



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:21 PM UTC

PDB ID : 7MIG / pdb_00007mig
EMDB ID : EMD-23850
Title : Human CTPS1 bound to inhibitor T35
Authors : Lynch, E.M.; Dimattia, M.A.; Kollman, J.M.
Deposited on : 2021-04-16
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

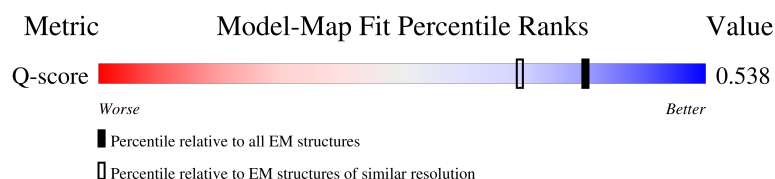
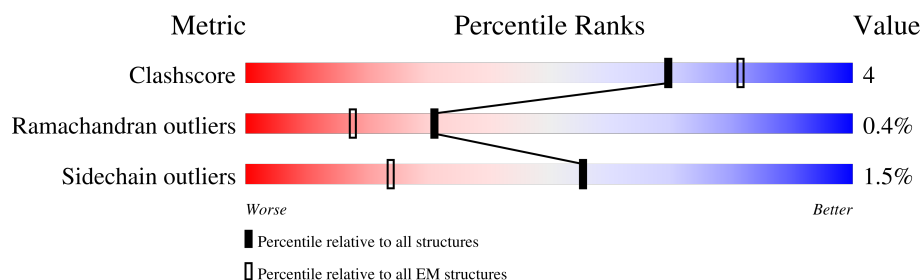
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	591	5% 81% 8% 10%
1	B	591	5% 81% 9% 10%
1	C	591	6% 81% 8% 10%
1	E	591	5% 81% 9% 10%

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
3	GLN	A	604	-	-	X	-
3	GLN	B	602	-	-	X	-
3	GLN	C	602	-	-	X	-
3	GLN	E	604	-	-	X	-

2 Entry composition [i](#)

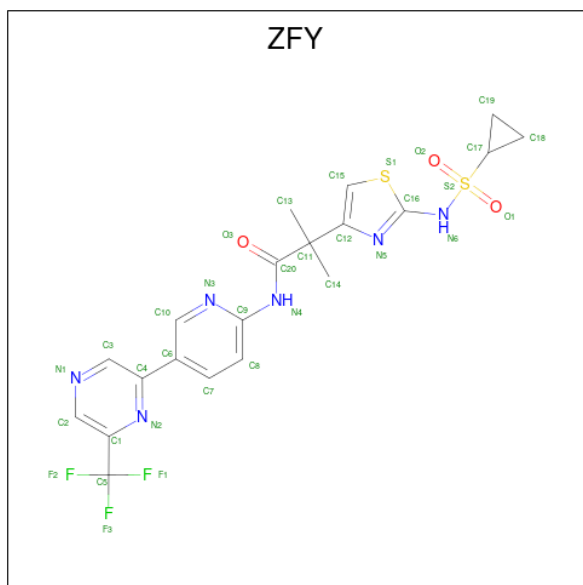
There are 5 unique types of molecules in this entry. The entry contains 34392 atoms, of which 17140 are hydrogens and 0 are deuteriums.

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 CTP synthase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	533	Total	C	H	N	O	S	0	0
			8484	2707	4245	726	784	22		
1	A	533	Total	C	H	N	O	S	0	0
			8484	2707	4245	726	784	22		
1	B	533	Total	C	H	N	O	S	0	0
			8484	2707	4245	726	784	22		
1	E	533	Total	C	H	N	O	S	0	0
			8484	2707	4245	726	784	22		

- Molecule 2 is 2-{2-[(cyclopropanesulfonyl)amino]-1,3-thiazol-4-yl}-2-methyl-N-{5-[6-(trifluoromethyl)pyrazin-2-yl]pyridin-2-yl}propanamide (CCD ID: ZFY) (formula: $C_{20}H_{19}F_3N_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



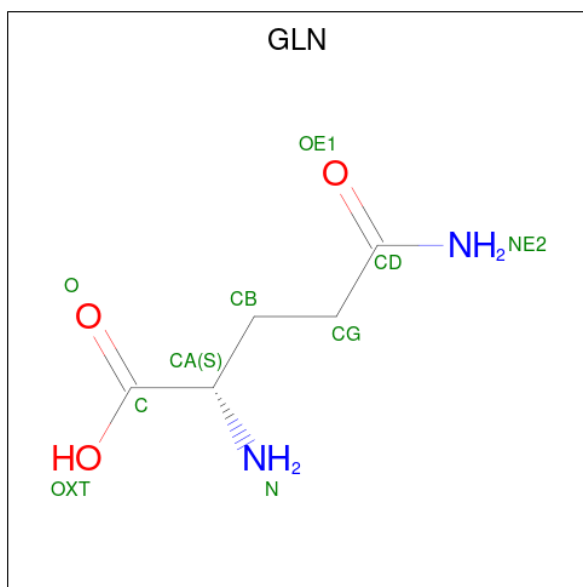
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	F	H	N	O	S
			53	20	3	19	6	3	2
2	A	1	Total	C	F	H	N	O	S
			53	20	3	19	6	3	2

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Mol	Chain	Residues	Atoms							AltConf
2	B	1	Total	C	F	H	N	O	S	0
			53	20	3	19	6	3	2	
2	E	1	Total	C	F	H	N	O	S	0
			53	20	3	19	6	3	2	

- Molecule 3 is GLUTAMINE (CCD ID: GLN) (formula: C₅H₁₀N₂O₃).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	N	O	0
			20	5	10	2	3	
3	A	1	Total	C	H	N	O	0
			20	5	10	2	3	
3	B	1	Total	C	H	N	O	0
			20	5	10	2	3	
3	E	1	Total	C	H	N	O	0
			20	5	10	2	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

