



## Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 02:27 PM JST

PDB ID : 8ZKP / pdb\_00008zkp  
EMDB ID : EMD-60202  
Title : Cryo-EM structure of the efflux transporter MmpL5/MmpS5 from Mycobacterium tuberculosis, C3 symmetry  
Authors : Zhang, B.; Xiong, Z.; Rao, Z.  
Deposited on : 2024-05-17  
Resolution : 2.64 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.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

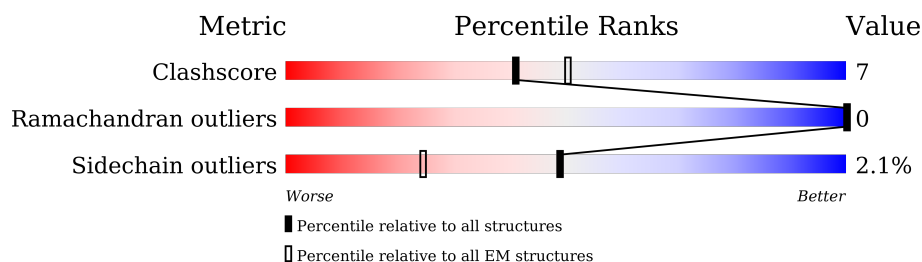
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.64 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	964	 68% 12% 20%
1	B	964	 67% 13% 20%
1	E	964	 67% 13% 20%
2	C	142	 21% • 76%
2	F	142	 21% • 76%
2	G	142	 20% • 76%
3	D	99	 71% 12% • 16%
3	H	99	 71% 12% • 16%

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Mol	Chain	Length	Quality of chain
3	I	99	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PN7	D	101	-	X	-	-
6	PN7	H	101	-	X	-	-
6	PN7	I	101	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21087 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 Siderophore exporter MmpL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	772	Total	C	N	O	S	0	0
			5810	3751	983	1046	30		
1	B	772	Total	C	N	O	S	0	0
			5810	3751	983	1046	30		
1	E	772	Total	C	N	O	S	0	0
			5810	3751	983	1046	30		

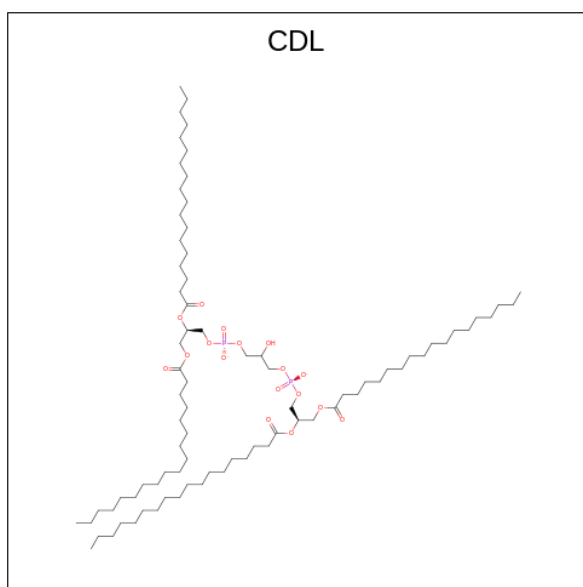
- Molecule 2 is a protein called Siderophore export accessory protein MmpS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	34	Total	C	N	O	S	0	0
			267	181	46	39	1		
2	C	34	Total	C	N	O	S	0	0
			267	181	46	39	1		
2	G	34	Total	C	N	O	S	0	0
			267	181	46	39	1		

- Molecule 3 is a protein called Meromycolate extension acyl carrier protein.

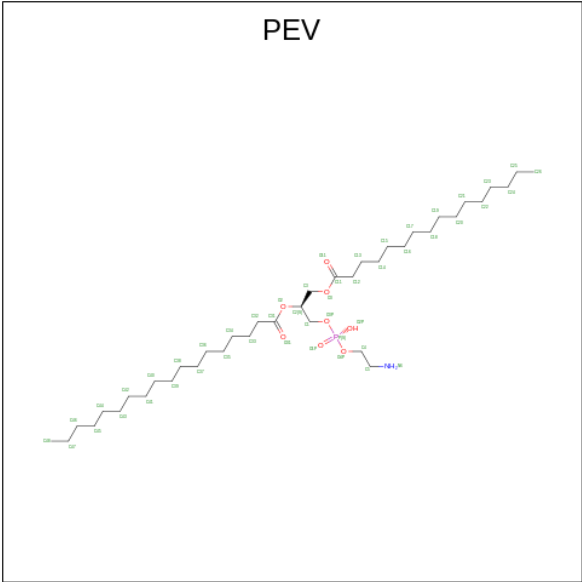
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	83	Total	C	N	O	S	0	0
			633	397	93	141	2		
3	D	83	Total	C	N	O	S	0	0
			633	397	93	141	2		
3	I	83	Total	C	N	O	S	0	0
			633	397	93	141	2		

- Molecule 4 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



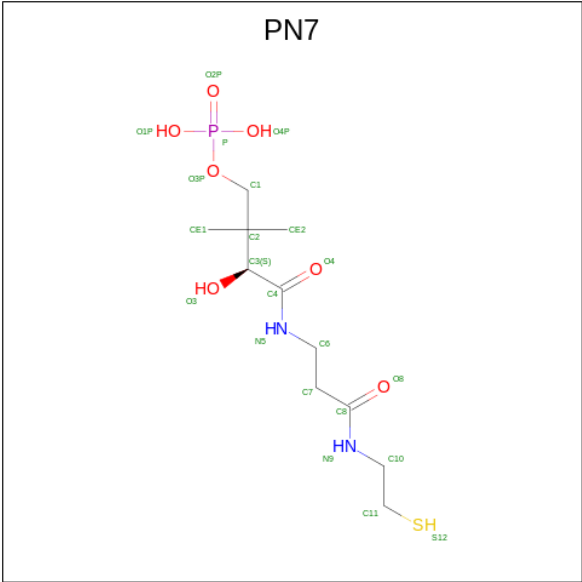
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			100	81	17	2	
4	A	1	Total	C	O	P	0
			100	81	17	2	
4	B	1	Total	C	O	P	0
			100	81	17	2	
4	B	1	Total	C	O	P	0
			100	81	17	2	
4	E	1	Total	C	O	P	0
			100	81	17	2	
4	E	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 5 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
5	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
5	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
5	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
5	E	1	Total	C	N	O	P	0
			49	39	1	8	1	
5	G	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 6 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanyl ethyl)-beta-alaninamide (CCD ID: PN7) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).

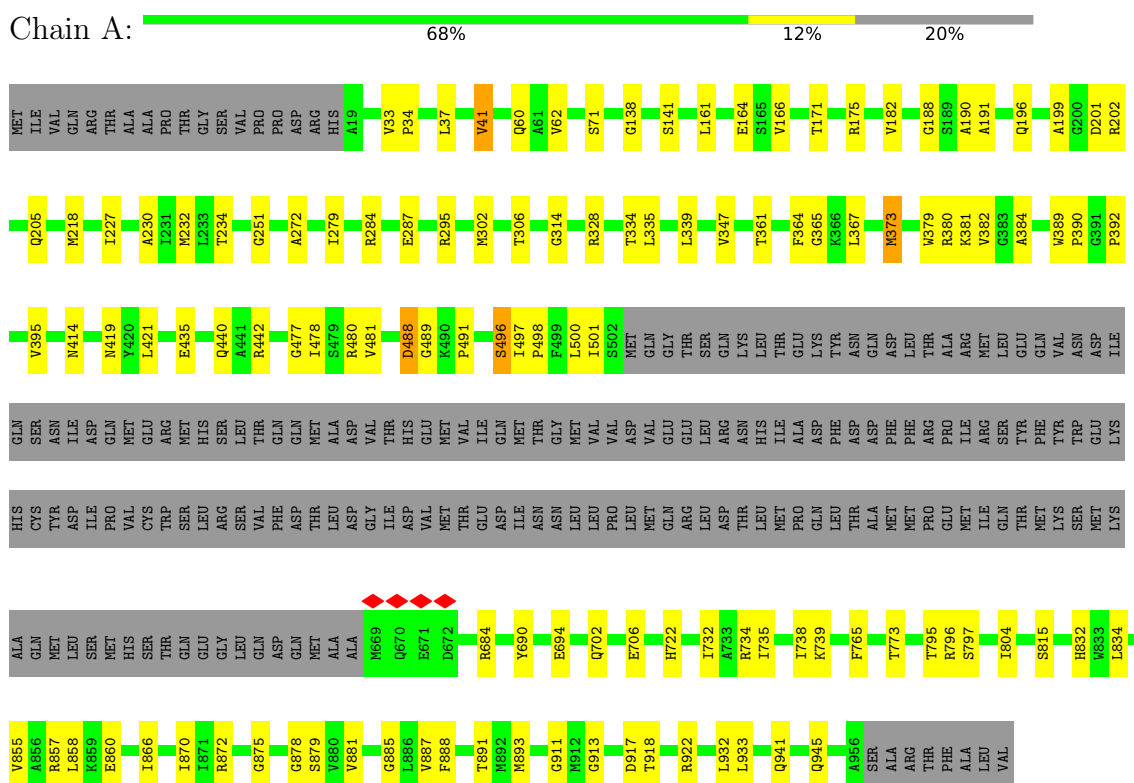


Mol	Chain	Residues	Atoms						AltConf
6	H	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
6	D	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
6	I	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

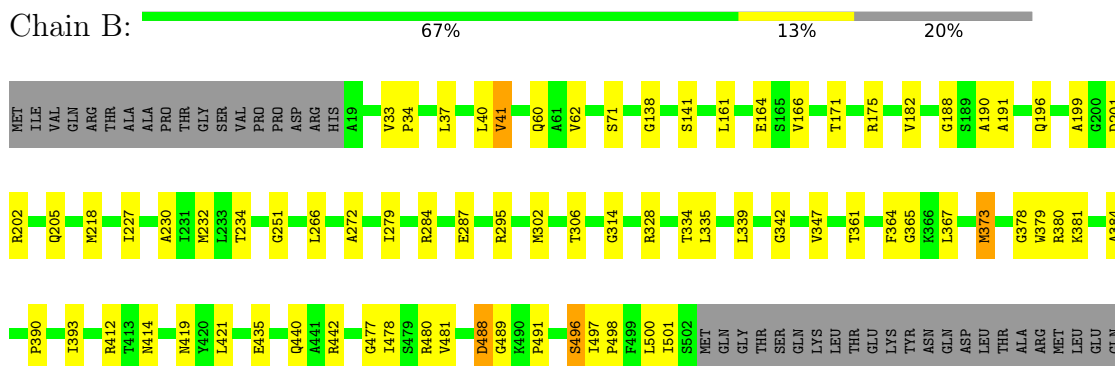
### 3 Residue-property plots

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: Siderophore exporter MmpL5



#### • Molecule 1: Siderophore exporter MmpL5









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.982	Depositor
Minimum map value	-1.982	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.252	Depositor
Map size ( $\text{\AA}$ )	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.832, 0.832, 0.832	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, CDL, PN7

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	0.21	0/5929	0.38	0/8072
1	B	0.21	0/5929	0.37	0/8072
1	E	0.21	0/5929	0.37	0/8072
2	C	0.17	0/272	0.36	0/368
2	F	0.17	0/272	0.36	0/368
2	G	0.17	0/272	0.36	0/368
3	D	0.21	0/638	0.39	0/866
3	H	0.21	0/638	0.39	0/866
3	I	0.21	0/638	0.39	0/866
All	All	0.21	0/20517	0.38	0/27918

