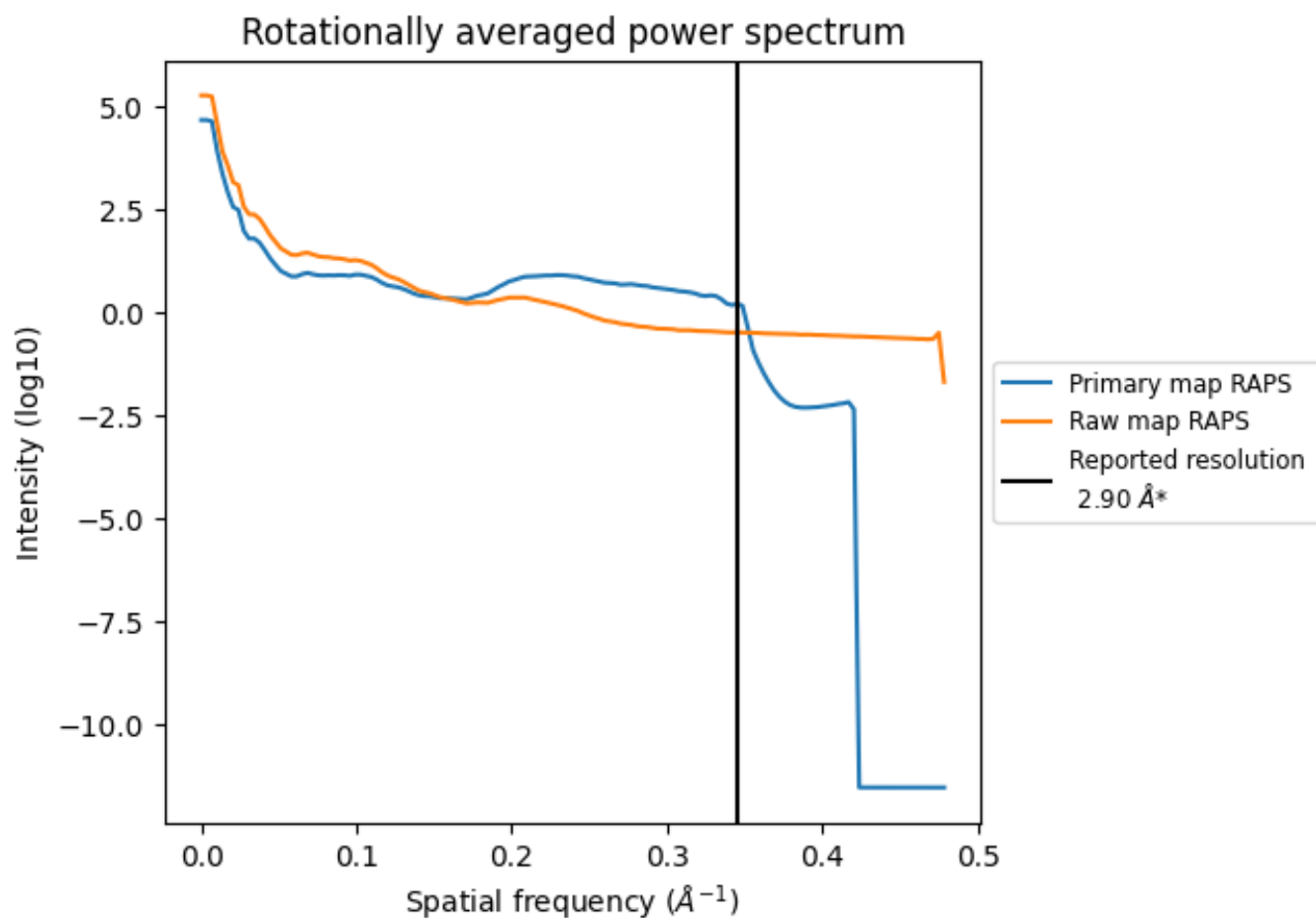


The volume at the recommended contour level is 135 nm<sup>3</sup>; this corresponds to an approximate mass of 122 kDa.