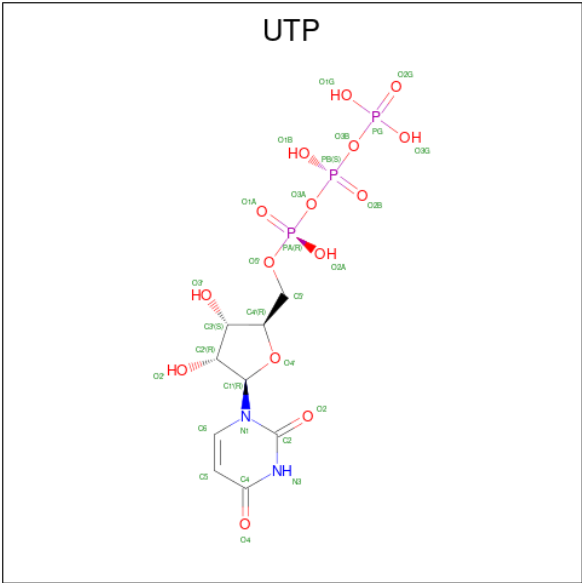
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

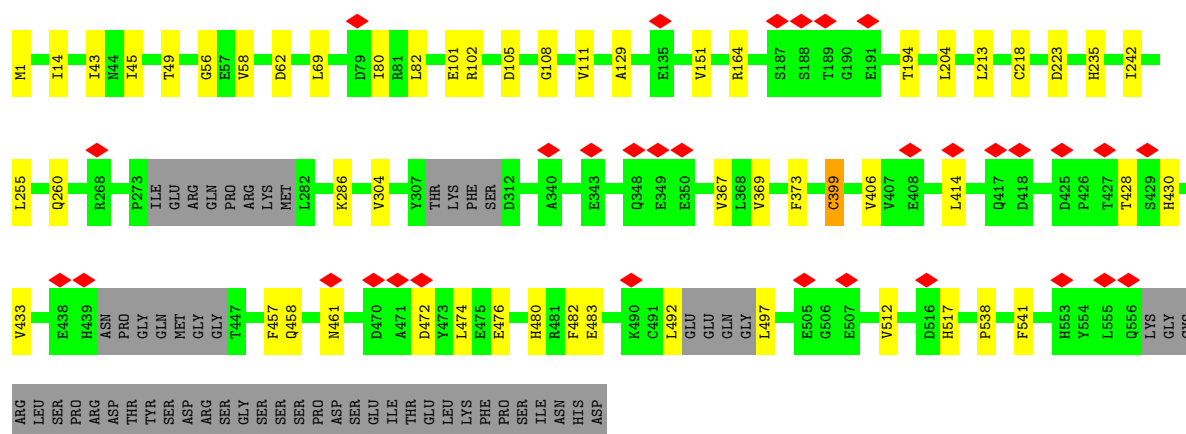
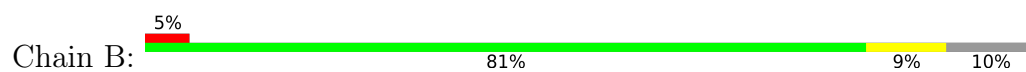
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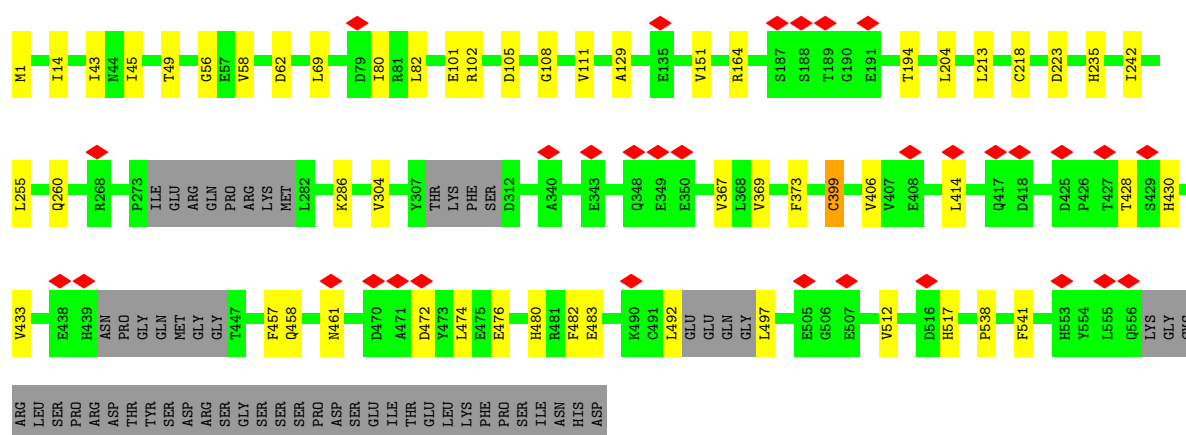
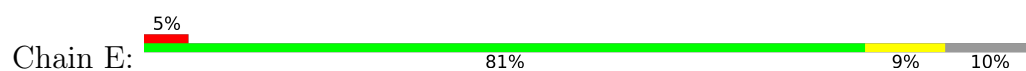
Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Mg	0
			1	1	

- Molecule 5 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).





• Molecule 1: CTP synthase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144655	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	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	12.673	Depositor
Minimum map value	-10.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.263	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: MG, UTP, ZFY