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

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	5810	0	5965	72	0
1	B	5810	0	5965	78	0
1	E	5810	0	5965	79	0
2	C	267	0	300	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	267	0	300	1	0
2	G	267	0	300	3	0
3	D	633	0	623	11	0
3	H	633	0	623	11	0
3	I	633	0	624	14	0
4	A	200	0	312	14	0
4	B	200	0	312	17	0
4	E	200	0	312	15	0
5	A	98	0	154	5	0
5	B	49	0	77	0	0
5	C	49	0	77	1	0
5	E	49	0	77	3	0
5	G	49	0	77	2	0
6	D	21	0	21	2	0
6	H	21	0	21	5	0
6	I	21	0	21	2	0
All	All	21087	0	22126	291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (291) 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)
3:I:41:SER:OG	6:I:101:PN7:P	2.02	1.18
1:A:804:ILE:HD11	1:A:855:VAL:HG11	1.62	0.81
1:E:804:ILE:HD11	1:E:855:VAL:HG11	1.62	0.80
1:B:804:ILE:HD11	1:B:855:VAL:HG11	1.62	0.80
4:A:1001:CDL:H873	5:A:1003:PEV:H221	1.68	0.76
6:H:101:PN7:O8	6:H:101:PN7:N5	2.21	0.73
1:A:488:ASP:N	1:A:488:ASP:OD1	2.23	0.71
1:E:885:GLY:HA3	1:E:918:THR:HG21	1.74	0.69
1:E:488:ASP:N	1:E:488:ASP:OD1	2.23	0.69
1:B:488:ASP:OD1	1:B:488:ASP:N	2.23	0.69
1:E:893:MET:HG3	1:E:911:GLY:HA3	1.75	0.69
1:A:893:MET:HG3	1:A:911:GLY:HA3	1.75	0.69
1:B:893:MET:HG3	1:B:911:GLY:HA3	1.75	0.69
1:A:885:GLY:HA3	1:A:918:THR:HG21	1.74	0.68
1:E:866:ILE:HD12	1:E:945:GLN:HA	1.76	0.68
1:A:227:ILE:HG21	1:A:367:LEU:HD22	1.76	0.68
1:B:885:GLY:HA3	1:B:918:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PRO:HB2	1:B:932:LEU:HD22	1.76	0.67
3:D:5:GLN:HG2	3:D:74:VAL:HG11	1.77	0.67
1:E:381:LYS:NZ	3:I:40:ASP:OD2	2.27	0.67
1:E:227:ILE:HG21	1:E:367:LEU:HD22	1.75	0.67
1:B:227:ILE:HG21	1:B:367:LEU:HD22	1.75	0.67
1:B:866:ILE:HD12	1:B:945:GLN:HA	1.76	0.67
1:A:866:ILE:HD12	1:A:945:GLN:HA	1.76	0.66
3:H:5:GLN:HG2	3:H:74:VAL:HG11	1.77	0.66
1:A:390:PRO:HB2	1:A:932:LEU:HD22	1.76	0.66
1:E:390:PRO:HB2	1:E:932:LEU:HD22	1.76	0.66
3:I:5:GLN:HG2	3:I:74:VAL:HG11	1.77	0.66
1:B:232:MET:HE2	1:B:279:ILE:HG13	1.79	0.65
1:A:232:MET:HE2	1:A:279:ILE:HG13	1.79	0.64
5:A:1003:PEV:H432	5:A:1003:PEV:H192	1.79	0.64
1:E:232:MET:HE2	1:E:279:ILE:HG13	1.79	0.64
1:B:872:ARG:NH1	3:D:18:GLU:OE2	2.30	0.64
1:E:496:SER:HB2	1:E:498:PRO:HD2	1.81	0.63
1:A:496:SER:HB2	1:A:498:PRO:HD2	1.81	0.62
1:B:496:SER:HB2	1:B:498:PRO:HD2	1.81	0.61
4:E:1001:CDL:H111	4:E:1001:CDL:H522	1.82	0.60
1:E:858:LEU:HD11	1:E:870:ILE:HG12	1.84	0.60
1:A:872:ARG:NH1	3:H:18:GLU:OE2	2.35	0.59
1:E:60:GLN:NE2	1:E:251:GLY:O	2.36	0.59
1:A:858:LEU:HD11	1:A:870:ILE:HG12	1.84	0.59
4:B:1001:CDL:H711	1:E:395:VAL:HG11	1.85	0.59
1:E:872:ARG:NH1	3:I:18:GLU:OE2	2.36	0.58
1:B:295:ARG:NH1	1:B:365:GLY:O	2.37	0.58
1:B:858:LEU:HD11	1:B:870:ILE:HG12	1.84	0.58
1:A:295:ARG:NH1	1:A:365:GLY:O	2.37	0.58
1:B:379:TRP:CD1	1:B:879:SER:HG	2.21	0.58
1:A:60:GLN:NE2	1:A:251:GLY:O	2.36	0.58
1:A:284:ARG:HG3	1:A:302:MET:HA	1.86	0.58
1:B:284:ARG:HG3	1:B:302:MET:HA	1.86	0.58
1:E:384:ALA:HB2	3:I:46:GLU:HB3	1.85	0.58
1:E:295:ARG:NH1	1:E:365:GLY:O	2.37	0.58
1:E:402:LEU:HD21	4:E:1001:CDL:H662	1.86	0.58
1:E:284:ARG:HG3	1:E:302:MET:HA	1.86	0.58
1:B:832:HIS:HD2	1:B:834:LEU:H	1.52	0.57
1:B:284:ARG:NH1	1:B:860:GLU:OE2	2.38	0.57
1:A:284:ARG:NH1	1:A:860:GLU:OE2	2.38	0.57
1:A:384:ALA:HB2	3:H:46:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:101:PN7:H8	6:H:101:PN7:O4	2.04	0.56
1:B:60:GLN:NE2	1:B:251:GLY:O	2.36	0.56
1:E:284:ARG:NH1	1:E:860:GLU:OE2	2.38	0.56
1:A:887:VAL:O	1:A:891:THR:HG23	2.05	0.56
1:E:887:VAL:O	1:E:891:THR:HG23	2.05	0.56
1:E:722:HIS:HD2	1:E:734:ARG:HE	1.53	0.56
1:A:722:HIS:HD2	1:A:734:ARG:HE	1.53	0.56
1:A:832:HIS:HD2	1:A:834:LEU:H	1.52	0.56
3:H:57:VAL:HG11	3:H:77:ILE:HG12	1.87	0.56
1:B:62:VAL:HG11	1:B:334:THR:HG21	1.88	0.56
1:B:932:LEU:HD12	4:B:1001:CDL:H122	1.88	0.56
3:I:57:VAL:HG11	3:I:77:ILE:HG12	1.87	0.56
1:B:722:HIS:HD2	1:B:734:ARG:HE	1.53	0.56
1:A:491:PRO:HD2	1:A:684:ARG:HG2	1.88	0.56
1:B:381:LYS:NZ	3:D:40:ASP:OD2	2.30	0.56
1:B:887:VAL:O	1:B:891:THR:HG23	2.05	0.55
1:E:62:VAL:HG11	1:E:334:THR:HG21	1.88	0.55
1:E:832:HIS:HD2	1:E:834:LEU:H	1.52	0.55
4:A:1002:CDL:H801	4:A:1002:CDL:H851	1.89	0.55
1:E:480:ARG:HD3	1:E:489:GLY:HA3	1.89	0.55
1:E:722:HIS:CD2	1:E:734:ARG:HE	2.25	0.55
1:A:381:LYS:NZ	3:H:40:ASP:OD2	2.34	0.55
1:A:395:VAL:HG11	4:E:1001:CDL:H311	1.88	0.55
1:A:722:HIS:CD2	1:A:734:ARG:HE	2.25	0.55
1:A:480:ARG:HD3	1:A:489:GLY:HA3	1.89	0.55
1:B:384:ALA:HB2	3:D:46:GLU:HB3	1.88	0.55
3:D:40:ASP:OD1	3:D:40:ASP:N	2.38	0.55
3:D:57:VAL:HG11	3:D:77:ILE:HG12	1.87	0.55
1:B:491:PRO:HD2	1:B:684:ARG:HG2	1.88	0.54
1:E:491:PRO:HD2	1:E:684:ARG:HG2	1.88	0.54
1:B:480:ARG:HD3	1:B:489:GLY:HA3	1.89	0.54
1:B:722:HIS:CD2	1:B:734:ARG:HE	2.25	0.54
1:E:912:MET:HG2	4:E:1002:CDL:H673	1.90	0.54
1:E:199:ALA:HA	1:E:202:ARG:HE	1.73	0.54
1:A:62:VAL:HG11	1:A:334:THR:HG21	1.88	0.54
1:A:379:TRP:CD1	1:A:879:SER:HG	2.27	0.53
3:I:40:ASP:OD1	3:I:40:ASP:N	2.38	0.53
1:B:218:MET:HE1	4:B:1002:CDL:H752	1.90	0.53
1:B:919:LEU:HB3	4:B:1002:CDL:H191	1.90	0.53
1:A:37:LEU:O	1:A:41:VAL:HG22	2.09	0.53
1:B:37:LEU:O	1:B:41:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:GLY:HA3	1:E:347:VAL:HG21	1.91	0.53
1:A:933:LEU:HD21	4:A:1001:CDL:H141	1.90	0.53
1:E:37:LEU:O	1:E:41:VAL:HG22	2.09	0.53
1:B:199:ALA:HA	1:B:202:ARG:HE	1.73	0.52
4:B:1001:CDL:HB31	1:E:392:PRO:HG3	1.92	0.52
1:B:314:GLY:HA3	1:B:347:VAL:HG21	1.91	0.52
1:A:199:ALA:HA	1:A:202:ARG:HE	1.73	0.52
1:B:917:ASP:OD2	1:B:922:ARG:NH2	2.41	0.52
1:B:435:GLU:HG2	1:B:440:GLN:HA	1.92	0.52
1:A:702:GLN:O	1:A:706:GLU:HG2	2.11	0.51
1:B:171:THR:O	1:B:175:ARG:HB2	2.10	0.51
1:E:393:ILE:HG23	4:E:1002:CDL:H792	1.90	0.51
3:H:40:ASP:N	3:H:40:ASP:OD1	2.38	0.51
1:E:171:THR:O	1:E:175:ARG:HB2	2.10	0.51
1:E:315:LEU:HD21	5:E:1003:PEV:H481	1.93	0.51
1:A:196:GLN:HG3	1:A:421:LEU:HD21	1.92	0.51
1:B:702:GLN:O	1:B:706:GLU:HG2	2.11	0.51
1:E:435:GLU:HG2	1:E:440:GLN:HA	1.92	0.51
1:B:196:GLN:HG3	1:B:421:LEU:HD21	1.92	0.51
1:E:33:VAL:HG23	1:E:34:PRO:HD3	1.93	0.51
1:A:171:THR:O	1:A:175:ARG:HB2	2.11	0.50
1:A:314:GLY:HA3	1:A:347:VAL:HG21	1.91	0.50
1:A:33:VAL:HG23	1:A:34:PRO:HD3	1.93	0.50
1:A:435:GLU:HG2	1:A:440:GLN:HA	1.92	0.50
1:E:196:GLN:HG3	1:E:421:LEU:HD21	1.92	0.50
1:E:384:ALA:CB	3:I:46:GLU:HB3	2.41	0.50
1:E:702:GLN:O	1:E:706:GLU:HG2	2.11	0.50
1:A:478:ILE:HD11	1:A:738:ILE:HD11	1.93	0.50
4:A:1002:CDL:H532	4:A:1002:CDL:H112	1.93	0.50
1:A:199:ALA:HB2	1:A:202:ARG:HH21	1.77	0.50
1:E:917:ASP:OD2	1:E:922:ARG:NH2	2.41	0.50
1:A:389:TRP:CE2	6:H:101:PN7:H16	2.47	0.49
1:E:199:ALA:HB2	1:E:202:ARG:HH21	1.77	0.49
1:B:199:ALA:HB2	1:B:202:ARG:HH21	1.77	0.49
1:B:478:ILE:HD11	1:B:738:ILE:HD11	1.93	0.49
1:E:138:GLY:O	1:E:442:ARG:NH2	2.45	0.49
1:A:287:GLU:OE2	1:A:857:ARG:NH2	2.31	0.49
1:A:481:VAL:O	1:A:489:GLY:HA2	2.13	0.49
1:B:138:GLY:O	1:B:442:ARG:NH2	2.45	0.49
1:E:481:VAL:O	1:E:489:GLY:HA2	2.13	0.49
1:E:478:ILE:HD11	1:E:738:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:O	1:A:442:ARG:NH2	2.45	0.49
1:E:328:ARG:NH2	2:G:29:ARG:O	2.46	0.49
1:B:33:VAL:HG23	1:B:34:PRO:HD3	1.94	0.48
4:A:1001:CDL:H772	4:A:1001:CDL:H462	1.96	0.48
1:B:481:VAL:O	1:B:489:GLY:HA2	2.13	0.48
1:A:384:ALA:CB	3:H:46:GLU:HB3	2.43	0.48
1:E:379:TRP:CD1	1:E:879:SER:HG	2.32	0.48
6:H:101:PN7:H15	1:E:936:TRP:CH2	2.49	0.48
4:A:1001:CDL:H522	4:A:1001:CDL:H142	1.96	0.48
1:B:201:ASP:O	1:B:205:GLN:HG2	2.14	0.48
1:B:832:HIS:CD2	1:B:834:LEU:H	2.30	0.48
1:E:201:ASP:O	1:E:205:GLN:HG2	2.14	0.48
1:E:832:HIS:CD2	1:E:834:LEU:H	2.30	0.48
1:A:392:PRO:HG3	4:E:1001:CDL:HA31	1.96	0.47
1:A:917:ASP:OD2	1:A:922:ARG:NH2	2.41	0.47
1:B:373:MET:HE2	1:B:373:MET:HA	1.97	0.47
1:B:393:ILE:HG12	4:B:1002:CDL:H392	1.96	0.47
1:E:373:MET:HE2	1:E:373:MET:HA	1.97	0.47
1:A:832:HIS:CD2	1:A:834:LEU:H	2.30	0.47
1:A:477:GLY:HA3	1:A:734:ARG:NH2	2.30	0.47
1:B:328:ARG:NH2	2:C:29:ARG:O	2.47	0.47
1:E:477:GLY:HA3	1:E:734:ARG:NH2	2.30	0.47
1:A:201:ASP:O	1:A:205:GLN:HG2	2.14	0.47
4:E:1002:CDL:H791	4:E:1002:CDL:H821	1.53	0.46
1:A:373:MET:HA	1:A:373:MET:HE2	1.97	0.46
1:B:414:ASN:HD21	1:B:419:ASN:HD22	1.64	0.46
4:A:1002:CDL:H762	5:G:201:PEV:H142	1.96	0.46
1:B:384:ALA:CB	3:D:46:GLU:HB3	2.46	0.46
1:B:477:GLY:HA3	1:B:734:ARG:NH2	2.30	0.46
4:E:1001:CDL:H142	4:E:1001:CDL:H112	1.69	0.46
1:B:272:ALA:HB2	1:B:888:PHE:CZ	2.51	0.45
1:E:272:ALA:HB2	1:E:888:PHE:CZ	2.51	0.45
1:E:414:ASN:HD21	1:E:419:ASN:HD22	1.64	0.45
1:B:890:PHE:HZ	4:B:1002:CDL:H592	1.82	0.45
1:B:886:LEU:HD11	4:B:1002:CDL:H541	1.97	0.45
1:A:414:ASN:HD21	1:A:419:ASN:HD22	1.64	0.45
4:B:1001:CDL:H461	4:B:1001:CDL:H432	1.78	0.45
1:B:287:GLU:OE2	1:B:857:ARG:NH2	2.31	0.45
4:A:1002:CDL:H382	4:A:1002:CDL:H411	1.70	0.45
1:E:796:ARG:O	1:E:941:GLN:NE2	2.50	0.45
1:A:796:ARG:O	1:A:941:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1004:PEV:H382	5:A:1004:PEV:H351	1.43	0.45
3:H:6:GLU:N	3:H:6:GLU:OE1	2.50	0.45
4:E:1002:CDL:H722	3:I:42:LEU:HD21	1.99	0.45
1:A:328:ARG:NH2	2:F:29:ARG:O	2.49	0.44
1:B:796:ARG:O	1:B:941:GLN:NE2	2.50	0.44
3:D:6:GLU:N	3:D:6:GLU:OE1	2.50	0.44
1:A:166:VAL:HG11	1:A:191:ALA:HA	2.00	0.44
4:B:1002:CDL:H531	4:B:1002:CDL:H562	1.67	0.44
3:I:6:GLU:OE1	3:I:6:GLU:N	2.50	0.44
1:A:272:ALA:HB2	1:A:888:PHE:CZ	2.51	0.44
1:B:40:LEU:HA	1:B:40:LEU:HD23	1.82	0.44
4:E:1002:CDL:H172	4:E:1002:CDL:H141	1.63	0.44
1:B:378:GLY:HA3	4:B:1002:CDL:HA4	2.00	0.44
1:E:166:VAL:HG11	1:E:191:ALA:HA	2.00	0.44
1:B:364:PHE:O	1:B:367:LEU:HG	2.17	0.44
1:B:166:VAL:HG11	1:B:191:ALA:HA	2.00	0.43
1:E:735:ILE:HG22	1:E:739:LYS:HE2	2.00	0.43
1:A:314:GLY:HA3	1:A:347:VAL:CG2	2.48	0.43
1:E:364:PHE:O	1:E:367:LEU:HG	2.17	0.43
1:A:735:ILE:HG22	1:A:739:LYS:HE2	2.00	0.43
4:B:1002:CDL:H361	6:D:101:PN7:H20	2.00	0.43
1:E:66:PRO:HG2	2:G:32:PHE:CE1	2.52	0.43
4:A:1001:CDL:H802	4:A:1001:CDL:H771	1.66	0.43
1:B:735:ILE:HG22	1:B:739:LYS:HE2	2.00	0.43
4:B:1002:CDL:H551	4:B:1002:CDL:H582	1.28	0.43
1:A:364:PHE:O	1:A:367:LEU:HG	2.18	0.43
1:B:890:PHE:CZ	4:B:1002:CDL:H592	2.54	0.43
1:A:795:THR:O	1:A:797:SER:N	2.51	0.43
5:A:1004:PEV:H451	5:A:1004:PEV:H421	1.72	0.43
1:B:161:LEU:O	1:B:164:GLU:HB2	2.19	0.43
1:E:265:LEU:HD12	1:E:265:LEU:HA	1.86	0.43
1:E:500:LEU:HD21	1:E:690:TYR:HB2	2.01	0.43
1:A:380:ARG:HG3	1:A:875:GLY:HA3	2.01	0.43
1:A:500:LEU:HD21	1:A:690:TYR:HB2	2.01	0.43
1:B:230:ALA:O	1:B:234:THR:HG23	2.19	0.43
1:E:732:ILE:HD11	1:E:765:PHE:HB3	2.01	0.43
4:E:1001:CDL:H712	4:E:1001:CDL:HB62	1.74	0.43
1:B:380:ARG:HG3	1:B:875:GLY:HA3	2.01	0.43
1:A:161:LEU:O	1:A:164:GLU:HB2	2.19	0.43
1:A:230:ALA:O	1:A:234:THR:HG23	2.19	0.43
1:B:314:GLY:HA3	1:B:347:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD21	1:B:690:TYR:HB2	2.01	0.43
1:E:497:ILE:N	1:E:498:PRO:HD2	2.34	0.43
1:B:732:ILE:HD11	1:B:765:PHE:HB3	2.01	0.42
5:A:1003:PEV:H263	5:A:1003:PEV:H231	1.81	0.42
4:E:1001:CDL:H862	4:E:1001:CDL:H341	2.00	0.42
1:E:161:LEU:O	1:E:164:GLU:HB2	2.19	0.42
3:I:33:PHE:O	3:I:39:ILE:N	2.36	0.42
1:A:732:ILE:HD11	1:A:765:PHE:HB3	2.01	0.42
1:E:380:ARG:HG3	1:E:875:GLY:HA3	2.01	0.42
5:E:1003:PEV:H251	5:E:1003:PEV:H222	1.70	0.42
1:B:497:ILE:N	1:B:498:PRO:HD2	2.34	0.42
1:E:230:ALA:O	1:E:234:THR:HG23	2.19	0.42
1:A:389:TRP:CE3	6:H:101:PN7:H18	2.54	0.42
1:E:795:THR:O	1:E:797:SER:N	2.51	0.42
4:E:1001:CDL:H341	4:E:1001:CDL:H372	1.73	0.42
1:A:497:ILE:N	1:A:498:PRO:HD2	2.34	0.42
1:A:878:GLY:HA2	1:A:881:VAL:HG22	2.02	0.42
1:E:231:ILE:O	1:E:234:THR:OG1	2.38	0.42
1:E:314:GLY:HA3	1:E:347:VAL:CG2	2.48	0.42
1:A:335:LEU:O	1:A:339:LEU:HB2	2.20	0.41
1:B:878:GLY:HA2	1:B:881:VAL:HG22	2.02	0.41
4:E:1001:CDL:H171	4:E:1001:CDL:H572	2.02	0.41
1:A:501:ILE:HA	1:B:501:ILE:HD13	2.02	0.41
1:B:795:THR:O	1:B:797:SER:N	2.51	0.41
4:B:1002:CDL:H602	4:B:1002:CDL:H571	1.39	0.41
1:A:361:THR:O	1:A:367:LEU:HD12	2.21	0.41
1:A:218:MET:HE1	4:A:1002:CDL:H352	2.02	0.41
1:B:335:LEU:O	1:B:339:LEU:HB2	2.20	0.41
1:B:361:THR:O	1:B:367:LEU:HD12	2.21	0.41
6:D:101:PN7:O4	6:D:101:PN7:H5	2.19	0.41
1:E:152:LYS:HB3	1:E:152:LYS:HE3	1.81	0.41
4:A:1002:CDL:H451	4:A:1002:CDL:H421	1.83	0.41
3:H:5:GLN:NE2	3:H:9:ILE:HD11	2.36	0.41
1:E:335:LEU:O	1:E:339:LEU:HB2	2.20	0.41
4:A:1001:CDL:H622	4:A:1001:CDL:H651	1.95	0.41
4:A:1002:CDL:H122	4:A:1002:CDL:HA4	2.02	0.41
5:C:201:PEV:H322	5:C:201:PEV:H2	1.78	0.41
1:E:822:ILE:HD13	1:E:826:ILE:HD12	2.03	0.41
2:G:13:LEU:HD11	5:G:201:PEV:H412	2.01	0.41
1:B:188:GLY:C	1:B:190:ALA:H	2.29	0.41
1:B:952:TRP:HA	1:B:953:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:23:GLU:HG3	3:D:24:PRO:HD2	2.03	0.41
1:E:360:VAL:O	1:E:363:ARG:HG2	2.21	0.41
1:E:858:LEU:HD12	1:E:858:LEU:HA	1.94	0.41
3:I:5:GLN:NE2	3:I:9:ILE:HD11	2.36	0.41
4:B:1001:CDL:H631	4:B:1001:CDL:H662	1.91	0.41
3:D:5:GLN:NE2	3:D:9:ILE:HD11	2.36	0.41
3:H:82:GLU:OE1	3:H:82:GLU:HA	2.21	0.40
1:B:412:ARG:H	1:B:824:GLN:HE22	1.69	0.40
1:E:878:GLY:HA2	1:E:881:VAL:HG22	2.02	0.40
5:E:1003:PEV:H182	5:E:1003:PEV:H212	1.78	0.40
1:A:188:GLY:C	1:A:190:ALA:H	2.29	0.40
1:A:815:SER:HB3	1:A:913:GLY:HA2	2.04	0.40
3:H:23:GLU:HG3	3:H:24:PRO:HD2	2.03	0.40
1:B:266:LEU:HD11	1:B:342:GLY:HA3	2.04	0.40
1:E:402:LEU:HD23	1:E:402:LEU:HA	1.92	0.40
6:I:101:PN7:O4	6:I:101:PN7:CE2	2.69	0.40
1:B:822:ILE:HD13	1:B:826:ILE:HD12	2.03	0.40
3:D:82:GLU:OE1	3:D:82:GLU:HA	2.21	0.40
1:E:361:THR:O	1:E:367:LEU:HD12	2.21	0.40
1:E:815:SER:HB3	1:E:913:GLY:HA2	2.04	0.40
1:E:836:LEU:O	1:E:840:VAL:HG13	2.22	0.40
4:E:1001:CDL:H441	4:E:1001:CDL:H411	1.92	0.40
3:I:23:GLU:HG3	3:I:24:PRO:HD2	2.03	0.40
3:I:82:GLU:HA	3:I:82:GLU:OE1	2.21	0.40
1:A:382:VAL:HG21	4:A:1002:CDL:H522	2.04	0.40
1:B:915:LEU:HD23	1:B:915:LEU:HA	1.92	0.40
4:B:1002:CDL:H342	4:B:1002:CDL:H371	1.82	0.40
1:E:188:GLY:C	1:E:190:ALA:H	2.29	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	768/964 (80%)	732 (95%)	36 (5%)	0	100	100
1	B	768/964 (80%)	733 (95%)	35 (5%)	0	100	100
1	E	768/964 (80%)	732 (95%)	36 (5%)	0	100	100
2	C	32/142 (22%)	32 (100%)	0	0	100	100
2	F	32/142 (22%)	31 (97%)	1 (3%)	0	100	100
2	G	32/142 (22%)	32 (100%)	0	0	100	100
3	D	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
3	H	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
3	I	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
All	All	2643/3615 (73%)	2529 (96%)	114 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	606/783 (77%)	596 (98%)	10 (2%)	56	74
1	B	606/783 (77%)	596 (98%)	10 (2%)	56	74
1	E	606/783 (77%)	596 (98%)	10 (2%)	56	74
2	C	28/117 (24%)	25 (89%)	3 (11%)	5	7
2	F	28/117 (24%)	25 (89%)	3 (11%)	5	7
2	G	28/117 (24%)	25 (89%)	3 (11%)	5	7
3	D	71/81 (88%)	69 (97%)	2 (3%)	38	58
3	H	71/81 (88%)	69 (97%)	2 (3%)	38	58
3	I	71/81 (88%)	69 (97%)	2 (3%)	38	58
All	All	2115/2943 (72%)	2070 (98%)	45 (2%)	49	69

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	71	SER
1	A	141	SER
1	A	182	VAL
1	A	306	THR
1	A	373	MET
1	A	488	ASP
1	A	496	SER
1	A	694	GLU
1	A	773	THR
2	F	2	ILE
2	F	5	LEU
2	F	24	THR
3	H	6	GLU
3	H	25	SER
1	B	41	VAL
1	B	71	SER
1	B	141	SER
1	B	182	VAL
1	B	306	THR
1	B	373	MET
1	B	488	ASP
1	B	496	SER
1	B	694	GLU
1	B	773	THR
2	C	2	ILE
2	C	5	LEU
2	C	24	THR
3	D	6	GLU
3	D	25	SER
1	E	41	VAL
1	E	71	SER
1	E	141	SER
1	E	182	VAL
1	E	306	THR
1	E	373	MET
1	E	488	ASP
1	E	496	SER
1	E	694	GLU
1	E	773	THR
2	G	2	ILE
2	G	5	LEU
2	G	24	THR