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

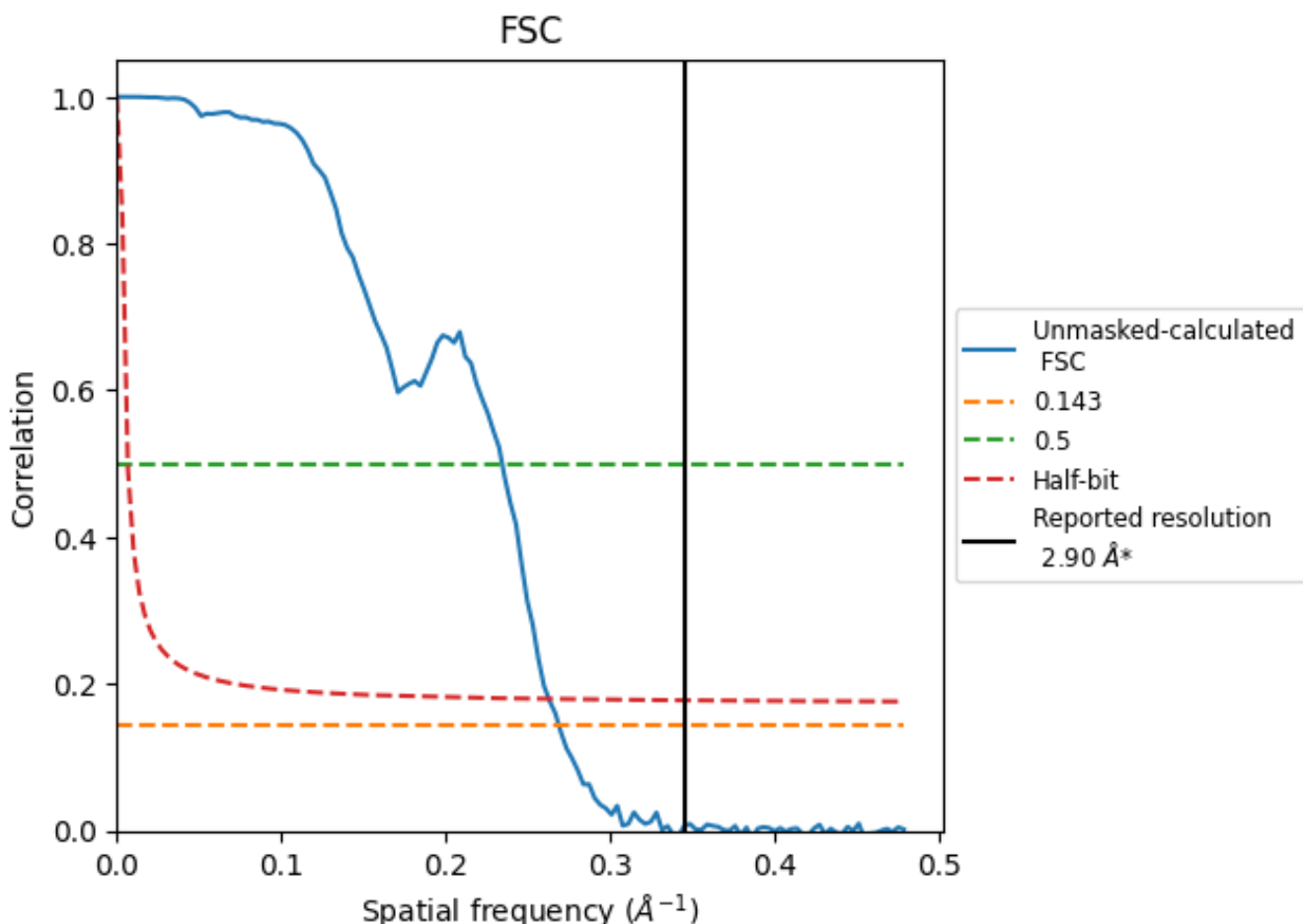


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

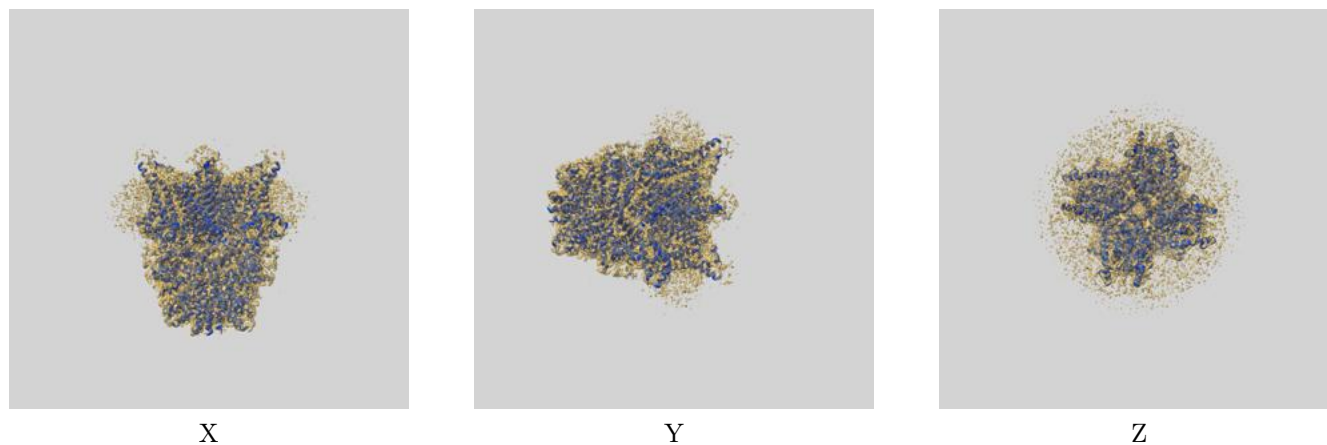
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.27	3.81

\*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 3.72 differs from the reported value 2.9 by more than 10 %