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	0.76	2/4331 (0.0%)	1.47	11/5861 (0.2%)
1	B	0.76	2/4331 (0.0%)	1.47	11/5861 (0.2%)
1	C	0.76	2/4331 (0.0%)	1.47	11/5861 (0.2%)
1	E	0.76	2/4331 (0.0%)	1.47	11/5861 (0.2%)
All	All	0.76	8/17324 (0.0%)	1.47	44/23444 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	GLU	CD-OE2	5.99	1.36	1.25
1	C	476	GLU	CD-OE2	5.98	1.36	1.25
1	E	476	GLU	CD-OE2	5.97	1.36	1.25
1	A	476	GLU	CD-OE2	5.96	1.36	1.25
1	B	483	GLU	CD-OE2	5.38	1.35	1.25
1	C	483	GLU	CD-OE2	5.38	1.35	1.25
1	E	483	GLU	CD-OE2	5.38	1.35	1.25
1	A	483	GLU	CD-OE2	5.37	1.35	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	PRO	N-CA-C	7.59	119.96	110.70
1	E	538	PRO	N-CA-C	7.58	119.94	110.70
1	C	538	PRO	N-CA-C	7.58	119.94	110.70
1	A	538	PRO	N-CA-C	7.54	119.90	110.70
1	A	461	ASN	CA-CB-CG	6.10	118.70	112.60
1	C	461	ASN	CA-CB-CG	6.10	118.70	112.60
1	E	461	ASN	CA-CB-CG	6.08	118.68	112.60
1	B	461	ASN	CA-CB-CG	6.07	118.67	112.60
1	E	105	ASP	CA-CB-CG	5.59	118.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	541	PHE	CA-C-N	5.59	126.19	119.98
1	E	541	PHE	C-N-CA	5.59	126.19	119.98
1	A	541	PHE	CA-C-N	5.58	126.18	119.98
1	A	541	PHE	C-N-CA	5.58	126.18	119.98
1	B	105	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	105	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	541	PHE	CA-C-N	5.55	126.14	119.98
1	C	541	PHE	C-N-CA	5.55	126.14	119.98
1	B	541	PHE	CA-C-N	5.53	126.11	119.98
1	B	541	PHE	C-N-CA	5.53	126.11	119.98
1	A	105	ASP	CA-CB-CG	5.51	118.11	112.60
1	E	62	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	62	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	62	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	62	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	472	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	472	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	472	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	223	ASP	CA-C-N	5.17	127.52	120.54
1	A	223	ASP	C-N-CA	5.17	127.52	120.54
1	B	223	ASP	CA-C-N	5.17	127.52	120.54
1	B	223	ASP	C-N-CA	5.17	127.52	120.54
1	E	472	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	517	HIS	CA-C-N	5.16	124.60	119.24
1	B	517	HIS	C-N-CA	5.16	124.60	119.24
1	C	223	ASP	CA-C-N	5.15	127.50	120.54
1	C	223	ASP	C-N-CA	5.15	127.50	120.54
1	E	223	ASP	CA-C-N	5.15	127.50	120.54
1	E	223	ASP	C-N-CA	5.15	127.50	120.54
1	C	517	HIS	CA-C-N	5.13	124.58	119.24
1	C	517	HIS	C-N-CA	5.13	124.58	119.24
1	E	517	HIS	CA-C-N	5.13	124.58	119.24
1	E	517	HIS	C-N-CA	5.13	124.58	119.24
1	A	517	HIS	CA-C-N	5.11	124.56	119.24
1	A	517	HIS	C-N-CA	5.11	124.56	119.24