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Mol	Chain	Res	Type
3	I	6	GLU
3	I	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	286	GLN
1	A	414	ASN
1	A	466	ASN
1	A	482	GLN
1	A	722	HIS
1	A	729	GLN
1	A	824	GLN
1	A	832	HIS
3	H	50	GLN
1	B	264	ASN
1	B	286	GLN
1	B	414	ASN
1	B	454	HIS
1	B	482	GLN
1	B	722	HIS
1	B	729	GLN
1	B	824	GLN
1	B	832	HIS
1	B	941	GLN
3	D	50	GLN
1	E	264	ASN
1	E	286	GLN
1	E	414	ASN
1	E	482	GLN
1	E	722	HIS
1	E	824	GLN
1	E	832	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	PEV	B	1003	-	48,48,48	0.88	4 (8%)	51,53,53	1.10	2 (3%)
6	PN7	I	101	-	13,20,21	3.39	7 (53%)	18,26,29	4.74	14 (77%)
4	CDL	B	1001	-	99,99,99	0.87	8 (8%)	105,111,111	1.12	4 (3%)
5	PEV	E	1003	-	48,48,48	0.88	4 (8%)	51,53,53	1.11	2 (3%)
5	PEV	G	201	-	48,48,48	0.87	4 (8%)	51,53,53	1.17	2 (3%)
5	PEV	A	1003	-	48,48,48	0.88	4 (8%)	51,53,53	1.18	2 (3%)
6	PN7	H	101	-	13,20,21	3.69	8 (61%)	18,26,29	6.39	12 (66%)
4	CDL	A	1001	-	99,99,99	0.87	8 (8%)	105,111,111	1.10	4 (3%)
4	CDL	E	1002	-	99,99,99	0.87	8 (8%)	105,111,111	1.10	4 (3%)
5	PEV	A	1004	-	48,48,48	0.87	4 (8%)	51,53,53	1.09	2 (3%)
6	PN7	D	101	3	13,20,21	3.59	9 (69%)	18,26,29	3.91	11 (61%)
4	CDL	A	1002	-	99,99,99	0.87	8 (8%)	105,111,111	1.15	4 (3%)
4	CDL	E	1001	-	99,99,99	0.87	8 (8%)	105,111,111	1.12	4 (3%)
4	CDL	B	1002	-	99,99,99	0.88	7 (7%)	105,111,111	1.12	5 (4%)
5	PEV	C	201	-	48,48,48	0.88	4 (8%)	51,53,53	1.15	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEV	B	1003	-	-	28/52/52/52	-
6	PN7	I	101	-	-	12/24/26/27	-
4	CDL	B	1001	-	-	62/110/110/110	-
5	PEV	E	1003	-	-	24/52/52/52	-
5	PEV	G	201	-	-	27/52/52/52	-
5	PEV	A	1003	-	-	28/52/52/52	-
6	PN7	H	101	-	-	11/24/26/27	-
4	CDL	A	1001	-	-	60/110/110/110	-
4	CDL	E	1002	-	-	60/110/110/110	-
5	PEV	A	1004	-	-	31/52/52/52	-
6	PN7	D	101	3	-	12/24/26/27	-
4	CDL	A	1002	-	-	61/110/110/110	-
4	CDL	E	1001	-	-	57/110/110/110	-
4	CDL	B	1002	-	-	62/110/110/110	-
5	PEV	C	201	-	-	25/52/52/52	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	101	PN7	O8-C8	-7.78	1.07	1.23
6	D	101	PN7	O8-C8	-7.44	1.08	1.23
6	I	101	PN7	O8-C8	-6.78	1.09	1.23
6	H	101	PN7	O4-C4	-5.52	1.12	1.23
6	I	101	PN7	O4-C4	-5.32	1.12	1.23
6	D	101	PN7	O4-C4	-5.26	1.12	1.23
6	D	101	PN7	C4-N5	4.95	1.44	1.33
6	I	101	PN7	O3P-C1	-4.71	1.33	1.44
6	H	101	PN7	C4-N5	4.34	1.43	1.33
6	H	101	PN7	O3P-C1	-4.29	1.34	1.44
6	I	101	PN7	C4-N5	4.09	1.42	1.33
6	H	101	PN7	O3-C3	-4.01	1.34	1.42
6	D	101	PN7	O3-C3	-3.59	1.35	1.42
6	D	101	PN7	O3P-C1	-3.55	1.36	1.44
6	I	101	PN7	O3-C3	-3.50	1.35	1.42
6	D	101	PN7	C8-N9	3.46	1.41	1.33
6	H	101	PN7	C10-N9	-3.10	1.39	1.46
6	I	101	PN7	C8-N9	2.96	1.40	1.33
6	H	101	PN7	C8-N9	2.89	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	CDL	OB6-CB4	-2.75	1.39	1.46
4	B	1001	CDL	OB6-CB4	-2.74	1.39	1.46
4	E	1001	CDL	OA6-CA4	-2.70	1.39	1.46
4	E	1002	CDL	OA6-CA4	-2.61	1.40	1.46
4	A	1001	CDL	OB6-CB4	-2.60	1.40	1.46
5	C	201	PEV	O2-C2	-2.59	1.40	1.46
5	E	1003	PEV	O2-C2	-2.56	1.40	1.46
5	A	1004	PEV	O2-C2	-2.54	1.40	1.46
5	B	1003	PEV	O2-C2	-2.49	1.40	1.46
4	B	1002	CDL	OB8-CB7	2.48	1.40	1.33
5	A	1003	PEV	O2-C2	-2.47	1.40	1.46
5	G	201	PEV	O2-C2	-2.47	1.40	1.46
4	E	1001	CDL	OB8-CB7	2.46	1.40	1.33
4	A	1002	CDL	OB6-CB4	-2.46	1.40	1.46
4	B	1001	CDL	OA8-CA7	2.44	1.40	1.33
4	A	1001	CDL	OA6-CA4	-2.44	1.40	1.46
4	A	1001	CDL	OA8-CA7	2.42	1.40	1.33
4	E	1002	CDL	OB6-CB4	-2.41	1.40	1.46
4	B	1001	CDL	OA6-CA4	-2.39	1.40	1.46
5	A	1004	PEV	O3-C11	2.39	1.40	1.33
4	E	1001	CDL	OA8-CA6	-2.39	1.39	1.45
6	D	101	PN7	CE1-C2	-2.38	1.48	1.53
4	E	1002	CDL	OB8-CB7	2.37	1.40	1.33
4	A	1002	CDL	OA8-CA7	2.37	1.40	1.33
5	G	201	PEV	O3-C11	2.36	1.40	1.33
4	E	1001	CDL	OB6-CB4	-2.36	1.40	1.46
5	B	1003	PEV	O3-C11	2.35	1.40	1.33
5	C	201	PEV	O3-C11	2.35	1.40	1.33
4	B	1002	CDL	OA8-CA6	-2.34	1.39	1.45
4	A	1001	CDL	OB8-CB7	2.34	1.40	1.33
4	B	1002	CDL	OA6-CA4	-2.33	1.40	1.46
4	B	1001	CDL	OB8-CB6	-2.32	1.39	1.45
5	A	1003	PEV	O3-C3	-2.32	1.39	1.45
4	A	1002	CDL	OB8-CB7	2.31	1.40	1.33
5	E	1003	PEV	O3-C11	2.31	1.40	1.33
4	E	1002	CDL	OA8-CA6	-2.29	1.39	1.45
4	A	1002	CDL	OB6-CB5	2.29	1.40	1.34
4	A	1002	CDL	OA6-CA4	-2.29	1.40	1.46
4	E	1002	CDL	OA8-CA7	2.26	1.39	1.33
4	A	1001	CDL	OA6-CA5	2.26	1.40	1.34
5	A	1003	PEV	O2-C31	2.25	1.40	1.34
6	H	101	PN7	CE2-C2	-2.25	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	CDL	OA6-CA5	2.24	1.40	1.34
4	A	1002	CDL	OA6-CA5	2.24	1.40	1.34
4	A	1001	CDL	OB8-CB6	-2.23	1.40	1.45
4	B	1002	CDL	OA8-CA7	2.23	1.39	1.33
4	A	1002	CDL	OB8-CB6	-2.22	1.40	1.45
6	I	101	PN7	C6-N5	-2.22	1.41	1.46
4	E	1001	CDL	OB6-CB5	2.21	1.40	1.34
4	E	1002	CDL	OB8-CB6	-2.21	1.40	1.45
5	A	1003	PEV	O3-C11	2.21	1.39	1.33
4	B	1001	CDL	OA6-CA5	2.20	1.40	1.34
5	E	1003	PEV	O3-C3	-2.19	1.40	1.45
5	A	1004	PEV	O3-C3	-2.17	1.40	1.45
4	E	1002	CDL	OB6-CB5	2.17	1.40	1.34
4	B	1001	CDL	OB8-CB7	2.16	1.39	1.33
5	E	1003	PEV	O2-C31	2.15	1.40	1.34
4	A	1001	CDL	OB6-CB5	2.15	1.40	1.34
5	B	1003	PEV	O2-C31	2.15	1.40	1.34
5	B	1003	PEV	O3-C3	-2.15	1.40	1.45
4	E	1002	CDL	OA6-CA5	2.14	1.40	1.34
5	G	201	PEV	O2-C31	2.14	1.40	1.34
4	B	1001	CDL	OA8-CA6	-2.13	1.40	1.45
5	C	201	PEV	O3-C3	-2.13	1.40	1.45
4	A	1002	CDL	OA8-CA6	-2.12	1.40	1.45
5	G	201	PEV	O3-C3	-2.10	1.40	1.45
5	C	201	PEV	O2-C31	2.09	1.40	1.34
4	E	1001	CDL	OA8-CA7	2.08	1.39	1.33
4	A	1001	CDL	OA8-CA6	-2.08	1.40	1.45
4	E	1001	CDL	OA6-CA5	2.08	1.40	1.34
5	A	1004	PEV	O2-C31	2.06	1.40	1.34
4	B	1002	CDL	OB8-CB6	-2.03	1.40	1.45
6	D	101	PN7	C10-N9	-2.03	1.41	1.46
4	E	1001	CDL	OB8-CB6	-2.02	1.40	1.45
6	D	101	PN7	CE2-C2	-2.01	1.49	1.53
4	B	1001	CDL	OB6-CB5	2.01	1.40	1.34

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	101	PN7	C7-C8-N9	17.19	145.37	116.42
6	I	101	PN7	CE1-C2-C1	-11.06	90.20	108.23
6	H	101	PN7	CE1-C2-C1	-10.21	91.58	108.23
6	H	101	PN7	O8-C8-N9	-9.55	105.00	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	101	PN7	C10-N9-C8	8.74	139.06	122.84
6	D	101	PN7	CE2-C2-C1	-8.26	94.75	108.23
6	I	101	PN7	O8-C8-N9	-7.90	108.10	123.01
6	I	101	PN7	C7-C8-N9	7.66	129.31	116.42
6	D	101	PN7	O8-C8-N9	-7.24	109.35	123.01
6	H	101	PN7	O8-C8-C7	-6.79	109.59	122.02
6	D	101	PN7	C7-C8-N9	6.78	127.84	116.42
6	I	101	PN7	C3-C4-N5	5.78	128.08	116.58
6	H	101	PN7	C6-N5-C4	5.48	132.37	122.59
6	D	101	PN7	C3-C4-N5	5.08	126.70	116.58
4	A	1002	CDL	OB6-CB5-C51	4.75	121.73	111.50
5	A	1003	PEV	O2-C31-C32	4.74	121.72	111.50
6	H	101	PN7	C7-C6-N5	-4.74	102.33	111.90
6	D	101	PN7	C10-N9-C8	4.66	131.48	122.84
5	G	201	PEV	O2-C31-C32	4.63	121.47	111.50
6	I	101	PN7	C11-C10-N9	-4.62	101.75	112.31
4	A	1002	CDL	OA6-CA5-C11	4.47	121.14	111.50
6	I	101	PN7	CE2-C2-CE1	4.45	118.24	109.17
5	C	201	PEV	O2-C31-C32	4.41	121.00	111.50
6	H	101	PN7	CE2-C2-CE1	4.30	117.94	109.17
6	I	101	PN7	CE2-C2-C3	4.28	116.25	108.82
4	B	1002	CDL	OA6-CA5-C11	4.24	120.63	111.50
4	A	1001	CDL	OB6-CB5-C51	4.16	120.47	111.50
6	I	101	PN7	C10-N9-C8	4.14	130.51	122.84
6	H	101	PN7	C6-C7-C8	4.09	119.17	112.36
5	E	1003	PEV	O2-C31-C32	4.07	120.27	111.50
4	E	1002	CDL	OA6-CA5-C11	4.06	120.25	111.50
4	B	1001	CDL	OA6-CA5-C11	4.05	120.22	111.50
5	B	1003	PEV	O2-C31-C32	4.03	120.18	111.50
4	E	1001	CDL	OA6-CA5-C11	4.01	120.14	111.50
5	A	1004	PEV	O2-C31-C32	3.96	120.04	111.50
4	E	1001	CDL	OB6-CB5-C51	3.94	120.00	111.50
4	B	1001	CDL	OB6-CB5-C51	3.93	119.97	111.50
4	A	1001	CDL	OA6-CA5-C11	3.89	119.89	111.50
4	E	1002	CDL	OB6-CB5-C51	3.87	119.85	111.50
6	I	101	PN7	CE2-C2-C1	-3.80	102.04	108.23
6	I	101	PN7	O4-C4-N5	-3.79	114.84	122.99
4	B	1002	CDL	OB6-CB5-C51	3.78	119.64	111.50
6	D	101	PN7	CE1-C2-C3	3.52	114.92	108.82
6	H	101	PN7	CE2-C2-C1	-3.41	102.67	108.23
6	D	101	PN7	CE2-C2-CE1	3.29	115.88	109.17
6	D	101	PN7	CE1-C2-C1	-3.22	102.98	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	101	PN7	C11-C10-N9	-3.07	105.29	112.31
4	E	1002	CDL	OB8-CB7-C71	2.80	120.70	111.91
4	E	1001	CDL	OB8-CB7-C71	2.75	120.55	111.91
4	A	1002	CDL	OA8-CA7-C31	2.75	120.53	111.91
4	B	1002	CDL	CB4-OB6-CB5	-2.74	111.04	117.79
5	G	201	PEV	O3-C11-C12	2.68	120.31	111.91
4	B	1001	CDL	OA8-CA7-C31	2.66	120.26	111.91
5	C	201	PEV	O3-C11-C12	2.66	120.25	111.91
6	D	101	PN7	O4-C4-N5	-2.66	117.29	122.99
6	D	101	PN7	CE2-C2-C3	-2.61	104.29	108.82
4	A	1002	CDL	OB8-CB7-C71	2.61	120.08	111.91
5	E	1003	PEV	O3-C11-C12	2.60	120.07	111.91
4	E	1002	CDL	OA8-CA7-C31	2.60	120.06	111.91
4	B	1002	CDL	OB8-CB7-C71	2.56	119.95	111.91
4	B	1002	CDL	OA8-CA7-C31	2.55	119.91	111.91
5	B	1003	PEV	O3-C11-C12	2.49	119.72	111.91
5	A	1004	PEV	O3-C11-C12	2.46	119.63	111.91
4	A	1001	CDL	OB8-CB7-C71	2.43	119.54	111.91
4	B	1001	CDL	OB8-CB7-C71	2.39	119.42	111.91
4	A	1001	CDL	OA8-CA7-C31	2.37	119.36	111.91
5	A	1003	PEV	O3-C11-C12	2.37	119.34	111.91
6	I	101	PN7	C6-N5-C4	2.31	126.71	122.59
6	D	101	PN7	C11-C10-N9	2.26	117.48	112.31
6	I	101	PN7	C6-C7-C8	-2.22	108.67	112.36
4	E	1001	CDL	OA8-CA7-C31	2.14	118.61	111.91
6	H	101	PN7	C3-C4-N5	2.07	120.70	116.58
6	I	101	PN7	O3-C3-C2	2.05	115.08	110.25
6	I	101	PN7	CE1-C2-C3	-2.04	105.29	108.82

There are no chirality outliers.