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

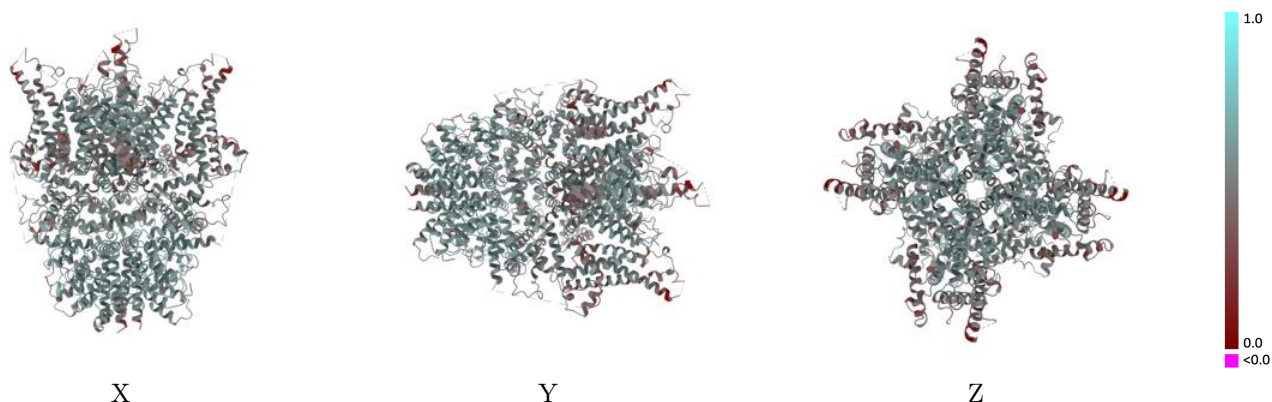
This section contains information regarding the fit between EMDB map EMD-30907 and PDB model 7DXF. Per-residue inclusion information can be found in section 3 on page 8.

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



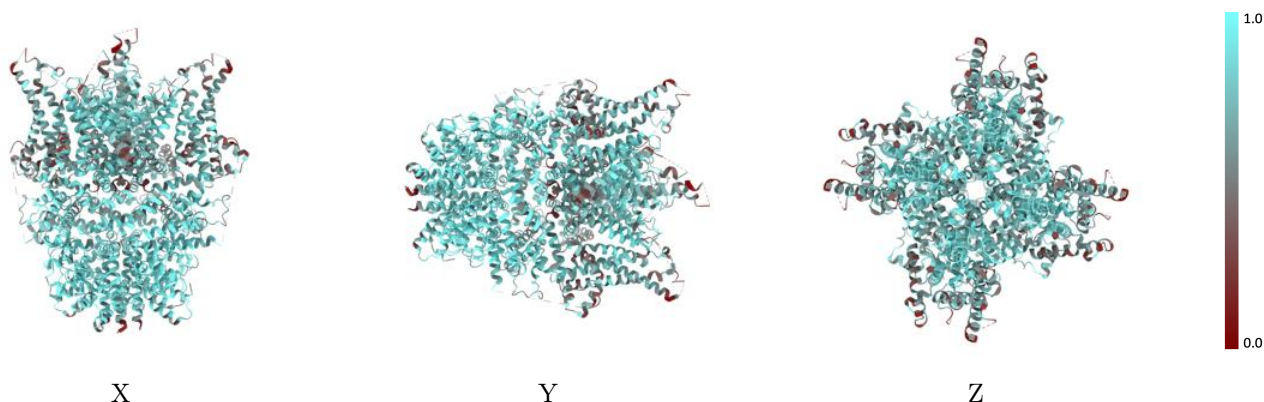
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