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	4239	4245	4240	41	0
1	B	4239	4245	4240	41	0
1	C	4239	4245	4240	41	0
1	E	4239	4245	4240	41	0
2	A	34	19	0	0	0
2	B	34	19	0	0	0
2	C	34	19	0	0	0
2	E	34	19	0	0	0
3	A	10	10	7	6	0
3	B	10	10	7	7	0
3	C	10	10	7	6	0
3	E	10	10	7	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	29	11	11	0	0
5	B	29	11	11	0	0
5	C	29	11	11	0	0
5	E	29	11	11	0	0
All	All	17252	17140	17032	122	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 4.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HB	1:E:111:VAL:CG2	1.80	1.10
1:C:43:ILE:HB	1:B:111:VAL:HG23	1.26	1.09
1:A:111:VAL:CG2	1:E:43:ILE:HB	1.81	1.09
1:A:43:ILE:HB	1:E:111:VAL:HG23	1.25	1.09
1:C:43:ILE:HB	1:B:111:VAL:CG2	1.82	1.08
1:C:111:VAL:CG2	1:B:43:ILE:HB	1.82	1.08
1:A:111:VAL:HG23	1:E:43:ILE:HB	1.23	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HG23	1:B:43:ILE:HB	1.26	1.06
1:A:43:ILE:CB	1:E:111:VAL:HG23	1.98	0.93
1:A:111:VAL:HG23	1:E:43:ILE:CB	1.98	0.92
1:C:43:ILE:CB	1:B:111:VAL:HG23	2.00	0.91
1:C:111:VAL:HG23	1:B:43:ILE:CB	2.00	0.90
1:C:45:ILE:O	1:B:102:ARG:NH2	2.03	0.90
1:A:45:ILE:O	1:E:102:ARG:NH2	2.04	0.90
1:A:102:ARG:NH2	1:E:45:ILE:O	2.05	0.90
1:C:102:ARG:NH2	1:B:45:ILE:O	2.05	0.90
1:C:235:HIS:CE1	1:E:164:ARG:HH22	1.96	0.83
1:A:235:HIS:CE1	1:B:164:ARG:HH22	1.97	0.83
1:C:164:ARG:HH22	1:E:235:HIS:CE1	1.96	0.82
1:A:164:ARG:HH22	1:B:235:HIS:CE1	1.98	0.82
1:C:399:CYS:SG	3:C:602:GLN:CD	2.65	0.79
1:A:399:CYS:SG	3:A:604:GLN:CD	2.65	0.79
1:E:399:CYS:SG	3:E:604:GLN:CD	2.65	0.79
1:B:399:CYS:SG	3:B:602:GLN:CD	2.66	0.79
1:A:480:HIS:HB2	3:A:604:GLN:OXT	1.87	0.75
1:C:480:HIS:HB2	3:C:602:GLN:O	1.87	0.75
1:C:45:ILE:O	1:B:102:ARG:CZ	2.35	0.74
1:A:45:ILE:O	1:E:102:ARG:CZ	2.35	0.74
1:C:102:ARG:CZ	1:B:45:ILE:O	2.36	0.74
1:B:480:HIS:HB2	3:B:602:GLN:OXT	1.87	0.74
1:E:480:HIS:HB2	3:E:604:GLN:O	1.87	0.73
1:A:102:ARG:CZ	1:E:45:ILE:O	2.38	0.72
1:A:43:ILE:HB	1:E:111:VAL:HG21	1.70	0.71
1:C:43:ILE:HB	1:B:111:VAL:HG21	1.72	0.69
1:C:235:HIS:CE1	1:E:164:ARG:NH2	2.63	0.66
1:C:164:ARG:NH2	1:E:235:HIS:CE1	2.63	0.65
1:A:235:HIS:CE1	1:B:164:ARG:NH2	2.63	0.65
1:A:111:VAL:HG21	1:E:43:ILE:HB	1.72	0.65
1:C:111:VAL:HG21	1:B:43:ILE:HB	1.73	0.64
1:A:164:ARG:NH2	1:B:235:HIS:CE1	2.64	0.64
1:B:151:VAL:HG11	1:B:204:LEU:HD13	1.83	0.61
1:E:151:VAL:HG11	1:E:204:LEU:HD13	1.83	0.61
1:A:151:VAL:HG11	1:A:204:LEU:HD13	1.83	0.60
1:C:151:VAL:HG11	1:C:204:LEU:HD13	1.83	0.59
1:C:101:GLU:OE2	1:B:49:THR:HG21	2.05	0.56
1:C:49:THR:HG21	1:B:101:GLU:OE2	2.05	0.56
1:B:80:ILE:HD12	1:B:82:LEU:HD21	1.87	0.56
1:E:80:ILE:HD12	1:E:82:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:HD12	1:C:82:LEU:HD21	1.87	0.55
1:A:80:ILE:HD12	1:A:82:LEU:HD21	1.87	0.55
1:A:49:THR:HG21	1:E:101:GLU:OE2	2.07	0.54
1:A:101:GLU:OE2	1:E:49:THR:HG21	2.07	0.54
1:C:406:VAL:HG22	1:C:497:LEU:HD21	1.91	0.52
1:A:406:VAL:HG22	1:A:497:LEU:HD21	1.91	0.52
1:B:406:VAL:HG22	1:B:497:LEU:HD21	1.91	0.52
1:E:406:VAL:HG22	1:E:497:LEU:HD21	1.91	0.52
1:C:399:CYS:SG	3:C:602:GLN:HB2	2.51	0.51
1:E:399:CYS:SG	3:E:604:GLN:HB2	2.51	0.51
1:A:399:CYS:SG	3:A:604:GLN:HB2	2.51	0.51
1:B:399:CYS:SG	3:B:602:GLN:HB2	2.51	0.51
1:C:399:CYS:SG	3:C:602:GLN:NE2	2.86	0.48
1:A:399:CYS:SG	3:A:604:GLN:NE2	2.86	0.48
1:B:399:CYS:SG	3:B:602:GLN:NE2	2.87	0.48
1:E:399:CYS:SG	3:E:604:GLN:NE2	2.86	0.48
1:C:482:PHE:HD2	3:C:602:GLN:C	2.22	0.47
1:A:482:PHE:HD2	3:A:604:GLN:C	2.22	0.47
1:E:482:PHE:HD2	3:E:604:GLN:C	2.22	0.47
1:A:108:GLY:HA2	1:E:49:THR:O	2.15	0.46
1:B:482:PHE:HD2	3:B:602:GLN:C	2.22	0.46
1:B:213:LEU:HD22	1:B:242:ILE:HD11	1.98	0.46
1:A:56:GLY:O	1:A:69:LEU:HD23	2.16	0.46
1:A:213:LEU:HD22	1:A:242:ILE:HD11	1.98	0.46
1:C:56:GLY:O	1:C:69:LEU:HD23	2.16	0.46
1:C:213:LEU:HD22	1:C:242:ILE:HD11	1.98	0.46
1:E:213:LEU:HD22	1:E:242:ILE:HD11	1.98	0.46
1:C:49:THR:O	1:B:108:GLY:HA2	2.16	0.45
1:C:108:GLY:HA2	1:B:49:THR:O	2.17	0.45
1:C:373:PHE:CD2	3:C:602:GLN:N	2.85	0.45
1:A:373:PHE:CD2	3:A:604:GLN:N	2.85	0.45
1:E:304:VAL:HG23	1:E:369:VAL:HG22	1.99	0.44
1:B:304:VAL:HG23	1:B:369:VAL:HG22	2.00	0.44
1:B:56:GLY:O	1:B:69:LEU:HD23	2.16	0.44
1:E:56:GLY:O	1:E:69:LEU:HD23	2.16	0.44
1:B:457:PHE:CE2	1:B:474:LEU:HD23	2.53	0.44
1:E:457:PHE:CE2	1:E:474:LEU:HD23	2.53	0.44
1:A:304:VAL:HG23	1:A:369:VAL:HG22	2.00	0.43
1:B:373:PHE:CD2	3:B:602:GLN:N	2.85	0.43
1:C:304:VAL:HG23	1:C:369:VAL:HG22	2.00	0.43
1:E:373:PHE:CD2	3:E:604:GLN:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:O	1:E:108:GLY:HA2	2.18	0.43
1:A:43:ILE:CG1	1:E:111:VAL:HG23	2.49	0.43
1:A:457:PHE:CE2	1:A:474:LEU:HD23	2.53	0.43
1:C:457:PHE:CE2	1:C:474:LEU:HD23	2.53	0.43
1:C:255:LEU:HD13	1:C:286:LYS:HD3	2.00	0.43
1:A:255:LEU:HD13	1:A:286:LYS:HD3	2.00	0.43
1:C:428:THR:HG22	1:C:430:HIS:H	1.84	0.42
1:B:428:THR:HG22	1:B:430:HIS:H	1.84	0.42
1:E:255:LEU:HD13	1:E:286:LYS:HD3	2.00	0.42
1:E:428:THR:HG22	1:E:430:HIS:H	1.84	0.42
1:A:428:THR:HG22	1:A:430:HIS:H	1.84	0.42
1:B:255:LEU:HD13	1:B:286:LYS:HD3	2.00	0.42
1:C:474:LEU:HD13	1:C:476:GLU:HG3	2.03	0.41
1:A:213:LEU:HD22	1:A:242:ILE:CD1	2.50	0.41
1:A:474:LEU:HD13	1:A:476:GLU:HG3	2.03	0.41
1:C:213:LEU:HD22	1:C:242:ILE:CD1	2.50	0.41
1:C:14:ILE:HG21	1:C:182:LEU:HD13	2.03	0.41
1:B:213:LEU:HD22	1:B:242:ILE:CD1	2.50	0.41
1:C:497:LEU:HG	1:C:512:VAL:HG21	2.03	0.41
1:A:1:MET:HE2	1:A:129:ALA:HB1	2.03	0.41
1:A:14:ILE:HG21	1:A:182:LEU:HD13	2.03	0.41
1:E:213:LEU:HD22	1:E:242:ILE:CD1	2.50	0.41
1:C:1:MET:HE2	1:C:129:ALA:HB1	2.03	0.41
1:A:497:LEU:HG	1:A:512:VAL:HG21	2.03	0.41
1:B:414:LEU:HD11	1:B:492:LEU:HD23	2.03	0.41
1:E:414:LEU:HD11	1:E:492:LEU:HD23	2.03	0.41
1:B:1:MET:HE2	1:B:129:ALA:HB1	2.03	0.40
1:E:1:MET:HE2	1:E:129:ALA:HB1	2.03	0.40
1:C:43:ILE:CG1	1:B:111:VAL:HG23	2.51	0.40
1:B:497:LEU:HG	1:B:512:VAL:HG21	2.03	0.40
1:E:497:LEU:HG	1:E:512:VAL:HG21	2.03	0.40
1:B:373:PHE:HE2	3:B:602:GLN:O	2.04	0.40
1:E:373:PHE:HE2	3:E:604:GLN:OXT	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/591 (88%)	502 (96%)	19 (4%)	2 (0%)	30	59
1	B	523/591 (88%)	502 (96%)	19 (4%)	2 (0%)	30	59
1	C	523/591 (88%)	502 (96%)	19 (4%)	2 (0%)	30	59
1	E	523/591 (88%)	502 (96%)	19 (4%)	2 (0%)	30	59
All	All	2092/2364 (88%)	2008 (96%)	76 (4%)	8 (0%)	31	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	ILE
1	A	14	ILE
1	B	14	ILE
1	E	14	ILE
1	C	399	CYS
1	A	399	CYS
1	B	399	CYS
1	E	399	CYS