All (560) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	CDL	CA2-OA2-PA1-OA3
4	A	1001	CDL	CA3-OA5-PA1-OA3
4	A	1001	CDL	CA3-OA5-PA1-OA4
4	A	1001	CDL	CB3-OB5-PB2-OB3
4	A	1001	CDL	CB3-OB5-PB2-OB4
4	A	1001	CDL	OB7-CB5-OB6-CB4
4	A	1001	CDL	C51-CB5-OB6-CB4
4	A	1002	CDL	CA2-OA2-PA1-OA3
4	A	1002	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
4	A	1002	CDL	C11-CA5-OA6-CA4
4	A	1002	CDL	OB7-CB5-OB6-CB4
4	B	1001	CDL	CA3-OA5-PA1-OA3
4	B	1001	CDL	CA3-OA5-PA1-OA4
4	B	1001	CDL	C11-CA5-OA6-CA4
4	B	1001	CDL	C31-CA7-OA8-CA6
4	B	1001	CDL	C51-CB5-OB6-CB4
4	B	1002	CDL	O1-C1-CB2-OB2
4	B	1002	CDL	CA2-C1-CB2-OB2
4	B	1002	CDL	CA3-OA5-PA1-OA2
4	B	1002	CDL	CA3-OA5-PA1-OA3
4	B	1002	CDL	CA3-OA5-PA1-OA4
4	B	1002	CDL	C11-CA5-OA6-CA4
4	B	1002	CDL	CB2-OB2-PB2-OB3
4	B	1002	CDL	CB3-OB5-PB2-OB3
4	B	1002	CDL	C51-CB5-OB6-CB4
4	E	1001	CDL	O1-C1-CA2-OA2
4	E	1001	CDL	CA3-OA5-PA1-OA3
4	E	1001	CDL	C11-CA5-OA6-CA4
4	E	1001	CDL	CB3-OB5-PB2-OB3
4	E	1001	CDL	CB3-OB5-PB2-OB4
4	E	1001	CDL	C51-CB5-OB6-CB4
4	E	1001	CDL	OB9-CB7-OB8-CB6
4	E	1001	CDL	C71-CB7-OB8-CB6
4	E	1002	CDL	O1-C1-CB2-OB2
4	E	1002	CDL	C11-CA5-OA6-CA4
4	E	1002	CDL	CB2-OB2-PB2-OB3
4	E	1002	CDL	OB7-CB5-OB6-CB4
5	A	1003	PEV	C32-C31-O2-C2
5	A	1003	PEV	O31-C31-O2-C2
5	A	1003	PEV	C1-O3P-P-O1P
5	A	1003	PEV	C1-O3P-P-O4P
5	A	1003	PEV	O11-C11-O3-C3
5	A	1004	PEV	O31-C31-O2-C2
5	A	1004	PEV	C1-O3P-P-O1P
5	A	1004	PEV	C4-O4P-P-O1P
5	A	1004	PEV	O4P-C4-C5-N6
5	B	1003	PEV	C1-O3P-P-O2P
5	B	1003	PEV	C4-O4P-P-O3P
5	B	1003	PEV	C4-O4P-P-O1P
5	B	1003	PEV	C4-O4P-P-O2P
5	B	1003	PEV	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
5	C	201	PEV	C32-C31-O2-C2
5	C	201	PEV	O31-C31-O2-C2
5	C	201	PEV	C4-O4P-P-O1P
5	C	201	PEV	C4-O4P-P-O2P
5	C	201	PEV	O4P-C4-C5-N6
5	E	1003	PEV	C32-C31-O2-C2
5	E	1003	PEV	C4-O4P-P-O3P
5	E	1003	PEV	O4P-C4-C5-N6
5	G	201	PEV	O31-C31-O2-C2
5	G	201	PEV	C4-O4P-P-O3P
5	G	201	PEV	C4-O4P-P-O1P
6	H	101	PN7	CE1-C2-C3-O3
6	H	101	PN7	CE1-C2-C3-C4
6	H	101	PN7	CE2-C2-C3-O3
6	H	101	PN7	O3-C3-C4-O4
6	H	101	PN7	N5-C6-C7-C8
6	H	101	PN7	N9-C10-C11-S12
6	D	101	PN7	C1-C2-C3-O3
6	D	101	PN7	C1-C2-C3-C4
6	D	101	PN7	CE1-C2-C3-O3
6	D	101	PN7	CE1-C2-C3-C4
6	D	101	PN7	CE2-C2-C3-O3
6	D	101	PN7	CE2-C2-C3-C4
6	D	101	PN7	O3-C3-C4-N5
6	D	101	PN7	C3-C4-N5-C6
6	D	101	PN7	N5-C6-C7-C8
6	D	101	PN7	N9-C10-C11-S12
6	I	101	PN7	C1-C2-C3-O3
6	I	101	PN7	C1-C2-C3-C4
6	I	101	PN7	CE1-C2-C3-O3
6	I	101	PN7	CE1-C2-C3-C4
6	I	101	PN7	CE2-C2-C3-O3
6	I	101	PN7	CE2-C2-C3-C4
6	I	101	PN7	O3-C3-C4-N5
6	I	101	PN7	C3-C4-N5-C6
6	I	101	PN7	N5-C6-C7-C8
6	I	101	PN7	N9-C10-C11-S12
4	B	1001	CDL	OA9-CA7-OA8-CA6
4	A	1001	CDL	OB9-CB7-OB8-CB6
4	E	1002	CDL	OB9-CB7-OB8-CB6
5	A	1004	PEV	O11-C11-O3-C3
5	E	1003	PEV	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
4	A	1001	CDL	OA7-CA5-OA6-CA4
4	B	1001	CDL	OA7-CA5-OA6-CA4
4	B	1001	CDL	OB7-CB5-OB6-CB4
4	B	1002	CDL	OA7-CA5-OA6-CA4
4	B	1002	CDL	OB7-CB5-OB6-CB4
4	E	1001	CDL	OA7-CA5-OA6-CA4
4	E	1001	CDL	OB7-CB5-OB6-CB4
4	E	1002	CDL	OA7-CA5-OA6-CA4
5	E	1003	PEV	O31-C31-O2-C2
4	A	1001	CDL	C71-CB7-OB8-CB6
5	A	1003	PEV	C12-C11-O3-C3
5	B	1003	PEV	C12-C11-O3-C3
5	E	1003	PEV	C12-C11-O3-C3
4	A	1001	CDL	C11-CA5-OA6-CA4
4	A	1002	CDL	C51-CB5-OB6-CB4
4	E	1002	CDL	C51-CB5-OB6-CB4
5	A	1004	PEV	C32-C31-O2-C2
5	G	201	PEV	C32-C31-O2-C2
6	H	101	PN7	C7-C8-N9-C10
4	E	1001	CDL	OA9-CA7-OA8-CA6
4	A	1002	CDL	C71-CB7-OB8-CB6
4	B	1001	CDL	C71-CB7-OB8-CB6
4	B	1002	CDL	C31-CA7-OA8-CA6
4	B	1002	CDL	C71-CB7-OB8-CB6
4	E	1001	CDL	C31-CA7-OA8-CA6
4	E	1002	CDL	C31-CA7-OA8-CA6
4	E	1002	CDL	C71-CB7-OB8-CB6
5	A	1004	PEV	C12-C11-O3-C3
5	G	201	PEV	C12-C11-O3-C3
4	A	1002	CDL	OA7-CA5-OA6-CA4
4	B	1002	CDL	OA9-CA7-OA8-CA6
4	B	1002	CDL	OB9-CB7-OB8-CB6
4	E	1002	CDL	OA9-CA7-OA8-CA6
4	A	1002	CDL	O1-C1-CA2-OA2
4	B	1002	CDL	O1-C1-CA2-OA2
4	A	1002	CDL	OB9-CB7-OB8-CB6
6	D	101	PN7	O4-C4-N5-C6
6	I	101	PN7	O4-C4-N5-C6
5	B	1003	PEV	C32-C31-O2-C2
4	E	1002	CDL	C73-C74-C75-C76
4	A	1002	CDL	C74-C75-C76-C77
4	B	1002	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
4	B	1001	CDL	OB9-CB7-OB8-CB6
5	G	201	PEV	O11-C11-O3-C3
6	H	101	PN7	O8-C8-N9-C10
4	A	1002	CDL	CB5-C51-C52-C53
4	A	1002	CDL	CB2-C1-CA2-OA2
4	E	1001	CDL	CB2-C1-CA2-OA2
4	E	1002	CDL	CA2-C1-CB2-OB2
5	B	1003	PEV	O31-C31-O2-C2
5	C	201	PEV	C12-C11-O3-C3
4	A	1001	CDL	C16-C17-C18-C19
4	B	1002	CDL	C55-C56-C57-C58
5	B	1003	PEV	C31-C32-C33-C34
5	C	201	PEV	O11-C11-O3-C3
4	A	1002	CDL	CA7-C31-C32-C33
4	B	1002	CDL	CB5-C51-C52-C53
4	B	1001	CDL	CB5-C51-C52-C53
4	A	1001	CDL	CA5-C11-C12-C13
4	A	1001	CDL	CB7-C71-C72-C73
4	A	1002	CDL	CA5-C11-C12-C13
4	A	1002	CDL	CB7-C71-C72-C73
4	E	1002	CDL	CA7-C31-C32-C33
4	E	1001	CDL	C11-C12-C13-C14
4	A	1001	CDL	CB5-C51-C52-C53
4	B	1001	CDL	CB7-C71-C72-C73
4	E	1001	CDL	CA7-C31-C32-C33
5	C	201	PEV	C31-C32-C33-C34
4	E	1002	CDL	C14-C15-C16-C17
5	E	1003	PEV	C18-C19-C20-C21
4	B	1002	CDL	C57-C58-C59-C60
4	E	1001	CDL	CA5-C11-C12-C13
4	A	1001	CDL	CA2-OA2-PA1-OA5
4	A	1001	CDL	CA3-OA5-PA1-OA2
4	A	1001	CDL	CB3-OB5-PB2-OB2
4	A	1002	CDL	CA3-OA5-PA1-OA2
4	B	1001	CDL	CA3-OA5-PA1-OA2
4	B	1002	CDL	CB3-OB5-PB2-OB2
4	E	1001	CDL	CB3-OB5-PB2-OB2
4	E	1002	CDL	CB2-OB2-PB2-OB5
5	A	1003	PEV	C4-O4P-P-O3P
5	B	1003	PEV	C1-O3P-P-O4P
5	C	201	PEV	C4-O4P-P-O3P
5	E	1003	PEV	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
5	G	201	PEV	C1-O3P-P-O4P
5	A	1004	PEV	C35-C36-C37-C38
4	A	1002	CDL	C31-CA7-OA8-CA6
4	A	1002	CDL	C80-C81-C82-C83
4	B	1002	CDL	C19-C20-C21-C22
4	E	1001	CDL	C77-C78-C79-C80
5	C	201	PEV	C33-C34-C35-C36
5	G	201	PEV	C32-C33-C34-C35
4	A	1001	CDL	C35-C36-C37-C38
4	A	1002	CDL	C21-C22-C23-C24
4	A	1002	CDL	C55-C56-C57-C58
4	B	1001	CDL	C77-C78-C79-C80
4	B	1002	CDL	C81-C82-C83-C84
4	E	1001	CDL	C14-C15-C16-C17
4	E	1002	CDL	C21-C22-C23-C24
4	E	1002	CDL	C54-C55-C56-C57
4	A	1002	CDL	C76-C77-C78-C79
4	B	1002	CDL	C14-C15-C16-C17
4	E	1002	CDL	C63-C64-C65-C66
4	E	1002	CDL	C74-C75-C76-C77
5	A	1004	PEV	C41-C42-C43-C44
4	E	1001	CDL	C17-C18-C19-C20
4	E	1002	CDL	C13-C14-C15-C16
4	E	1002	CDL	C76-C77-C78-C79
5	A	1004	PEV	C17-C18-C19-C20
5	C	201	PEV	C15-C16-C17-C18
4	A	1001	CDL	C13-C14-C15-C16
4	B	1001	CDL	C20-C21-C22-C23
4	B	1002	CDL	C32-C33-C34-C35
4	E	1002	CDL	C62-C63-C64-C65
4	E	1002	CDL	C79-C80-C81-C82
5	G	201	PEV	C12-C13-C14-C15
4	B	1002	CDL	C39-C40-C41-C42
4	A	1002	CDL	C73-C74-C75-C76
4	A	1002	CDL	C77-C78-C79-C80
4	B	1001	CDL	C16-C17-C18-C19
4	B	1002	CDL	C22-C23-C24-C25
4	E	1002	CDL	C75-C76-C77-C78
4	A	1002	CDL	C41-C42-C43-C44
5	A	1004	PEV	C32-C33-C34-C35
5	E	1003	PEV	C15-C16-C17-C18
4	A	1001	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
4	A	1001	CDL	C52-C53-C54-C55
4	A	1001	CDL	C56-C57-C58-C59
4	A	1001	CDL	C59-C60-C61-C62
4	A	1002	CDL	C79-C80-C81-C82
4	A	1002	CDL	C82-C83-C84-C85
4	E	1001	CDL	C16-C17-C18-C19
4	E	1001	CDL	C39-C40-C41-C42
4	E	1001	CDL	C63-C64-C65-C66
4	E	1002	CDL	C15-C16-C17-C18
5	C	201	PEV	C43-C44-C45-C46
5	G	201	PEV	C44-C45-C46-C47
5	G	201	PEV	C41-C42-C43-C44
4	A	1002	CDL	OA9-CA7-OA8-CA6
4	A	1002	CDL	C75-C76-C77-C78
5	A	1003	PEV	C42-C43-C44-C45
5	A	1004	PEV	C44-C45-C46-C47
5	E	1003	PEV	C41-C42-C43-C44
4	A	1002	CDL	C31-C32-C33-C34
4	B	1001	CDL	C11-C12-C13-C14
4	B	1002	CDL	C75-C76-C77-C78
4	E	1001	CDL	C33-C34-C35-C36
4	E	1001	CDL	C75-C76-C77-C78
4	E	1002	CDL	CA5-C11-C12-C13
4	A	1002	CDL	C35-C36-C37-C38
4	A	1002	CDL	C81-C82-C83-C84
4	B	1001	CDL	C17-C18-C19-C20
4	B	1002	CDL	C71-C72-C73-C74
4	E	1001	CDL	C19-C20-C21-C22
5	E	1003	PEV	C36-C37-C38-C39
4	B	1001	CDL	C32-C33-C34-C35
4	B	1002	CDL	C20-C21-C22-C23
4	E	1001	CDL	C82-C83-C84-C85
4	E	1002	CDL	C39-C40-C41-C42
5	A	1003	PEV	C16-C17-C18-C19
4	B	1001	CDL	C74-C75-C76-C77
4	B	1002	CDL	C38-C39-C40-C41
4	E	1001	CDL	C73-C74-C75-C76
4	E	1002	CDL	C20-C21-C22-C23
4	B	1001	CDL	CA5-C11-C12-C13
4	A	1001	CDL	C23-C24-C25-C26
4	B	1001	CDL	C71-C72-C73-C74
4	E	1001	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
5	G	201	PEV	C17-C18-C19-C20
4	A	1002	CDL	C61-C62-C63-C64
5	A	1004	PEV	C43-C44-C45-C46
5	A	1004	PEV	C12-C13-C14-C15
5	C	201	PEV	C12-C13-C14-C15
4	A	1001	CDL	C78-C79-C80-C81
4	A	1002	CDL	C18-C19-C20-C21
4	E	1001	CDL	C56-C57-C58-C59
4	E	1001	CDL	C76-C77-C78-C79
4	A	1002	CDL	C19-C20-C21-C22
4	B	1002	CDL	C83-C84-C85-C86
4	E	1001	CDL	C23-C24-C25-C26
5	G	201	PEV	C35-C36-C37-C38
4	E	1002	CDL	CA3-CA4-CA6-OA8
4	A	1001	CDL	C71-C72-C73-C74
4	A	1002	CDL	C11-C12-C13-C14
4	B	1001	CDL	C22-C23-C24-C25
4	E	1002	CDL	C32-C33-C34-C35
5	B	1003	PEV	C12-C13-C14-C15
4	A	1002	CDL	CA4-CA6-OA8-CA7
4	B	1002	CDL	C72-C73-C74-C75
4	A	1001	CDL	C58-C59-C60-C61
4	B	1001	CDL	C34-C35-C36-C37
4	A	1001	CDL	C63-C64-C65-C66
4	A	1002	CDL	C22-C23-C24-C25
5	A	1003	PEV	C14-C15-C16-C17
4	A	1002	CDL	C13-C14-C15-C16
4	B	1001	CDL	C15-C16-C17-C18
4	E	1002	CDL	C77-C78-C79-C80
4	E	1001	CDL	C31-C32-C33-C34
4	E	1002	CDL	C52-C53-C54-C55
4	E	1002	CDL	C83-C84-C85-C86
4	E	1001	CDL	C58-C59-C60-C61
4	A	1002	CDL	C14-C15-C16-C17
5	A	1004	PEV	C14-C15-C16-C17
5	G	201	PEV	C18-C19-C20-C21
4	E	1002	CDL	C37-C38-C39-C40
4	E	1002	CDL	C40-C41-C42-C43
4	E	1001	CDL	CB5-C51-C52-C53
5	E	1003	PEV	C31-C32-C33-C34
5	A	1003	PEV	C20-C21-C22-C23
5	B	1003	PEV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	E	1003	PEV	C43-C44-C45-C46
4	E	1001	CDL	C35-C36-C37-C38
4	B	1002	CDL	C80-C81-C82-C83
5	G	201	PEV	C34-C35-C36-C37
4	A	1002	CDL	OA5-CA3-CA4-OA6
4	A	1001	CDL	C72-C73-C74-C75
4	A	1001	CDL	CA7-C31-C32-C33
4	A	1001	CDL	OB6-CB4-CB6-OB8
4	B	1002	CDL	C34-C35-C36-C37
5	B	1003	PEV	C18-C19-C20-C21
5	G	201	PEV	C33-C34-C35-C36
4	A	1001	CDL	C15-C16-C17-C18
4	B	1002	CDL	C13-C14-C15-C16
4	E	1001	CDL	C21-C22-C23-C24
4	E	1002	CDL	C58-C59-C60-C61
5	B	1003	PEV	C17-C18-C19-C20
5	C	201	PEV	C34-C35-C36-C37
4	B	1002	CDL	C16-C17-C18-C19
5	A	1003	PEV	C19-C20-C21-C22
4	A	1001	CDL	C14-C15-C16-C17
4	A	1002	CDL	C17-C18-C19-C20
4	B	1001	CDL	C75-C76-C77-C78
5	B	1003	PEV	C14-C15-C16-C17
4	B	1002	CDL	CB2-OB2-PB2-OB5
4	E	1001	CDL	CA3-OA5-PA1-OA2
5	A	1004	PEV	C1-O3P-P-O4P
5	A	1004	PEV	C4-O4P-P-O3P
4	E	1002	CDL	C51-C52-C53-C54
4	E	1002	CDL	C60-C61-C62-C63
5	E	1003	PEV	C2-C1-O3P-P
4	B	1001	CDL	OB5-CB3-CB4-CB6
4	E	1001	CDL	OA5-CA3-CA4-CA6
4	E	1001	CDL	C12-C13-C14-C15
4	B	1002	CDL	C54-C55-C56-C57
4	A	1001	CDL	C54-C55-C56-C57
4	B	1001	CDL	C82-C83-C84-C85
4	A	1002	CDL	C20-C21-C22-C23
4	A	1002	CDL	CA3-CA4-CA6-OA8
4	B	1001	CDL	C18-C19-C20-C21
4	B	1002	CDL	CB3-CB4-CB6-OB8
5	C	201	PEV	C1-C2-C3-O3
5	G	201	PEV	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	E	1002	CDL	C23-C24-C25-C26
4	A	1001	CDL	C64-C65-C66-C67
4	B	1002	CDL	C63-C64-C65-C66
5	A	1004	PEV	C21-C22-C23-C24
4	E	1001	CDL	C24-C25-C26-C27
4	E	1002	CDL	C84-C85-C86-C87
5	A	1003	PEV	C43-C44-C45-C46
6	D	101	PN7	O3-C3-C4-O4
6	I	101	PN7	O3-C3-C4-O4
4	A	1001	CDL	C31-C32-C33-C34
4	E	1001	CDL	C74-C75-C76-C77
4	E	1002	CDL	C12-C13-C14-C15
5	A	1004	PEV	C45-C46-C47-C48
4	E	1001	CDL	C43-C44-C45-C46
4	E	1002	CDL	C11-C12-C13-C14
4	B	1001	CDL	C33-C34-C35-C36
4	E	1002	CDL	C55-C56-C57-C58
4	B	1001	CDL	CA7-C31-C32-C33
5	G	201	PEV	C19-C20-C21-C22
4	A	1001	CDL	O1-C1-CA2-OA2
4	B	1002	CDL	C58-C59-C60-C61
4	E	1001	CDL	C34-C35-C36-C37
4	E	1001	CDL	C84-C85-C86-C87
4	B	1001	CDL	OA6-CA4-CA6-OA8
5	A	1003	PEV	O2-C2-C3-O3
4	B	1002	CDL	C18-C19-C20-C21
4	A	1002	CDL	C62-C63-C64-C65
4	B	1002	CDL	C64-C65-C66-C67
4	B	1001	CDL	C72-C73-C74-C75
4	B	1002	CDL	C52-C53-C54-C55
5	A	1003	PEV	C17-C18-C19-C20
4	A	1002	CDL	C72-C71-CB7-OB8
4	A	1001	CDL	OA5-CA3-CA4-CA6
4	A	1002	CDL	OA5-CA3-CA4-CA6
4	E	1001	CDL	OB5-CB3-CB4-CB6
5	B	1003	PEV	C21-C22-C23-C24
5	C	201	PEV	C20-C21-C22-C23
5	B	1003	PEV	C22-C23-C24-C25
5	A	1004	PEV	C22-C23-C24-C25
4	B	1001	CDL	C13-C14-C15-C16
5	A	1003	PEV	C41-C42-C43-C44
4	A	1002	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
4	A	1001	CDL	C81-C82-C83-C84
4	A	1001	CDL	CA3-CA4-CA6-OA8
4	A	1001	CDL	CB3-CB4-CB6-OB8
4	B	1001	CDL	C57-C58-C59-C60
4	E	1002	CDL	CA3-OA5-PA1-OA2
4	E	1002	CDL	CB3-OB5-PB2-OB2
5	C	201	PEV	C41-C42-C43-C44
4	A	1001	CDL	C77-C78-C79-C80
4	B	1002	CDL	C11-C12-C13-C14
4	B	1002	CDL	OA5-CA3-CA4-OA6
4	E	1001	CDL	OA5-CA3-CA4-OA6
5	A	1004	PEV	C42-C43-C44-C45
4	A	1001	CDL	C34-C35-C36-C37
4	A	1001	CDL	C60-C61-C62-C63
5	C	201	PEV	O2-C2-C3-O3
5	G	201	PEV	O2-C2-C3-O3
4	E	1002	CDL	CB2-C1-CA2-OA2
4	B	1002	CDL	C56-C57-C58-C59
5	A	1003	PEV	C40-C41-C42-C43
4	B	1001	CDL	CA4-CA3-OA5-PA1
5	B	1003	PEV	C38-C39-C40-C41
5	A	1004	PEV	C36-C37-C38-C39
4	B	1002	CDL	C60-C61-C62-C63
5	B	1003	PEV	C33-C34-C35-C36
4	A	1002	CDL	OB5-CB3-CB4-CB6
5	A	1003	PEV	O3P-C1-C2-C3
4	B	1001	CDL	C19-C20-C21-C22
5	E	1003	PEV	C40-C41-C42-C43
4	A	1002	CDL	C58-C59-C60-C61
5	E	1003	PEV	C44-C45-C46-C47
4	E	1001	CDL	C44-C45-C46-C47
4	A	1001	CDL	C79-C80-C81-C82
5	A	1004	PEV	C39-C40-C41-C42
5	E	1003	PEV	C19-C20-C21-C22
5	A	1003	PEV	C18-C19-C20-C21
4	B	1002	CDL	C40-C41-C42-C43
4	B	1001	CDL	C31-C32-C33-C34
4	B	1002	CDL	CB2-C1-CA2-OA2
4	A	1002	CDL	OA6-CA4-CA6-OA8
4	B	1002	CDL	OB6-CB4-CB6-OB8
5	E	1003	PEV	C33-C34-C35-C36
5	G	201	PEV	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
4	B	1001	CDL	C52-C53-C54-C55
5	B	1003	PEV	C39-C40-C41-C42
5	E	1003	PEV	C37-C38-C39-C40
5	C	201	PEV	C37-C38-C39-C40
4	A	1001	CDL	C38-C39-C40-C41
4	B	1001	CDL	C60-C61-C62-C63
4	B	1002	CDL	C76-C77-C78-C79
5	C	201	PEV	C36-C37-C38-C39
4	A	1001	CDL	CA2-OA2-PA1-OA4
4	A	1002	CDL	CB3-OB5-PB2-OB4
4	B	1002	CDL	CB3-OB5-PB2-OB4
4	E	1001	CDL	CA3-OA5-PA1-OA4
4	E	1002	CDL	CB2-OB2-PB2-OB4
5	A	1003	PEV	C4-O4P-P-O2P
5	A	1004	PEV	C1-O3P-P-O2P
5	B	1003	PEV	C1-O3P-P-O1P
5	E	1003	PEV	C1-O3P-P-O1P
5	E	1003	PEV	C1-O3P-P-O2P
5	E	1003	PEV	C4-O4P-P-O2P
5	G	201	PEV	C1-O3P-P-O2P
4	B	1002	CDL	OA5-CA3-CA4-CA6
5	A	1004	PEV	O3P-C1-C2-C3
4	E	1001	CDL	C72-C73-C74-C75
4	E	1002	CDL	C61-C62-C63-C64
5	C	201	PEV	C18-C19-C20-C21
4	A	1001	CDL	OA5-CA3-CA4-OA6
4	A	1002	CDL	OB5-CB3-CB4-OB6
4	B	1001	CDL	OB5-CB3-CB4-OB6
4	E	1001	CDL	OB5-CB3-CB4-OB6
5	A	1003	PEV	O3P-C1-C2-O2
5	A	1004	PEV	O3P-C1-C2-O2
5	G	201	PEV	C16-C17-C18-C19
4	E	1002	CDL	O1-C1-CA2-OA2
4	A	1001	CDL	OA6-CA4-CA6-OA8
4	E	1002	CDL	OA6-CA4-CA6-OA8
4	B	1002	CDL	C36-C37-C38-C39
5	E	1003	PEV	C21-C22-C23-C24
5	A	1003	PEV	C15-C16-C17-C18
4	B	1001	CDL	C61-C62-C63-C64
4	E	1001	CDL	C42-C43-C44-C45
4	E	1002	CDL	C34-C35-C36-C37
4	E	1002	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
4	E	1002	CDL	C56-C57-C58-C59
4	A	1001	CDL	C1-CA2-OA2-PA1
4	B	1001	CDL	C1-CB2-OB2-PB2
4	B	1002	CDL	CA4-CA3-OA5-PA1
5	C	201	PEV	C19-C20-C21-C22
4	A	1002	CDL	C24-C25-C26-C27
4	A	1001	CDL	CB2-OB2-PB2-OB5
4	B	1001	CDL	CA2-OA2-PA1-OA5
4	B	1001	CDL	CB2-OB2-PB2-OB5
4	E	1001	CDL	CA2-OA2-PA1-OA5
4	E	1001	CDL	C13-C14-C15-C16
4	B	1001	CDL	CA3-CA4-CA6-OA8
4	B	1001	CDL	CB3-CB4-CB6-OB8
5	A	1003	PEV	C1-C2-C3-O3
5	G	201	PEV	C37-C38-C39-C40
5	A	1003	PEV	C2-C1-O3P-P
4	B	1002	CDL	C53-C54-C55-C56
4	A	1001	CDL	C12-C13-C14-C15
4	A	1001	CDL	C43-C44-C45-C46
5	G	201	PEV	C20-C21-C22-C23
4	A	1001	CDL	C1-CB2-OB2-PB2
4	E	1002	CDL	CB4-CB3-OB5-PB2
5	A	1003	PEV	C13-C14-C15-C16
4	E	1002	CDL	C24-C25-C26-C27
4	B	1001	CDL	C54-C55-C56-C57
5	A	1004	PEV	C20-C21-C22-C23
4	A	1001	CDL	CB2-C1-CA2-OA2
6	H	101	PN7	O3P-C1-C2-CE2
5	B	1003	PEV	C3-C2-O2-C31
5	G	201	PEV	C3-C2-O2-C31
5	A	1004	PEV	C33-C34-C35-C36
5	E	1003	PEV	O3P-C1-C2-C3
4	B	1001	CDL	OB6-CB4-CB6-OB8
4	B	1001	CDL	C59-C60-C61-C62
4	B	1001	CDL	C36-C37-C38-C39
4	A	1001	CDL	C32-C31-CA7-OA8
4	B	1001	CDL	C78-C79-C80-C81
4	B	1002	CDL	OB5-CB3-CB4-CB6
4	E	1002	CDL	OA5-CA3-CA4-CA6
4	A	1002	CDL	C72-C71-CB7-OB9
5	A	1003	PEV	C37-C38-C39-C40
4	E	1002	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
6	H	101	PN7	O3-C3-C4-N5
5	B	1003	PEV	C41-C42-C43-C44
5	A	1003	PEV	C33-C34-C35-C36
5	G	201	PEV	O2-C31-C32-C33
4	A	1002	CDL	C53-C54-C55-C56
4	A	1002	CDL	C84-C85-C86-C87
4	B	1001	CDL	C40-C41-C42-C43
5	B	1003	PEV	C1-C2-C3-O3
4	A	1002	CDL	C56-C57-C58-C59
5	C	201	PEV	O3P-C1-C2-O2
5	B	1003	PEV	O2-C2-C3-O3
5	B	1003	PEV	C16-C17-C18-C19
5	A	1003	PEV	C35-C36-C37-C38
5	B	1003	PEV	C11-C12-C13-C14
4	B	1001	CDL	C80-C81-C82-C83
4	A	1002	CDL	C1-CB2-OB2-PB2
4	B	1001	CDL	C52-C51-CB5-OB6
4	E	1002	CDL	C17-C18-C19-C20
4	E	1002	CDL	CB3-CB4-CB6-OB8
5	G	201	PEV	O31-C31-C32-C33
4	A	1001	CDL	C37-C38-C39-C40
4	B	1002	CDL	C61-C62-C63-C64
4	B	1001	CDL	C52-C51-CB5-OB7
4	B	1001	CDL	C83-C84-C85-C86
4	B	1001	CDL	CA2-OA2-PA1-OA3
4	B	1001	CDL	CB2-OB2-PB2-OB3
4	E	1001	CDL	C32-C31-CA7-OA8
4	A	1002	CDL	C38-C39-C40-C41
4	E	1001	CDL	C71-C72-C73-C74
6	H	101	PN7	O3P-C1-C2-CE1
4	E	1002	CDL	C33-C34-C35-C36
4	B	1001	CDL	C38-C39-C40-C41
4	A	1002	CDL	C52-C53-C54-C55
5	A	1004	PEV	C40-C41-C42-C43
5	C	201	PEV	C5-C4-O4P-P
4	A	1002	CDL	C83-C84-C85-C86
4	B	1001	CDL	C76-C77-C78-C79
5	B	1003	PEV	O3P-C1-C2-O2
4	B	1002	CDL	C12-C11-CA5-OA6
4	B	1002	CDL	C52-C51-CB5-OB6
5	A	1004	PEV	O2-C31-C32-C33
4	E	1001	CDL	C32-C31-CA7-OA9