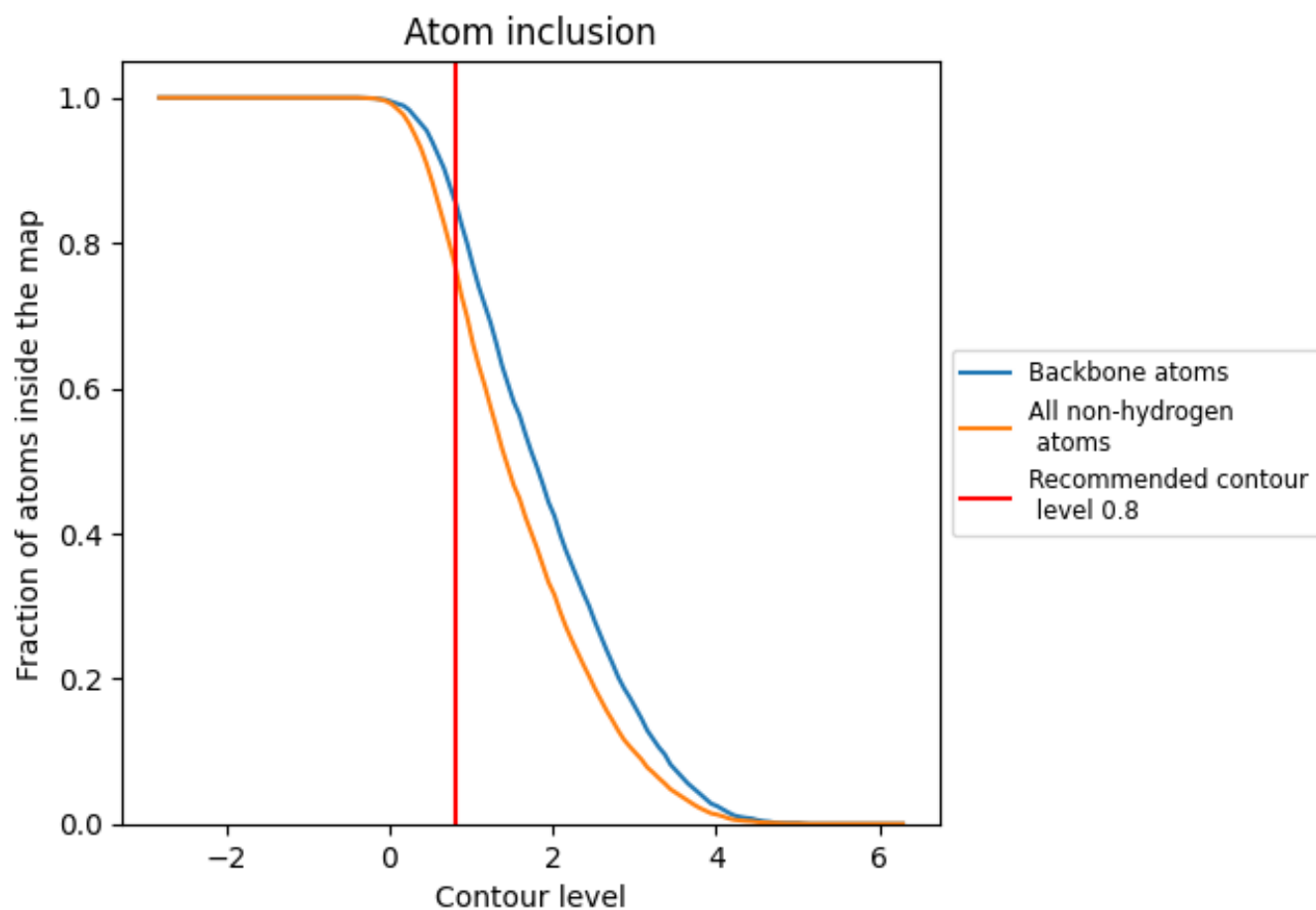
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 77% 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	 0.7721	 0.5150
A	 0.7718	 0.5140
B	 0.7725	 0.5150
C	 0.7718	 0.5160
D	 0.7720	 0.5160