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	472/524 (90%)	465 (98%)	7 (2%)	57	84
1	B	472/524 (90%)	465 (98%)	7 (2%)	57	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	472/524 (90%)	465 (98%)	7 (2%)	57	84
1	E	472/524 (90%)	465 (98%)	7 (2%)	57	84
All	All	1888/2096 (90%)	1860 (98%)	28 (2%)	55	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	VAL
1	C	194	THR
1	C	218	CYS
1	C	260	GLN
1	C	367	VAL
1	C	433	VAL
1	C	458	GLN
1	A	58	VAL
1	A	194	THR
1	A	218	CYS
1	A	260	GLN
1	A	367	VAL
1	A	433	VAL
1	A	458	GLN
1	B	58	VAL
1	B	194	THR
1	B	218	CYS
1	B	260	GLN
1	B	367	VAL
1	B	433	VAL
1	B	458	GLN
1	E	58	VAL
1	E	194	THR
1	E	218	CYS
1	E	260	GLN
1	E	367	VAL
1	E	433	VAL
1	E	458	GLN

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

Mol	Chain	Res	Type
1	C	95	GLN

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Mol	Chain	Res	Type
1	C	122	GLN
1	C	185	GLN
1	C	220	ASN
1	C	365	HIS
1	C	390	ASN
1	C	391	GLN
1	A	95	GLN
1	A	122	GLN
1	A	185	GLN
1	A	220	ASN
1	A	365	HIS
1	A	390	ASN
1	A	391	GLN
1	B	95	GLN
1	B	122	GLN
1	B	185	GLN
1	B	220	ASN
1	B	365	HIS
1	B	390	ASN
1	B	391	GLN
1	E	95	GLN
1	E	122	GLN
1	E	185	GLN
1	E	220	ASN
1	E	365	HIS
1	E	390	ASN
1	E	391	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	UTP	C	604	4	29,30,30	2.73	5 (17%)	43,47,47	1.35	6 (13%)
2	ZFY	B	601	-	34,37,37	1.25	4 (11%)	50,57,57	1.52	7 (14%)
3	GLN	B	602	-	8,9,9	0.87	0	8,11,11	0.60	0
2	ZFY	A	603	-	34,37,37	1.26	4 (11%)	50,57,57	1.51	7 (14%)
2	ZFY	E	603	-	34,37,37	1.25	4 (11%)	50,57,57	1.51	7 (14%)
5	UTP	E	602	4	29,30,30	2.72	5 (17%)	43,47,47	1.35	6 (13%)
3	GLN	E	604	-	8,9,9	0.80	0	8,11,11	0.61	0
3	GLN	A	604	-	8,9,9	0.86	0	8,11,11	0.60	0
5	UTP	B	604	4	29,30,30	2.73	5 (17%)	43,47,47	1.37	6 (13%)
5	UTP	A	602	4	29,30,30	2.73	5 (17%)	43,47,47	1.36	6 (13%)
2	ZFY	C	601	-	34,37,37	1.25	4 (11%)	50,57,57	1.51	7 (14%)
3	GLN	C	602	-	8,9,9	0.79	0	8,11,11	0.61	0

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	UTP	C	604	4	-	8/22/38/38	0/2/2/2
2	ZFY	B	601	-	-	0/33/39/39	0/4/4/4
3	GLN	B	602	-	-	0/9/9/9	-
2	ZFY	A	603	-	-	0/33/39/39	0/4/4/4
2	ZFY	E	603	-	-	0/33/39/39	0/4/4/4
5	UTP	E	602	4	-	8/22/38/38	0/2/2/2
3	GLN	E	604	-	-	0/9/9/9	-
3	GLN	A	604	-	-	0/9/9/9	-
5	UTP	B	604	4	-	8/22/38/38	0/2/2/2
5	UTP	A	602	4	-	8/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZFY	C	601	-	-	0/33/39/39	0/4/4/4
3	GLN	C	602	-	-	0/9/9/9	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	UTP	PA-O3A	8.19	1.68	1.59
5	A	602	UTP	PA-O3A	8.18	1.68	1.59
5	B	604	UTP	PA-O3A	8.14	1.68	1.59
5	E	602	UTP	PA-O3A	8.14	1.68	1.59
5	B	604	UTP	PB-O3B	7.89	1.68	1.59
5	C	604	UTP	PB-O3B	7.84	1.68	1.59
5	A	602	UTP	PB-O3B	7.84	1.68	1.59
5	E	602	UTP	PB-O3B	7.76	1.67	1.59
5	C	604	UTP	PB-O3A	7.74	1.67	1.59
5	E	602	UTP	PB-O3A	7.73	1.67	1.59
5	A	602	UTP	PB-O3A	7.72	1.67	1.59
5	B	604	UTP	PB-O3A	7.72	1.67	1.59
2	B	601	ZFY	C15-C12	3.95	1.39	1.35
2	E	603	ZFY	C15-C12	3.89	1.39	1.35
2	C	601	ZFY	C15-C12	3.87	1.39	1.35
2	A	603	ZFY	C15-C12	3.87	1.39	1.35
5	C	604	UTP	PA-O5'	3.18	1.71	1.59
5	A	602	UTP	PA-O5'	3.15	1.71	1.59
5	B	604	UTP	PA-O5'	3.15	1.71	1.59
5	E	602	UTP	PA-O5'	3.15	1.71	1.59
2	A	603	ZFY	O2-S2	3.03	1.47	1.43
2	E	603	ZFY	O2-S2	3.02	1.47	1.43
2	C	601	ZFY	O2-S2	3.01	1.47	1.43
2	B	601	ZFY	O2-S2	2.94	1.47	1.43
5	A	602	UTP	C4-N3	-2.53	1.34	1.38
5	C	604	UTP	C4-N3	-2.53	1.34	1.38
5	E	602	UTP	C4-N3	-2.53	1.34	1.38
5	B	604	UTP	C4-N3	-2.48	1.34	1.38
2	C	601	ZFY	O1-S2	2.47	1.46	1.43
2	A	603	ZFY	O1-S2	2.47	1.46	1.43
2	B	601	ZFY	O1-S2	2.46	1.46	1.43
2	E	603	ZFY	O1-S2	2.42	1.46	1.43
2	A	603	ZFY	C12-N5	-2.26	1.33	1.38
2	C	601	ZFY	C12-N5	-2.22	1.33	1.38
2	B	601	ZFY	C12-N5	-2.22	1.33	1.38
2	E	603	ZFY	C12-N5	-2.22	1.33	1.38