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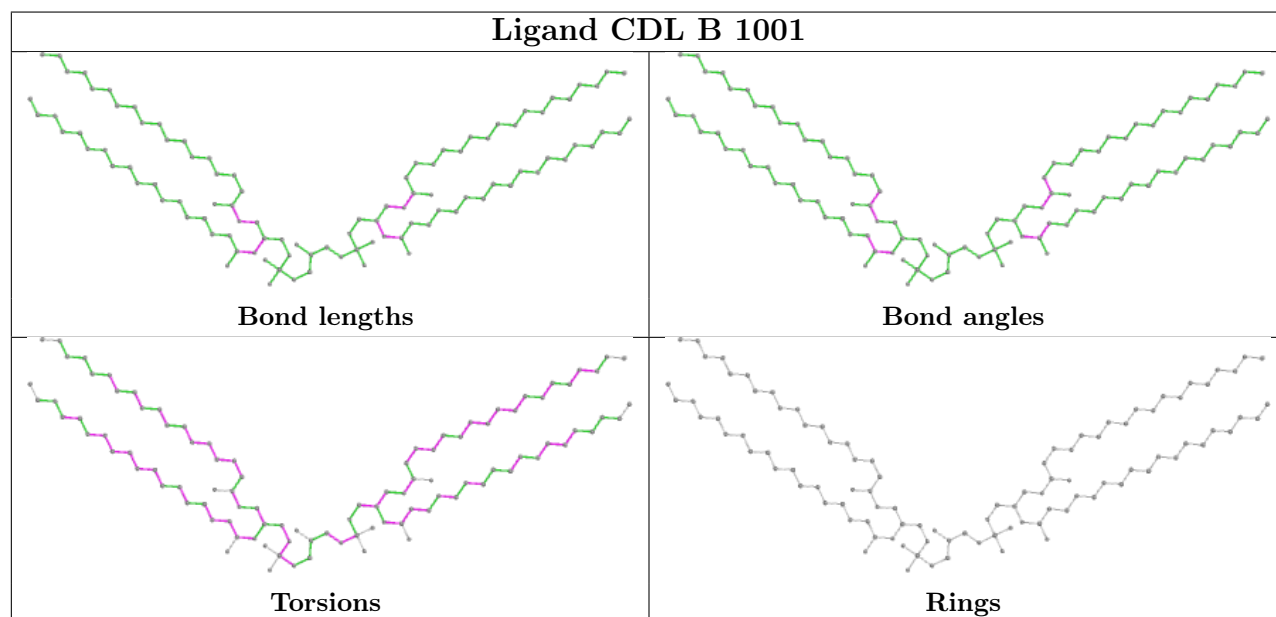
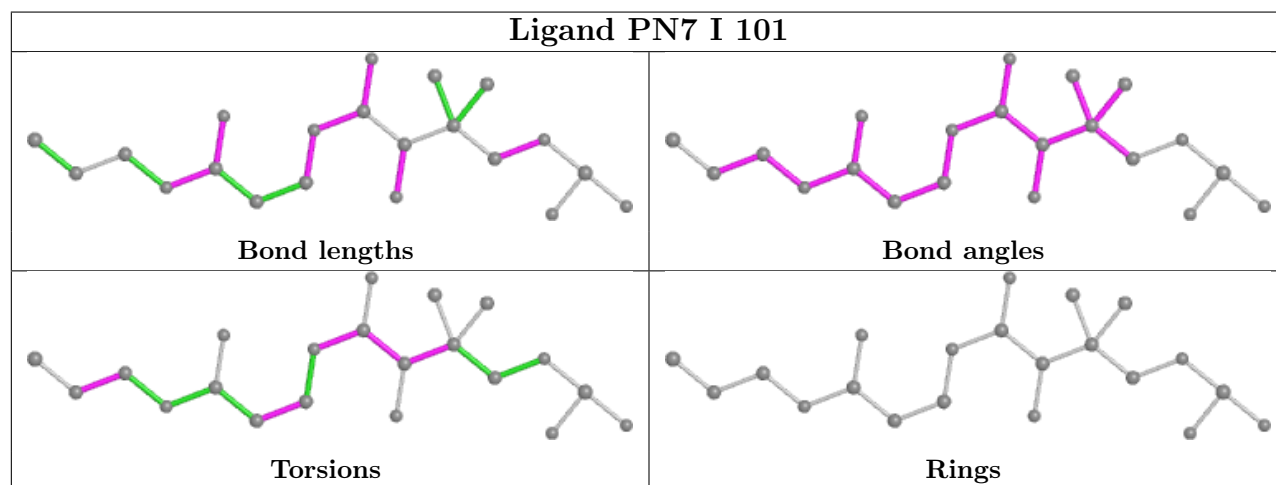
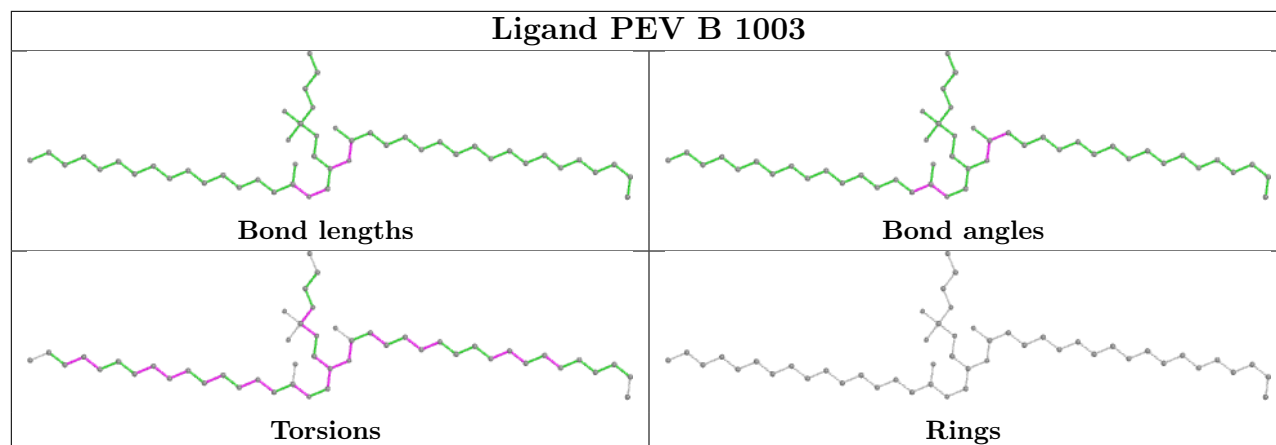
Mol	Chain	Res	Type	Atoms
4	A	1001	CDL	C32-C33-C34-C35
4	A	1001	CDL	C42-C43-C44-C45
5	A	1004	PEV	O31-C31-C32-C33
5	C	201	PEV	C42-C43-C44-C45
4	B	1001	CDL	C12-C11-CA5-OA6

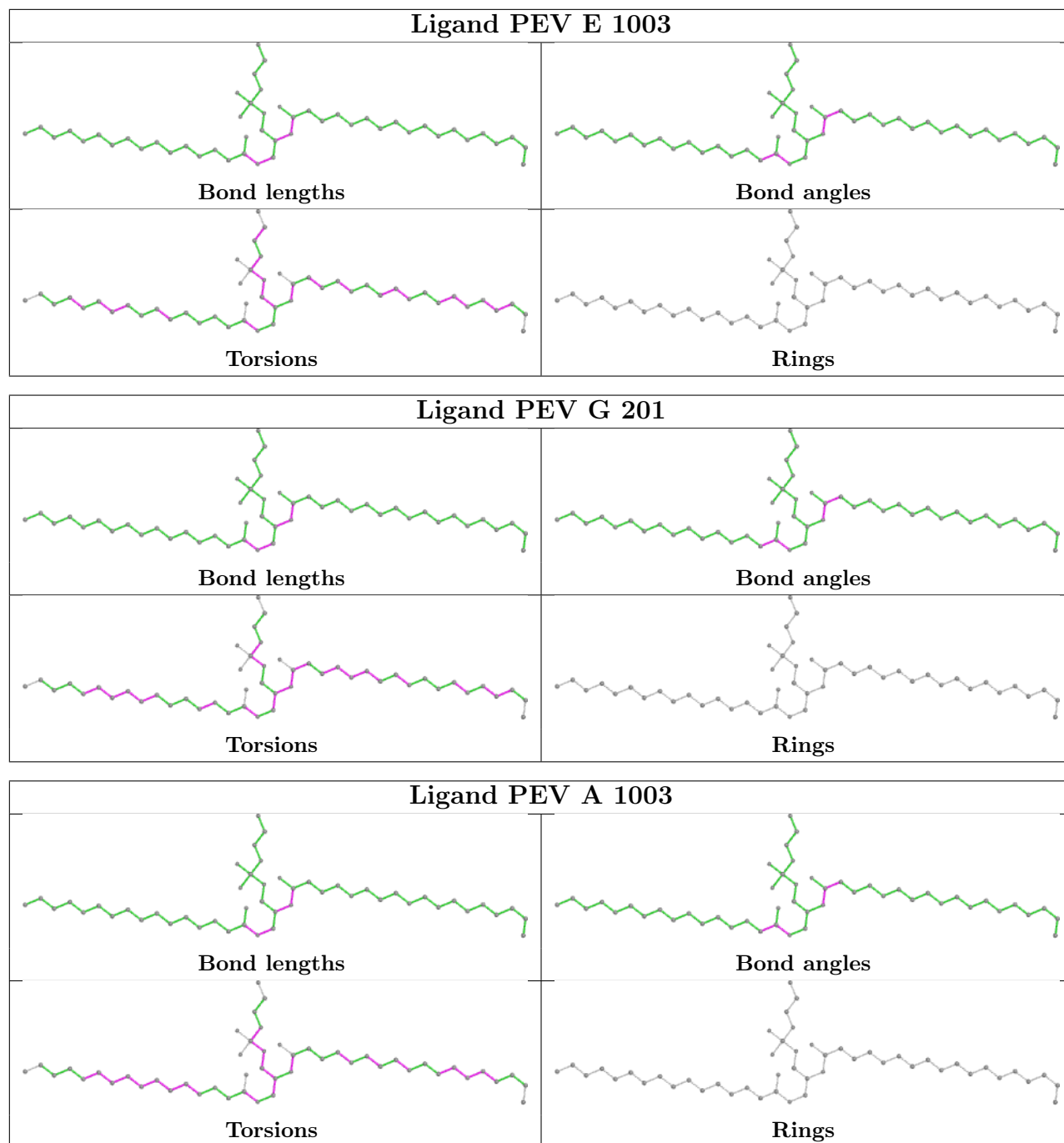
There are no ring outliers.