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ZFY	C16-N5-C12	6.53	114.16	110.01
2	E	603	ZFY	C16-N5-C12	6.52	114.15	110.01
2	A	603	ZFY	C16-N5-C12	6.52	114.15	110.01
2	C	601	ZFY	C16-N5-C12	6.50	114.14	110.01
5	B	604	UTP	O2-C2-N1	5.00	129.31	122.80
5	E	602	UTP	O2-C2-N1	4.99	129.29	122.80
5	C	604	UTP	O2-C2-N1	4.98	129.27	122.80
5	A	602	UTP	O2-C2-N1	4.98	129.27	122.80
2	B	601	ZFY	S1-C16-N6	-3.78	123.32	129.14
2	E	603	ZFY	S1-C16-N6	-3.78	123.33	129.14
2	C	601	ZFY	S1-C16-N6	-3.77	123.34	129.14
2	A	603	ZFY	S1-C16-N6	-3.76	123.36	129.14
5	B	604	UTP	O2-C2-N3	-3.28	115.44	121.49
5	E	602	UTP	O2-C2-N3	-3.26	115.47	121.49
5	A	602	UTP	O2-C2-N3	-3.26	115.47	121.49
5	C	604	UTP	O2-C2-N3	-3.24	115.51	121.49
2	B	601	ZFY	O1-S2-C17	-2.85	104.18	107.98
2	C	601	ZFY	O1-S2-C17	-2.85	104.19	107.98
2	E	603	ZFY	O1-S2-C17	-2.83	104.21	107.98
2	A	603	ZFY	O1-S2-C17	-2.82	104.22	107.98
5	C	604	UTP	C2'-C1'-N1	2.79	121.01	113.25
5	A	602	UTP	C2'-C1'-N1	2.78	120.98	113.25
5	B	604	UTP	C2'-C1'-N1	2.77	120.97	113.25
5	E	602	UTP	C2'-C1'-N1	2.76	120.93	113.25
2	A	603	ZFY	S1-C16-N5	-2.64	112.92	115.69
2	E	603	ZFY	S1-C16-N5	-2.61	112.94	115.69
2	C	601	ZFY	S1-C16-N5	-2.61	112.94	115.69
2	B	601	ZFY	S1-C16-N5	-2.61	112.95	115.69
5	C	604	UTP	C4-N3-C2	2.57	129.81	126.61
5	A	602	UTP	C4-N3-C2	2.56	129.80	126.61
5	B	604	UTP	C4-N3-C2	2.55	129.78	126.61
5	E	602	UTP	C4-N3-C2	2.55	129.78	126.61
5	C	604	UTP	O2A-PA-O1A	2.45	123.86	112.44
5	A	602	UTP	O2A-PA-O1A	2.45	123.85	112.44
5	B	604	UTP	O2A-PA-O1A	2.45	123.82	112.44
5	E	602	UTP	O2A-PA-O1A	2.45	123.82	112.44
5	C	604	UTP	O1B-PB-O2B	2.44	123.80	112.44
5	B	604	UTP	O1B-PB-O2B	2.43	123.76	112.44
5	A	602	UTP	O1B-PB-O2B	2.43	123.76	112.44
5	E	602	UTP	O1B-PB-O2B	2.43	123.73	112.44
2	B	601	ZFY	N6-C16-N5	2.40	123.64	120.40
2	A	603	ZFY	N6-C16-N5	2.39	123.63	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	603	ZFY	N6-C16-N5	2.39	123.63	120.40
2	C	601	ZFY	N6-C16-N5	2.38	123.62	120.40
2	B	601	ZFY	C16-N6-S2	2.11	125.99	121.90
2	E	603	ZFY	C16-N6-S2	2.09	125.95	121.90
2	C	601	ZFY	C16-N6-S2	2.09	125.94	121.90
2	A	603	ZFY	C16-N6-S2	2.07	125.91	121.90
2	E	603	ZFY	C11-C12-N5	-2.05	117.83	120.52
2	C	601	ZFY	C11-C12-N5	-2.04	117.85	120.52
2	A	603	ZFY	C11-C12-N5	-2.04	117.85	120.52
2	B	601	ZFY	C11-C12-N5	-2.03	117.86	120.52

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	604	UTP	PB-O3B-PG-O3G
5	A	602	UTP	C5'-O5'-PA-O1A
5	A	602	UTP	PB-O3B-PG-O3G
5	B	604	UTP	C5'-O5'-PA-O1A
5	B	604	UTP	PB-O3B-PG-O3G
5	E	602	UTP	PB-O3B-PG-O3G
5	C	604	UTP	O4'-C4'-C5'-O5'
5	B	604	UTP	O4'-C4'-C5'-O5'
5	A	602	UTP	O4'-C4'-C5'-O5'
5	E	602	UTP	O4'-C4'-C5'-O5'
5	C	604	UTP	PA-O3A-PB-O1B
5	A	602	UTP	PA-O3A-PB-O2B
5	B	604	UTP	PA-O3A-PB-O2B
5	E	602	UTP	PA-O3A-PB-O1B
5	C	604	UTP	O4'-C1'-N1-C6
5	A	602	UTP	O4'-C1'-N1-C6
5	B	604	UTP	O4'-C1'-N1-C6
5	E	602	UTP	O4'-C1'-N1-C6
5	C	604	UTP	O4'-C1'-N1-C2
5	A	602	UTP	O4'-C1'-N1-C2
5	B	604	UTP	O4'-C1'-N1-C2
5	E	602	UTP	O4'-C1'-N1-C2
5	C	604	UTP	PA-O3A-PB-O2B
5	E	602	UTP	PA-O3A-PB-O2B
5	C	604	UTP	PB-O3B-PG-O2G
5	A	602	UTP	PB-O3B-PG-O2G
5	B	604	UTP	PB-O3B-PG-O2G

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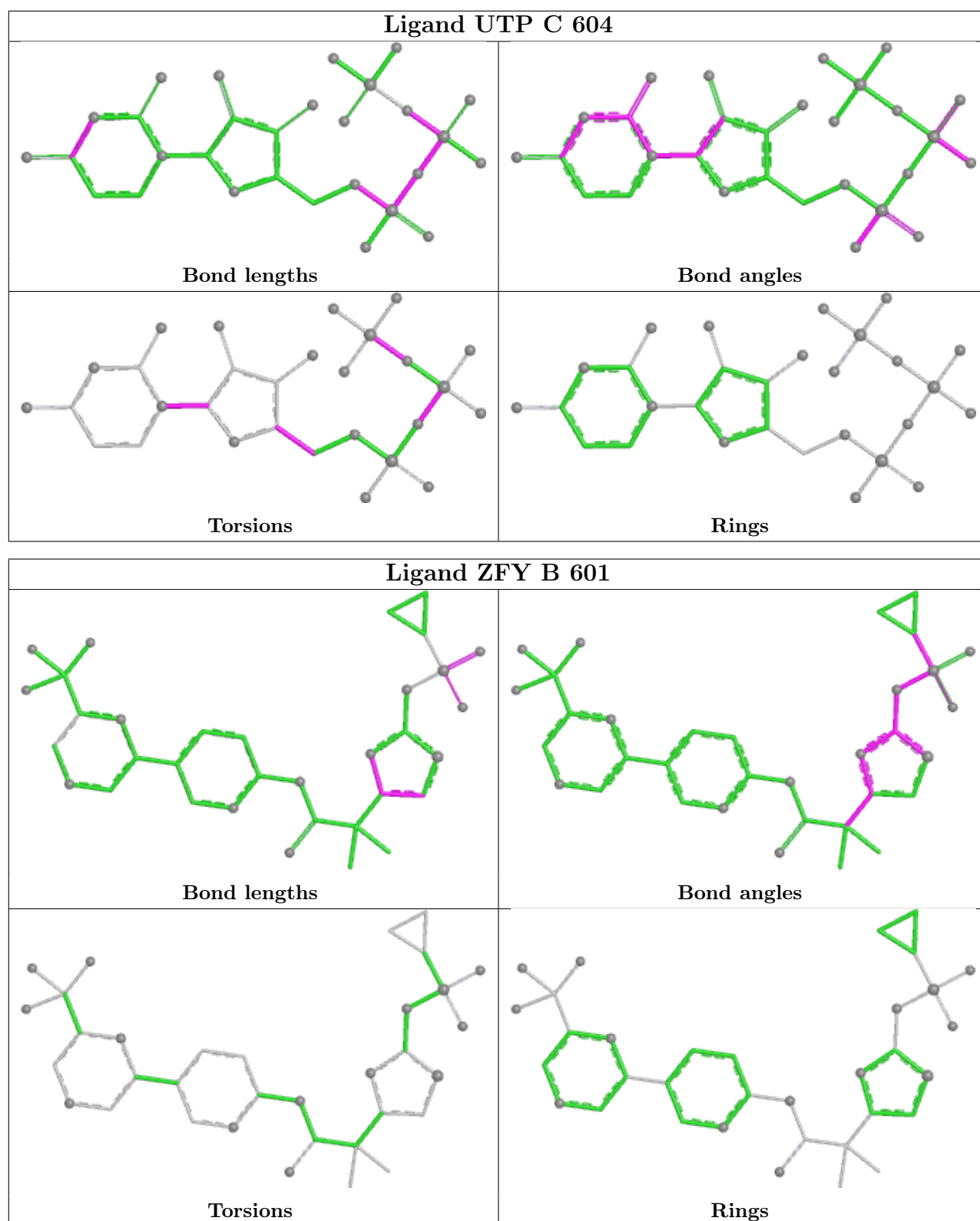
Mol	Chain	Res	Type	Atoms
5	E	602	UTP	PB-O3B-PG-O2G
5	C	604	UTP	PB-O3B-PG-O1G
5	E	602	UTP	PB-O3B-PG-O1G
5	A	602	UTP	PA-O3A-PB-O1B
5	B	604	UTP	PA-O3A-PB-O1B