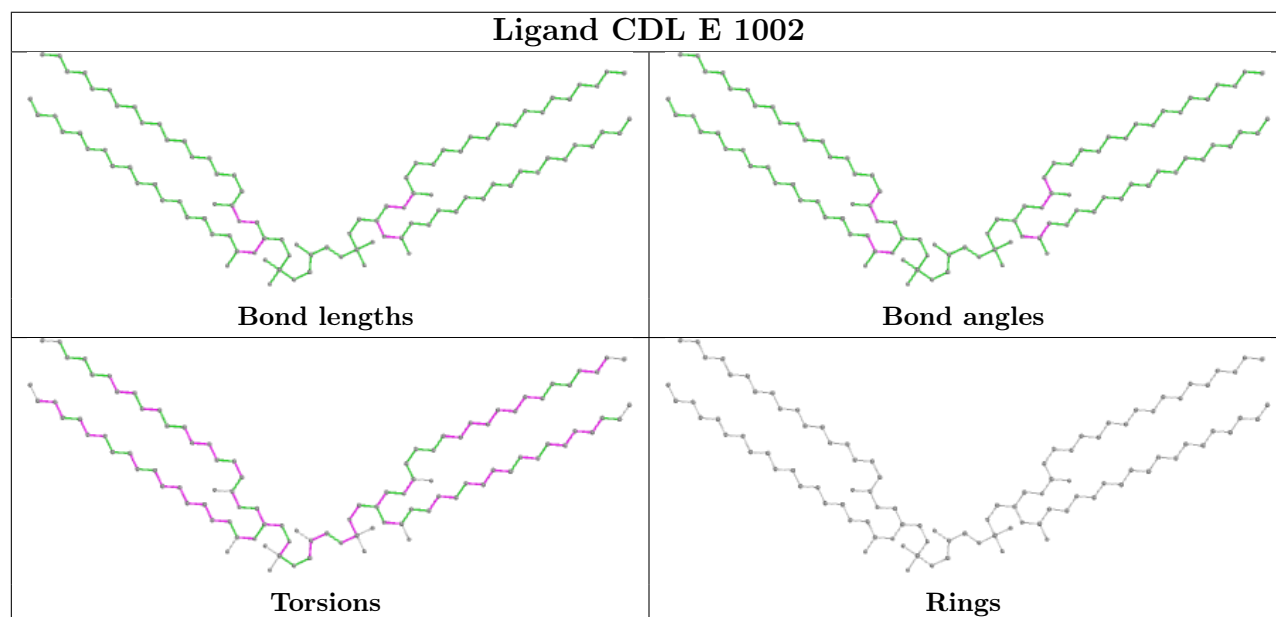
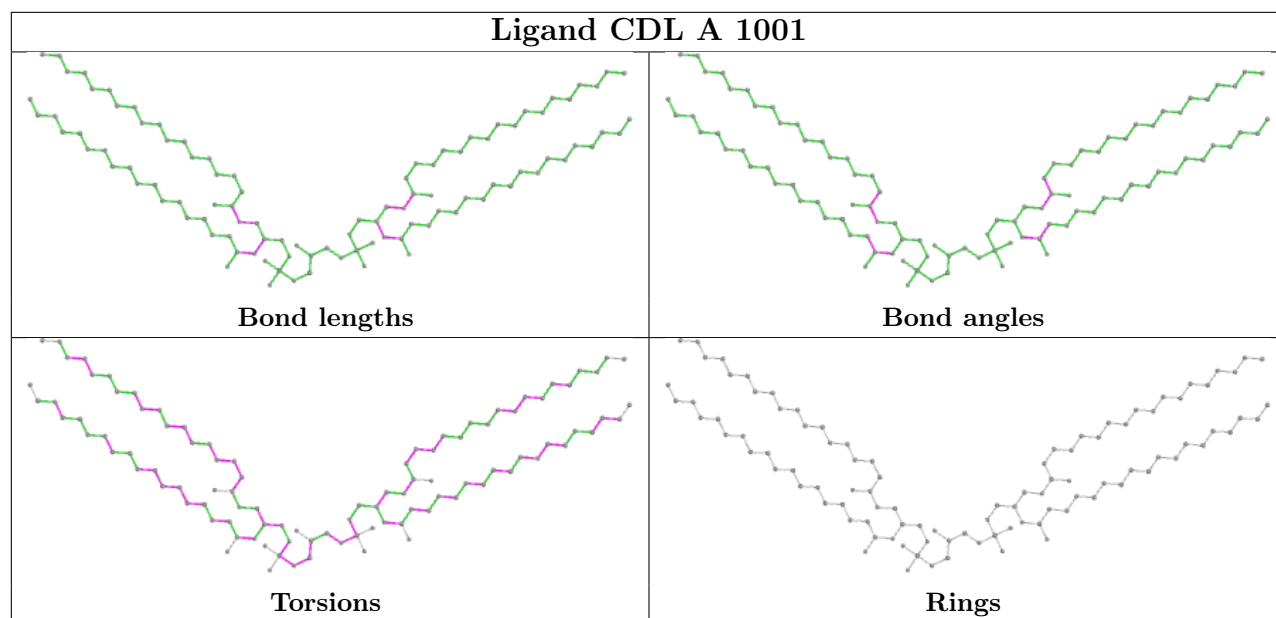
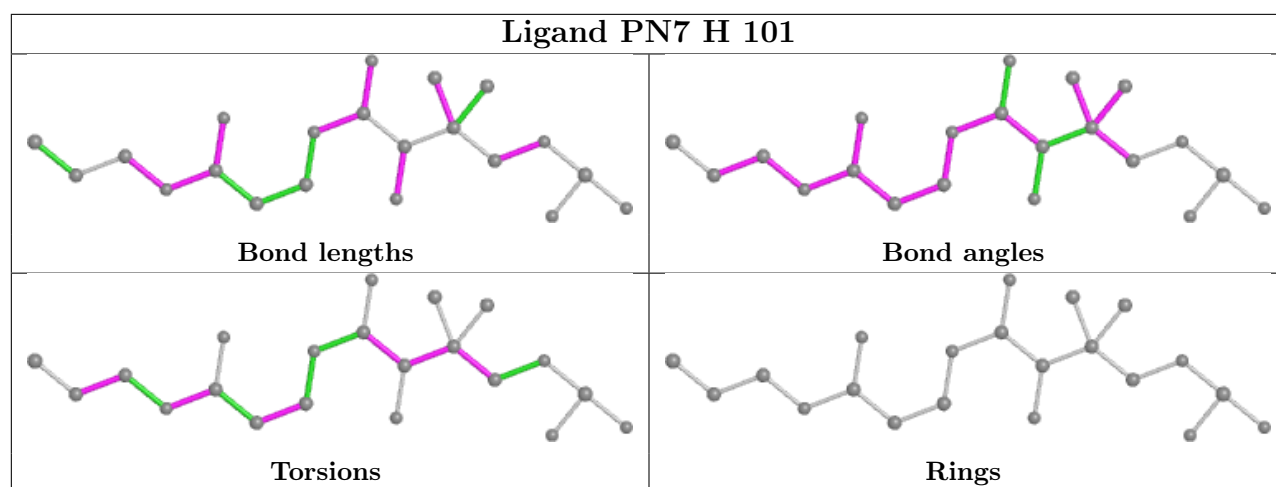
14 monomers are involved in 63 short contacts:

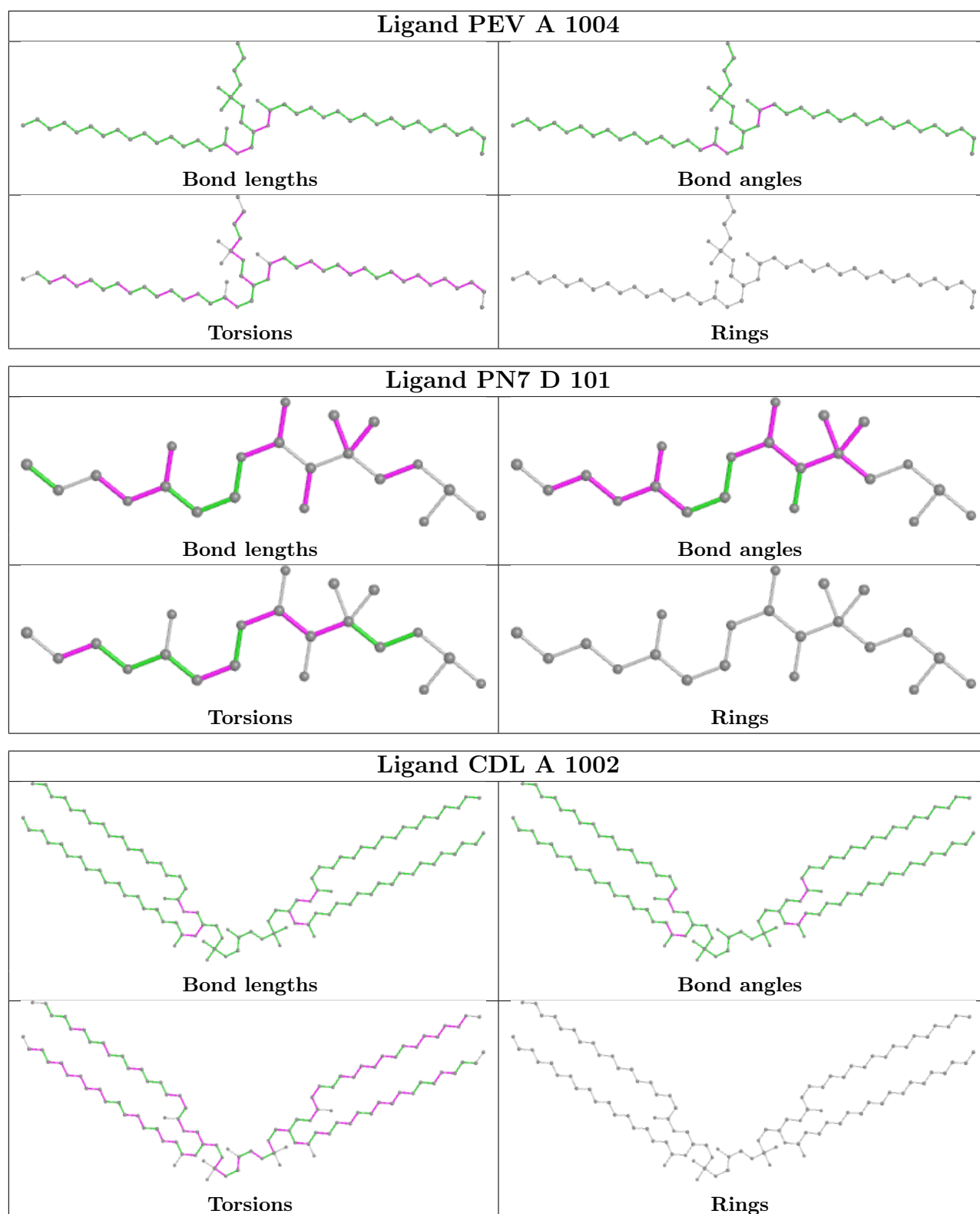
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	101	PN7	2	0
4	B	1001	CDL	5	0
5	E	1003	PEV	3	0
5	G	201	PEV	2	0
5	A	1003	PEV	3	0
6	H	101	PN7	5	0
4	A	1001	CDL	6	0
4	E	1002	CDL	5	0
5	A	1004	PEV	2	0
6	D	101	PN7	2	0
4	A	1002	CDL	8	0
4	E	1001	CDL	10	0
4	B	1002	CDL	12	0
5	C	201	PEV	1	0

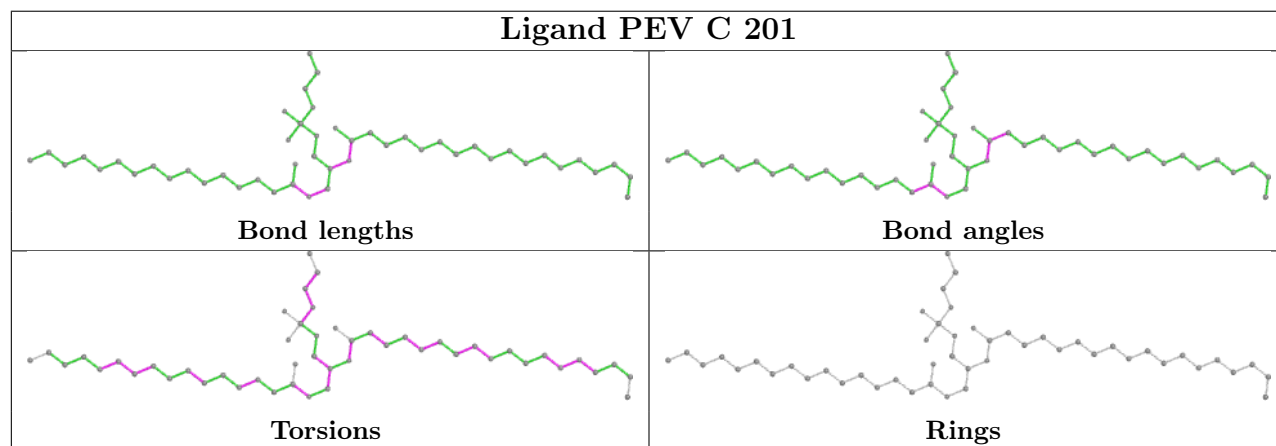
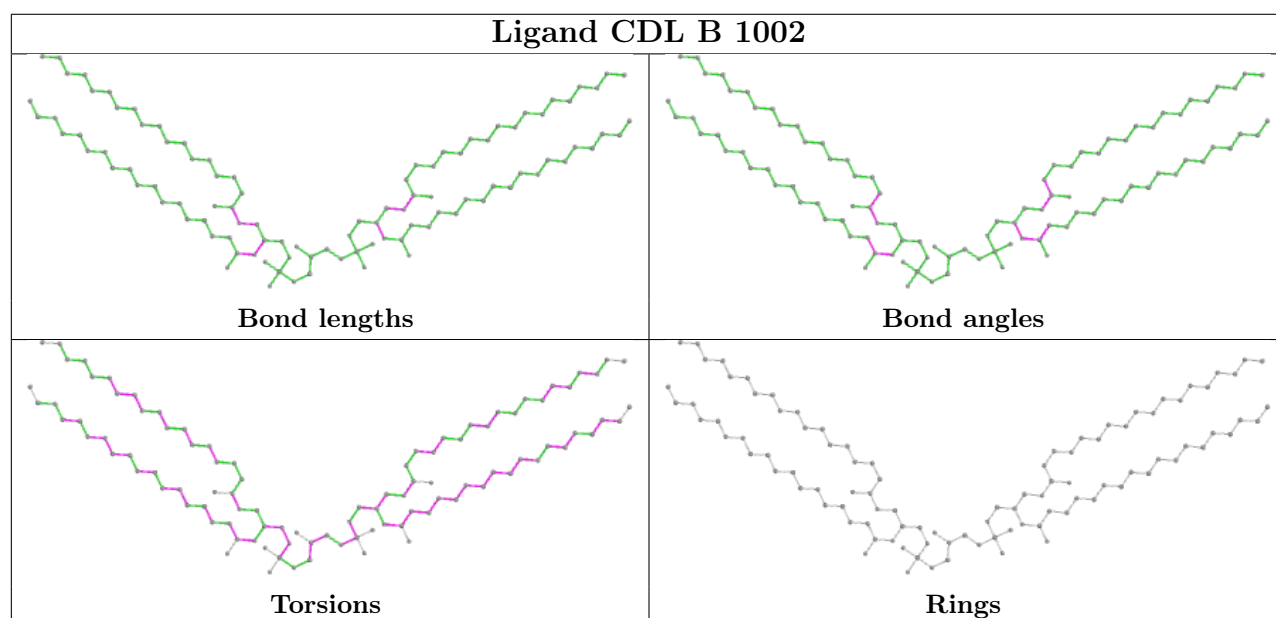
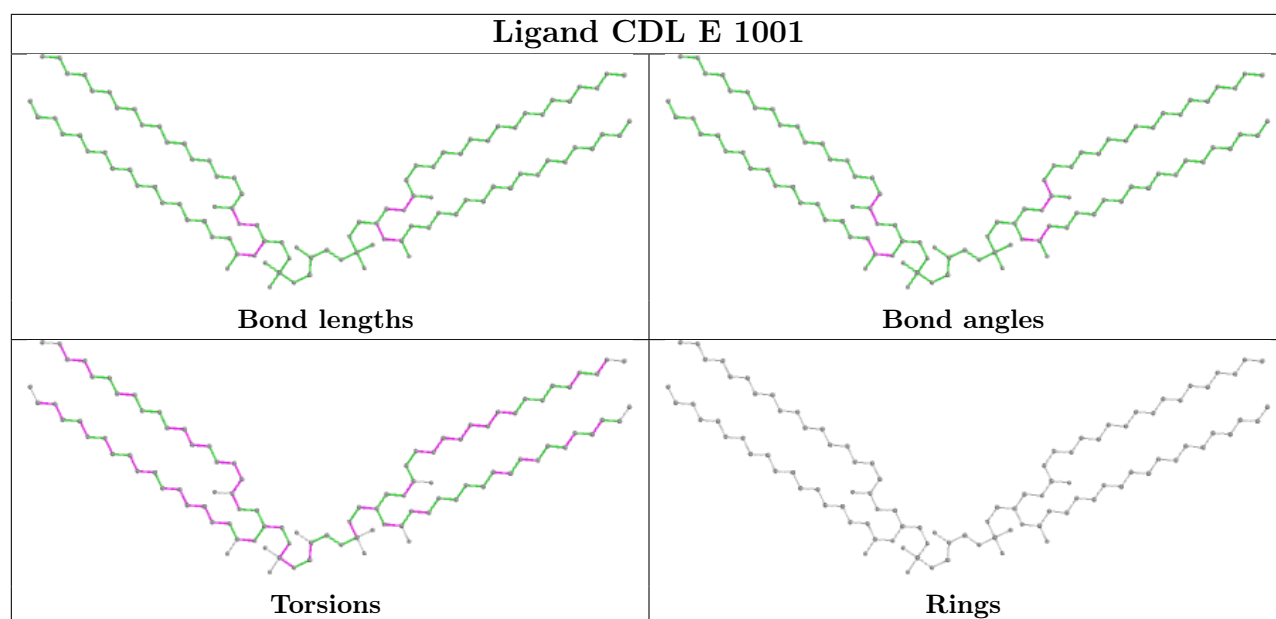
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

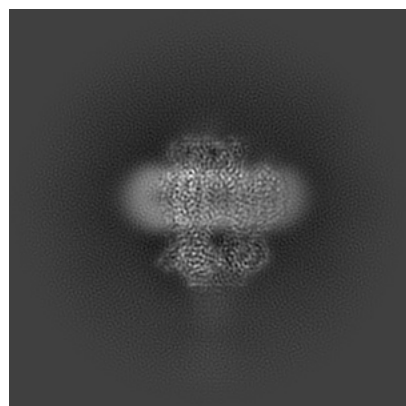
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60202. These allow visual inspection of the internal detail of the map and identification of artifacts.

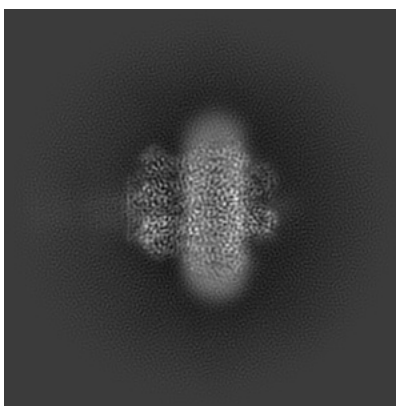
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

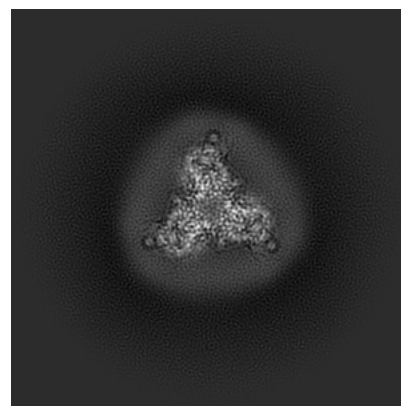
#### 6.1.1 Primary map



X

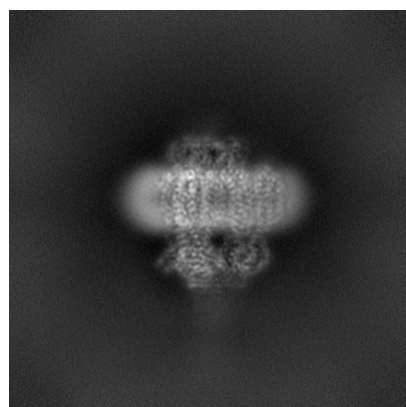


Y

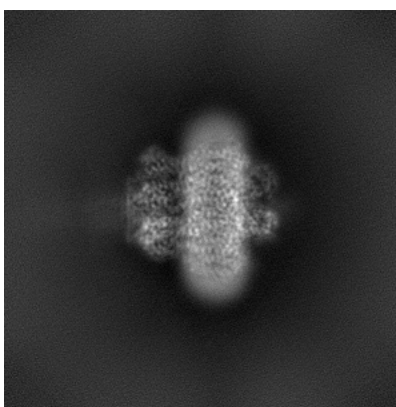


Z

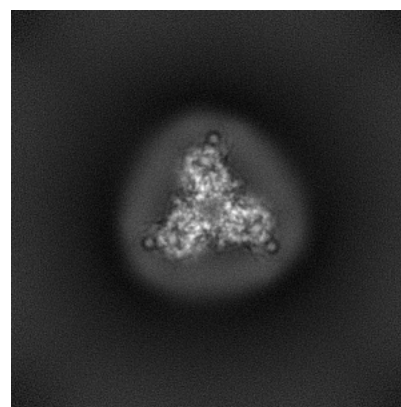
#### 6.1.2 Raw map



X



Y

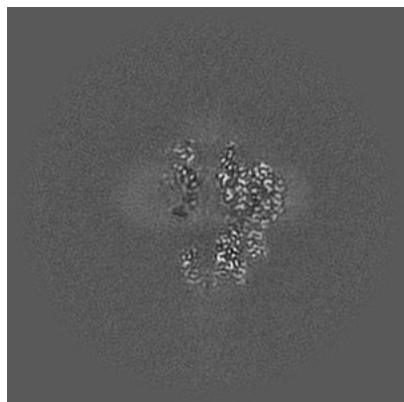


Z

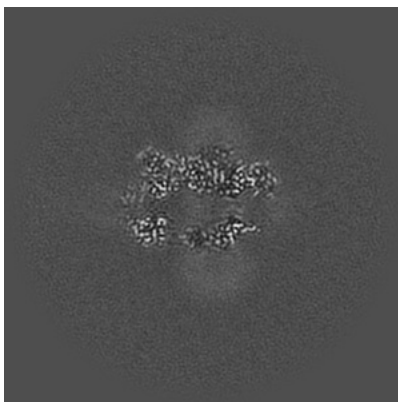
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

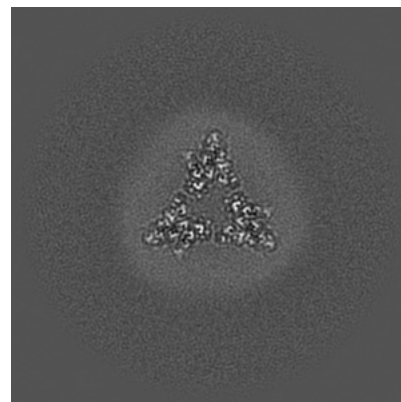
### 6.2.1 Primary map



X Index: 192

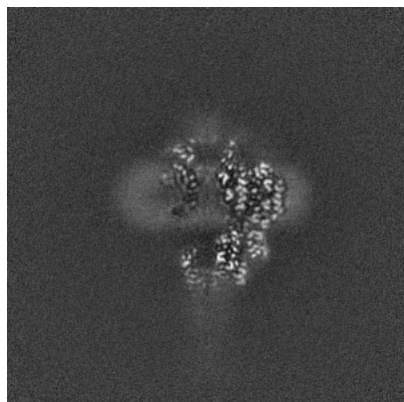


Y Index: 192

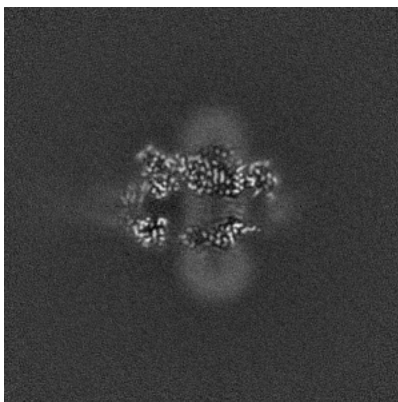


Z Index: 192

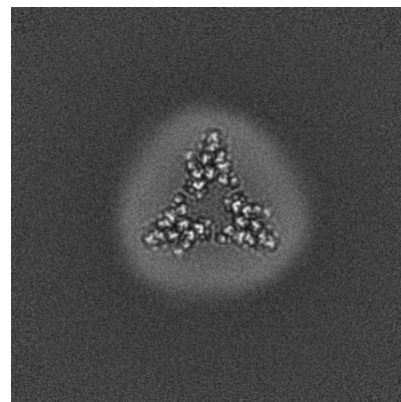
### 6.2.2 Raw map



X Index: 192



Y Index: 192

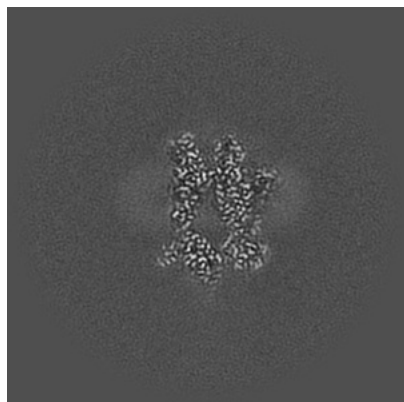


Z Index: 192

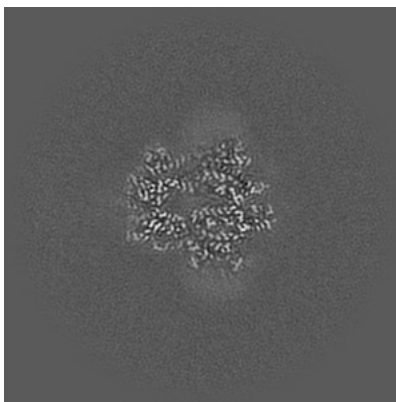
The images above show central slices of the map in three orthogonal directions.

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

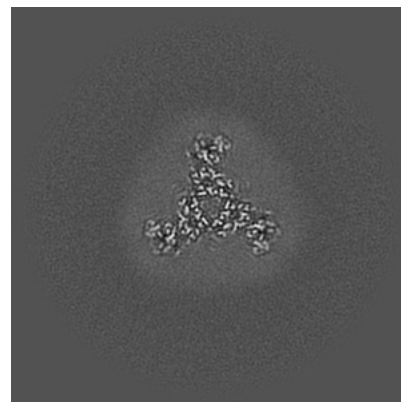
### 6.3.1 Primary map



X Index: 178

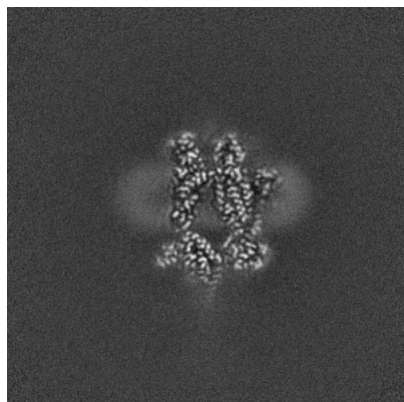


Y Index: 177

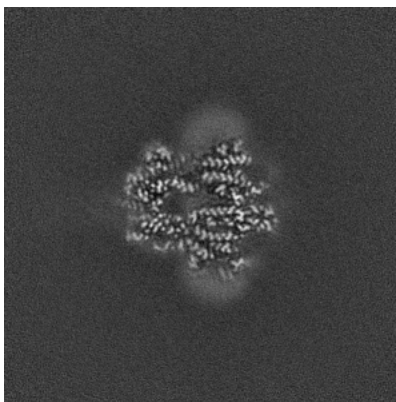


Z Index: 223

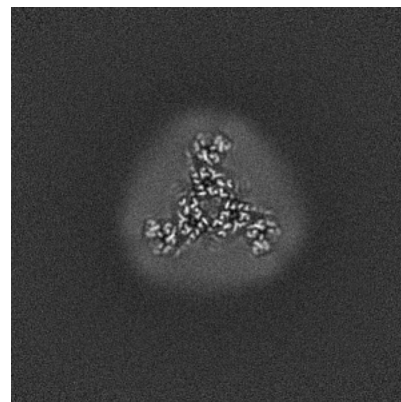
### 6.3.2 Raw map



X Index: 178



Y Index: 176

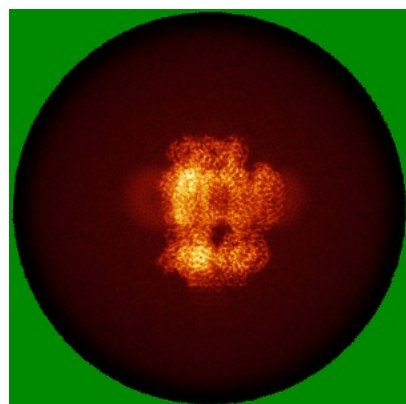


Z Index: 223

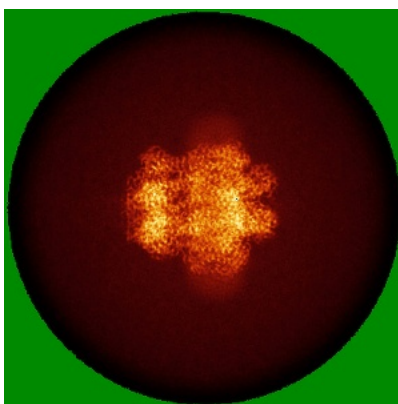
The images above show the largest variance slices of the map in three orthogonal directions.

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

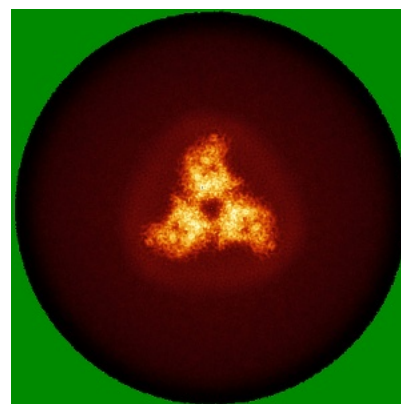
### 6.4.1 Primary map



X

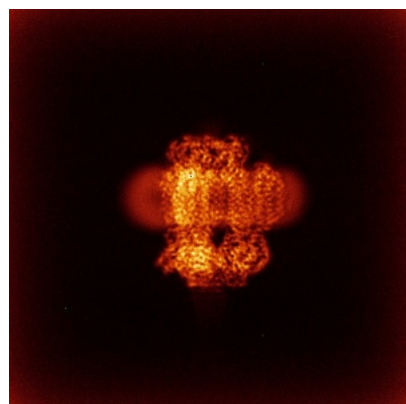


Y

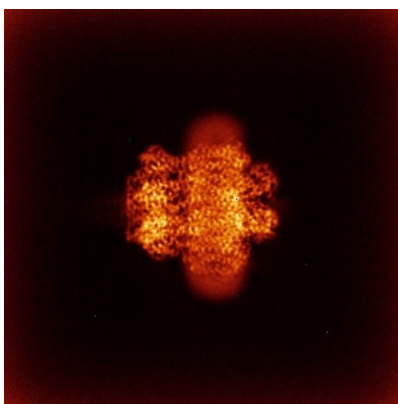


Z

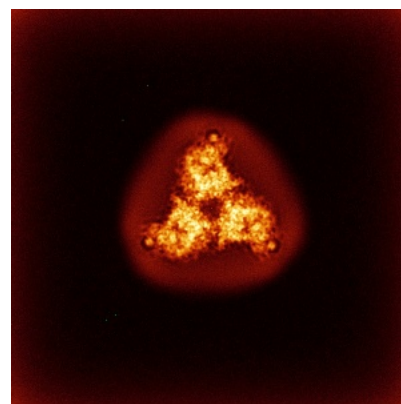
### 6.4.2 Raw map



X



Y



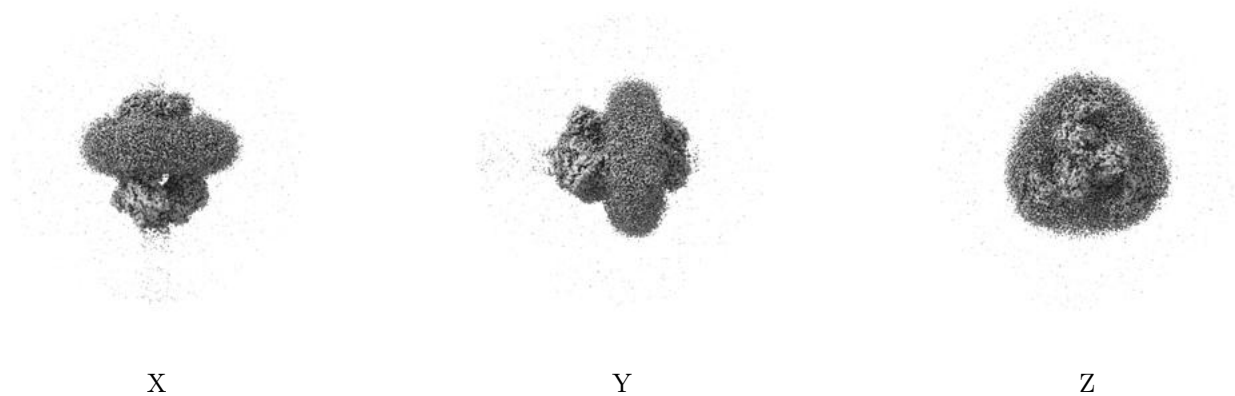
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



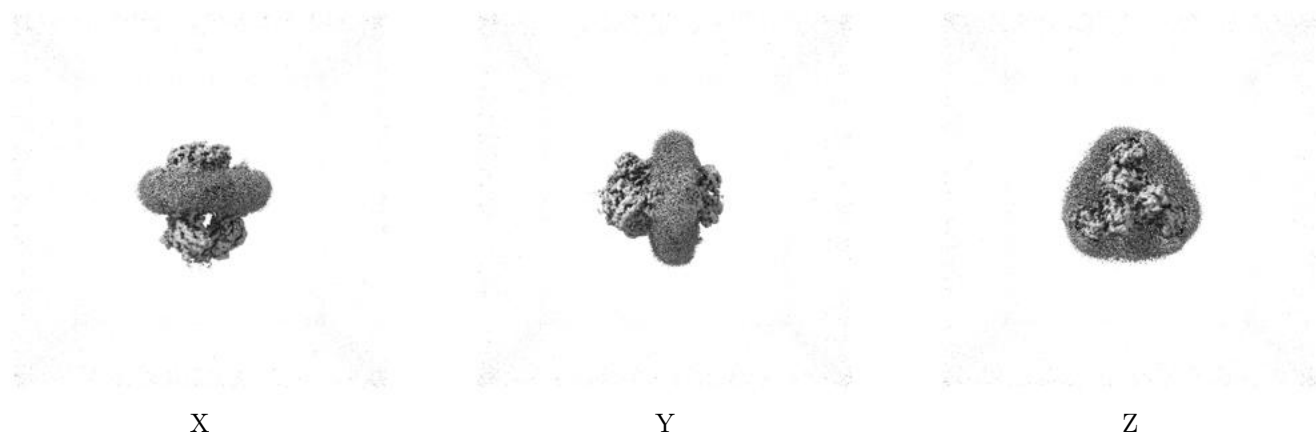
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.252. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 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.

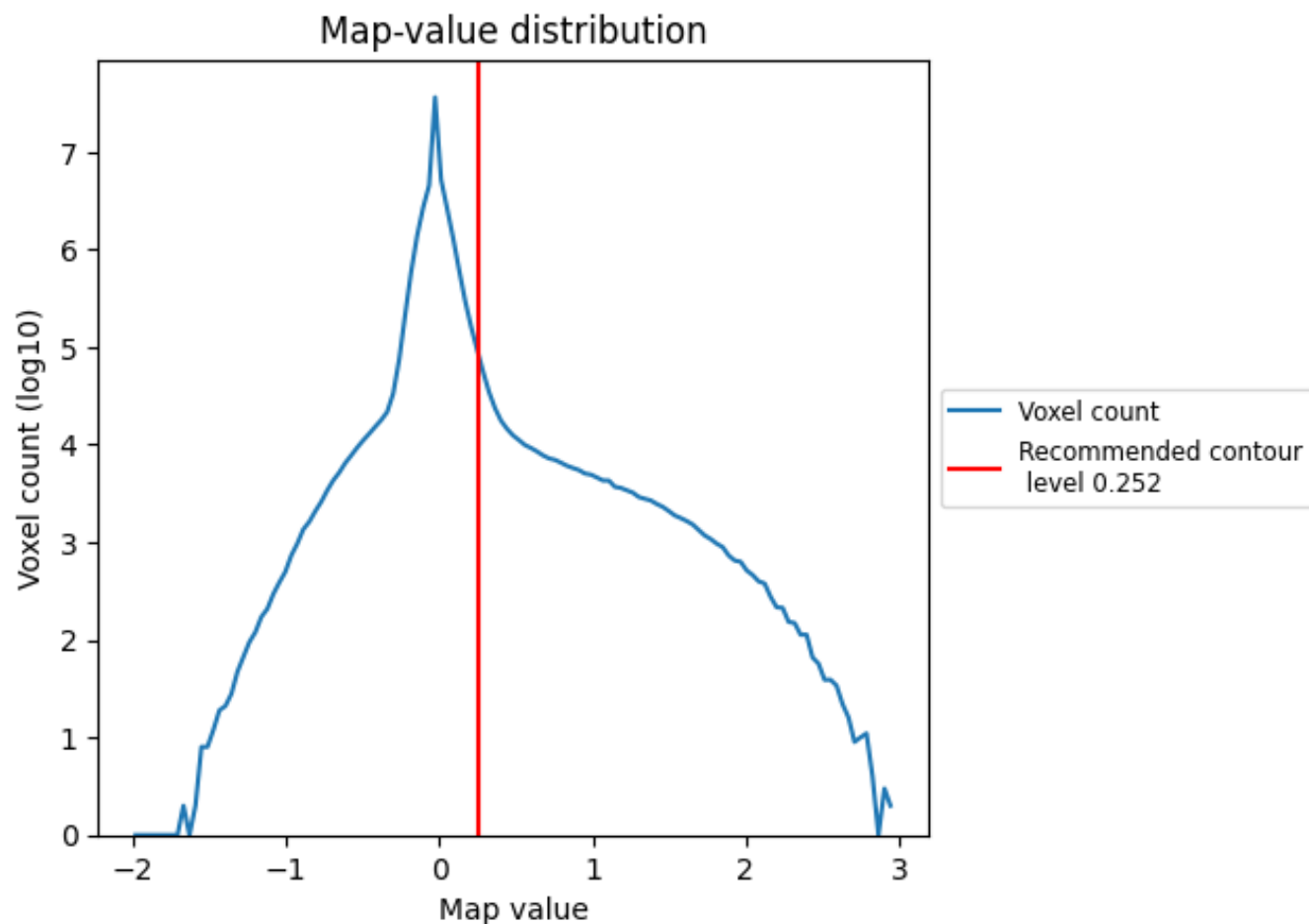
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

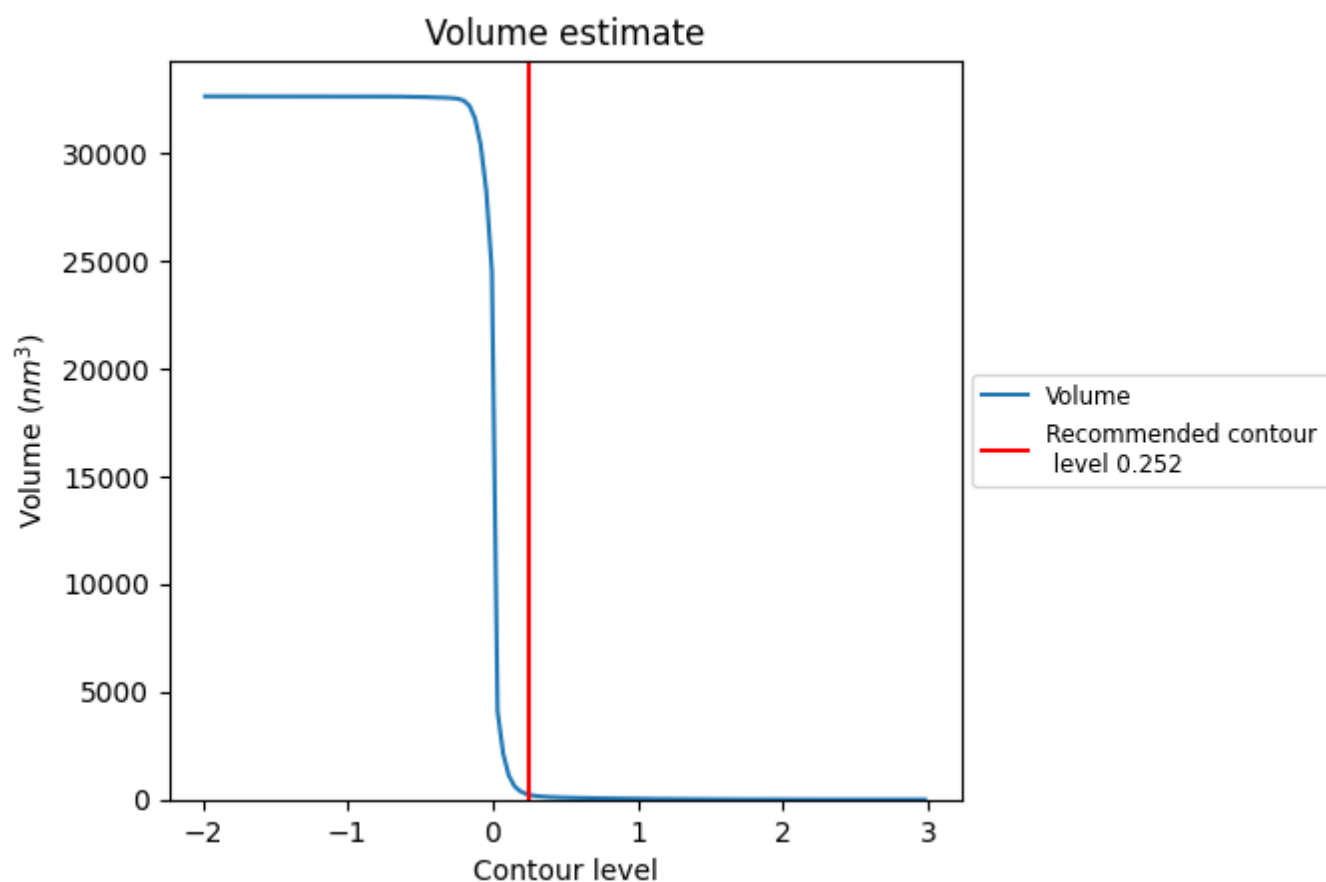
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

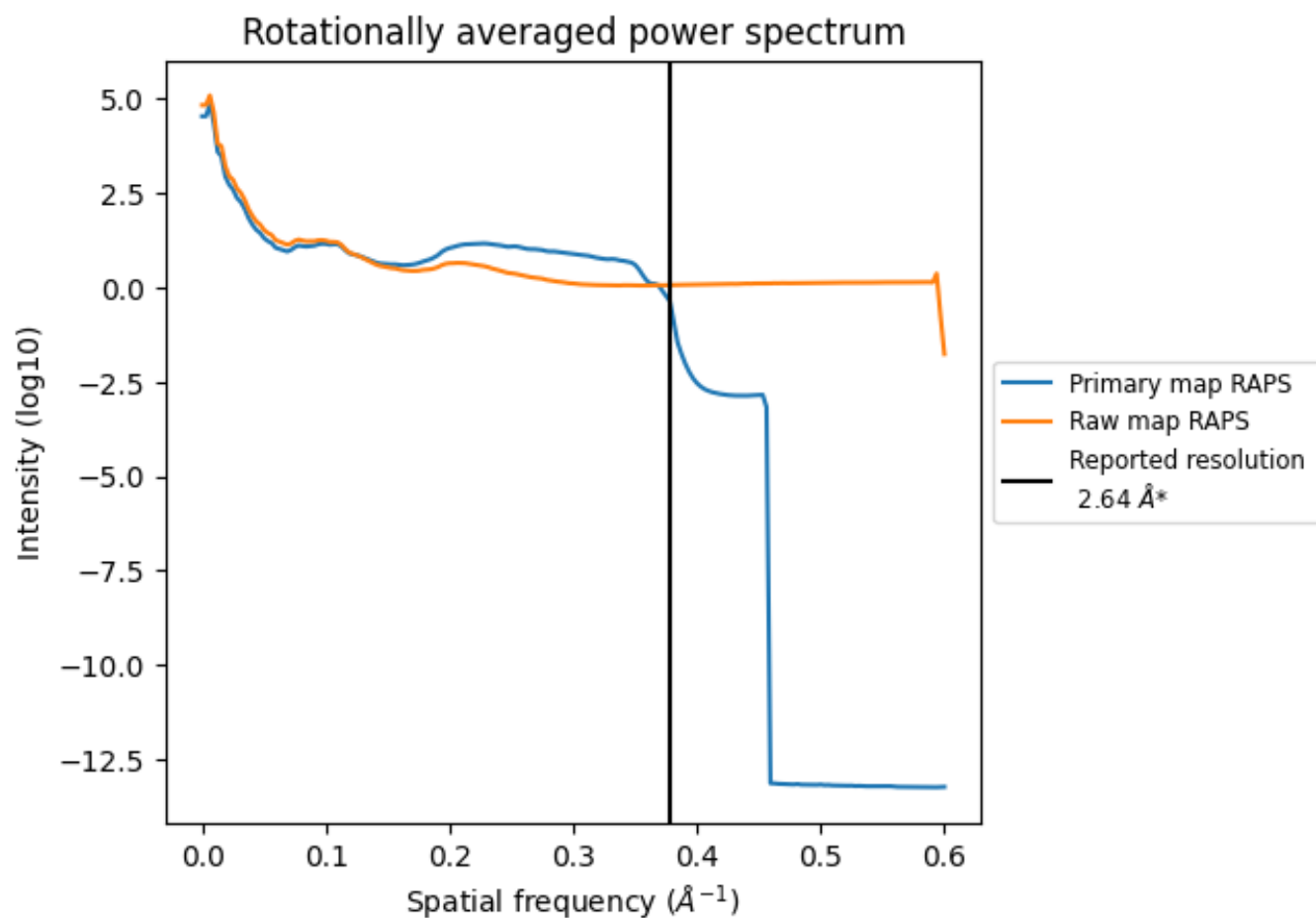


The volume at the recommended contour level is 229 nm<sup>3</sup>; this corresponds to an approximate mass of 207 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

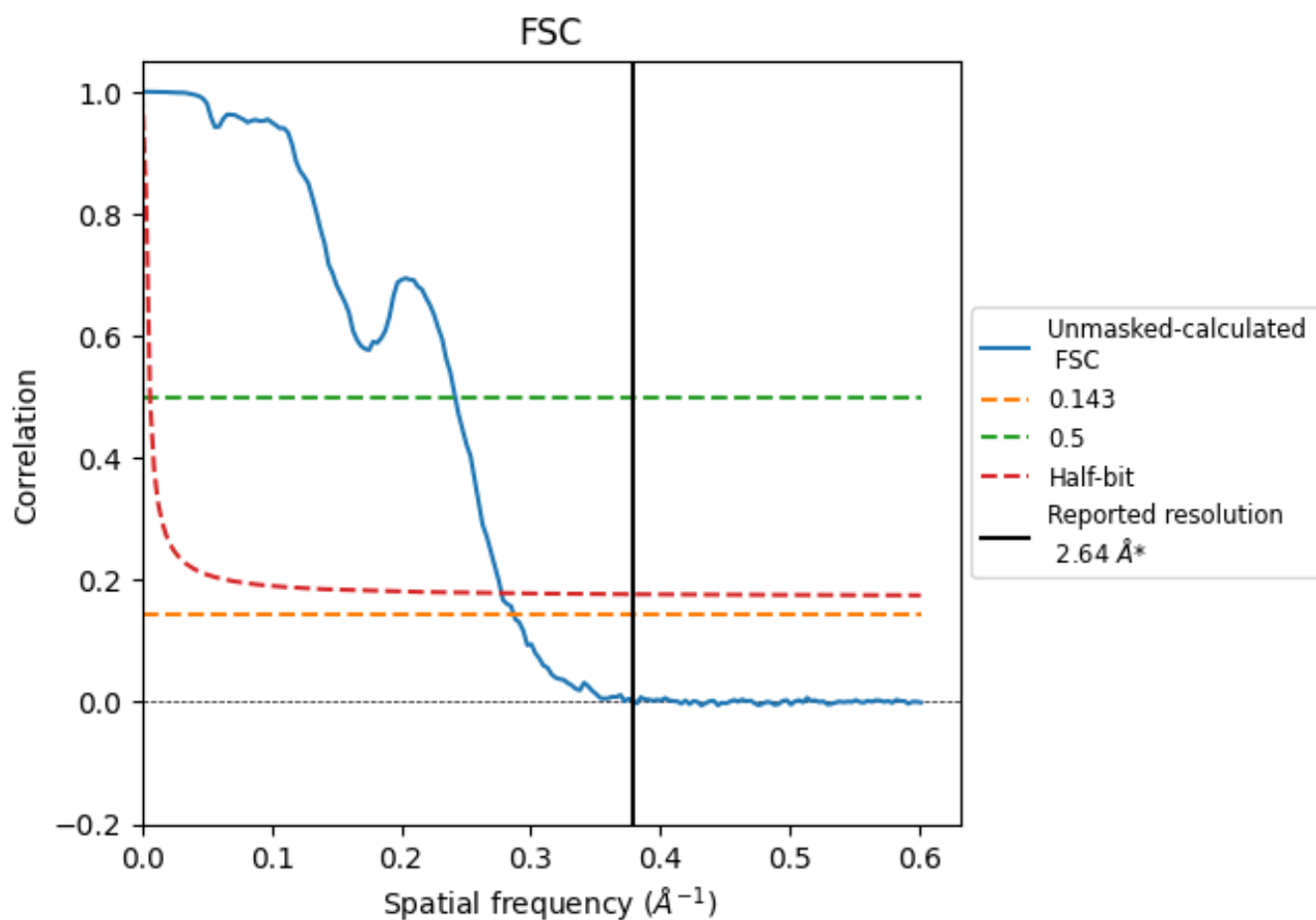


\*Reported resolution corresponds to spatial frequency of 0.379 Å<sup>-1</sup>

## 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 0.379  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

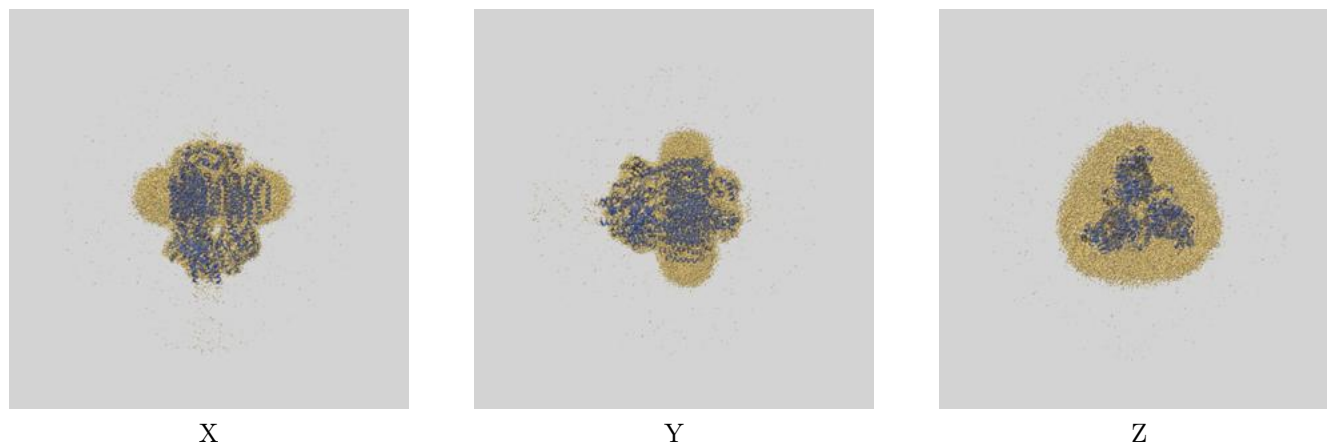
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	4.14	3.60

\*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 3.49 differs from the reported value 2.64 by more than 10 %

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

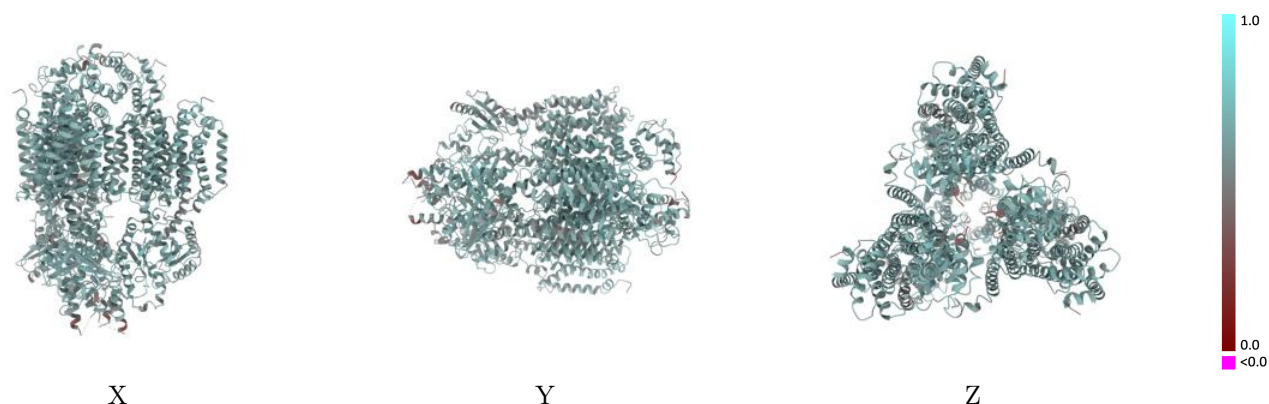
This section contains information regarding the fit between EMDB map EMD-60202 and PDB model 8ZKP. Per-residue inclusion information can be found in section 3 on page 8.

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



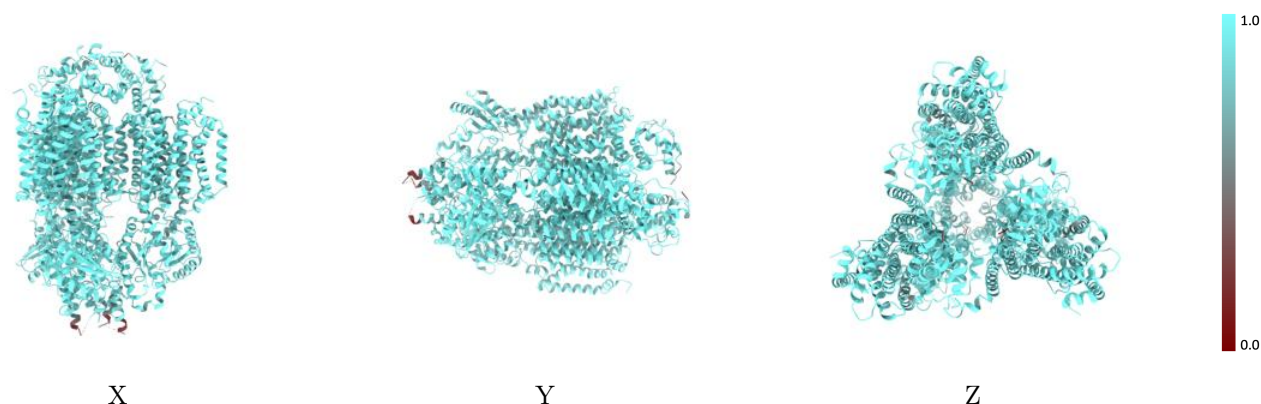
The images above show the 3D surface view of the map at the recommended contour level 0.252 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



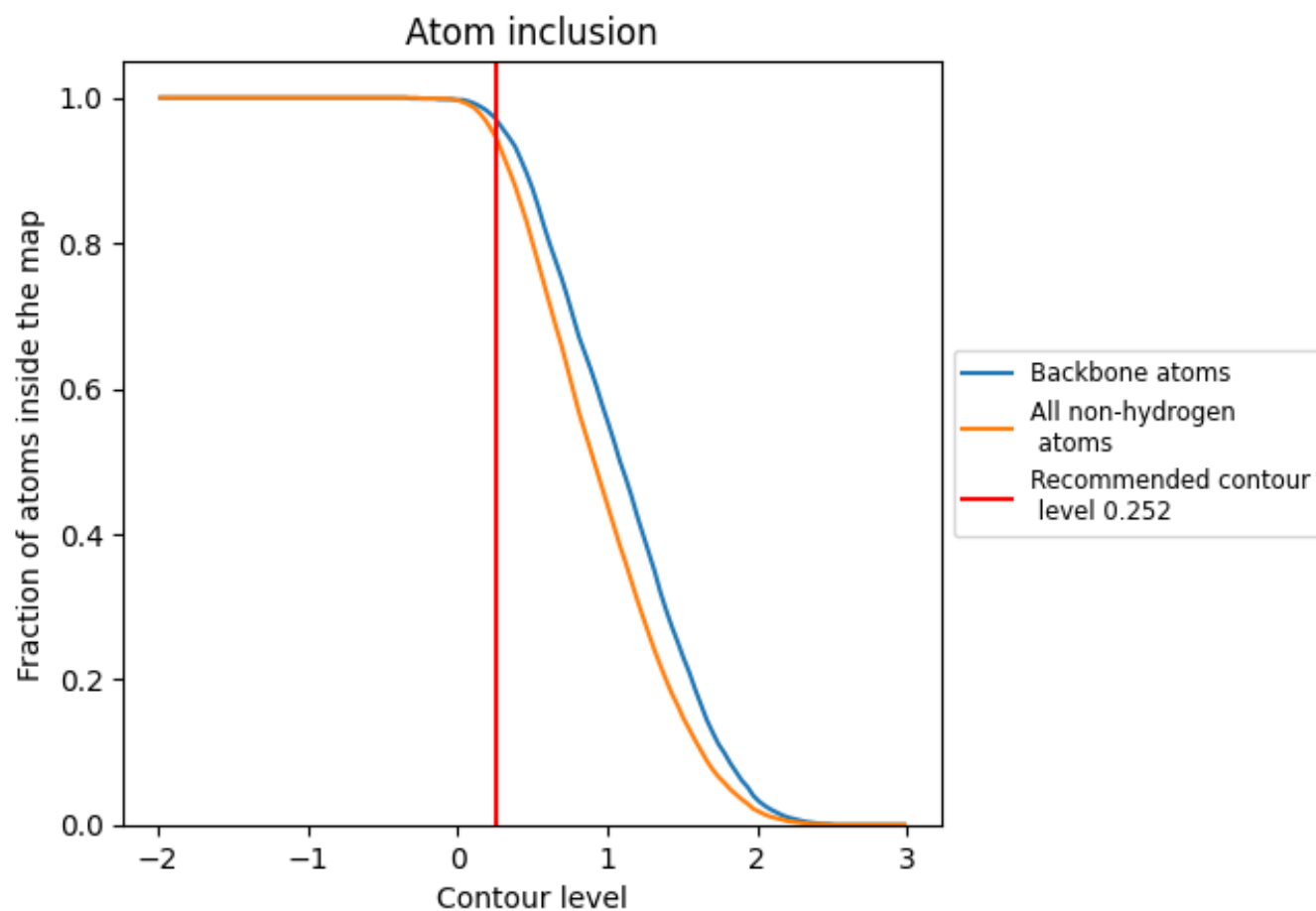
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.252).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.252) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9470	<div><div></div></div> 0.6080
A	<div><div></div></div> 0.9500	<div><div></div></div> 0.6090
B	<div><div></div></div> 0.9510	<div><div></div></div> 0.6100
C	<div><div></div></div> 0.9480	<div><div></div></div> 0.6100
D	<div><div></div></div> 0.9180	<div><div></div></div> 0.5940
E	<div><div></div></div> 0.9480	<div><div></div></div> 0.6090
F	<div><div></div></div> 0.9650	<div><div></div></div> 0.6030
G	<div><div></div></div> 0.9480	<div><div></div></div> 0.6080
H	<div><div></div></div> 0.9260	<div><div></div></div> 0.5940
I	<div><div></div></div> 0.9200	<div><div></div></div> 0.5910

1.0

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