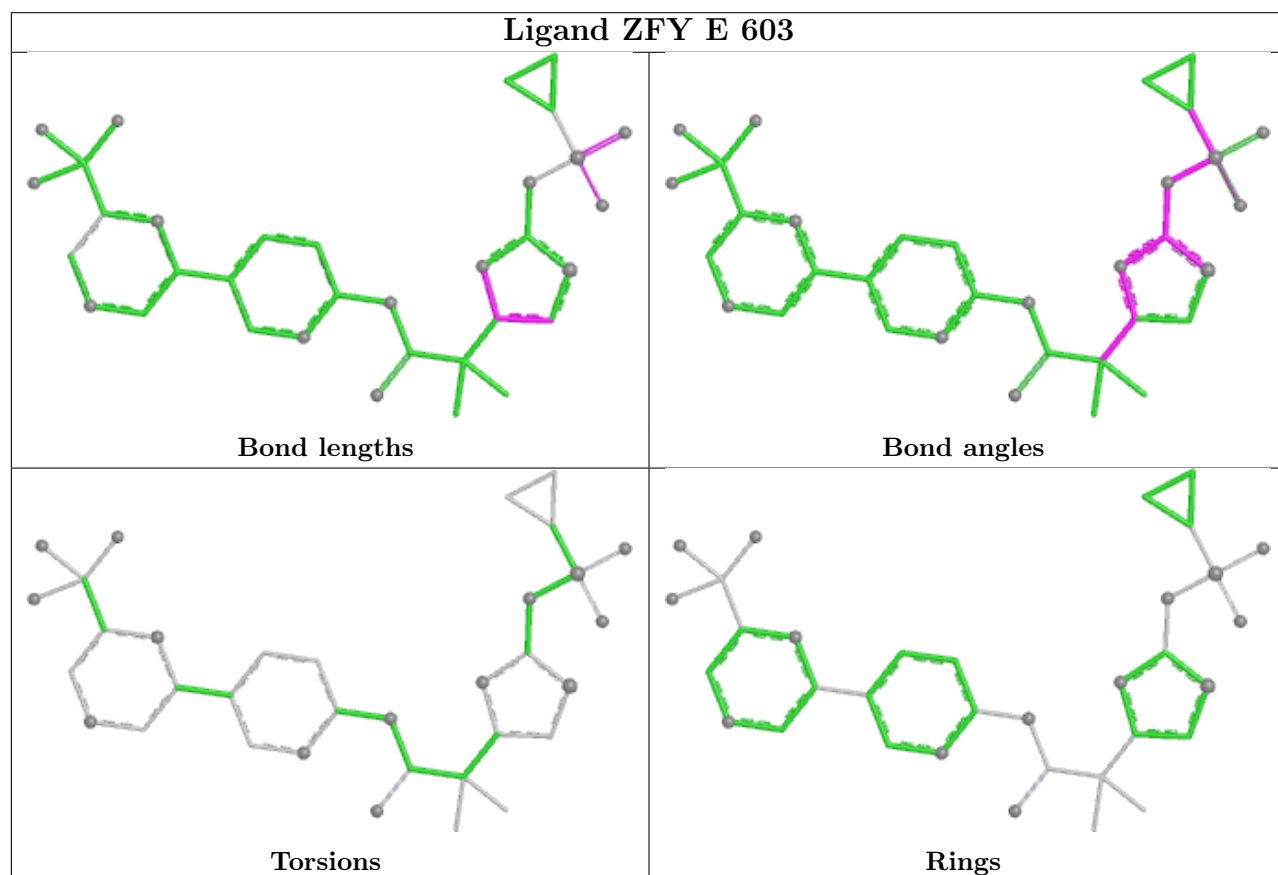
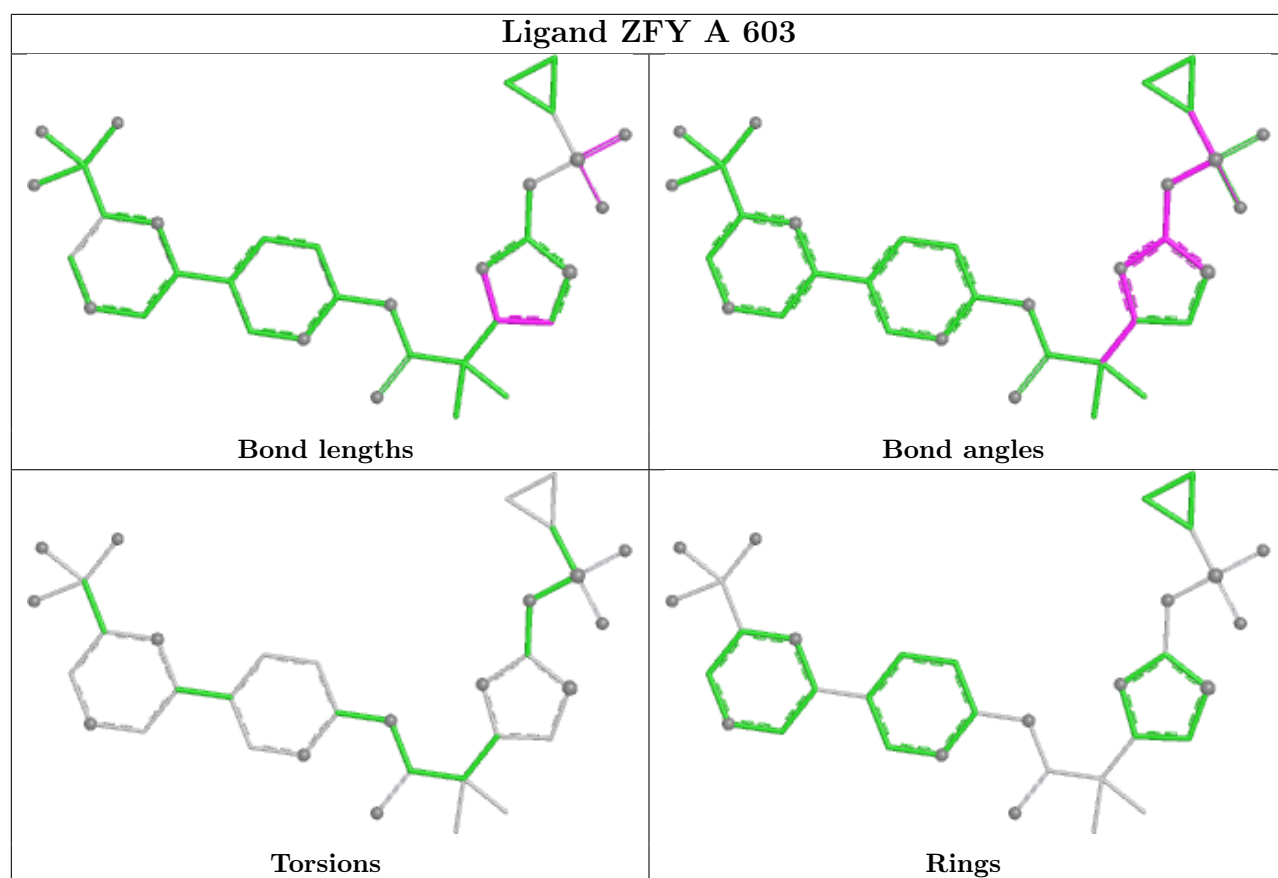
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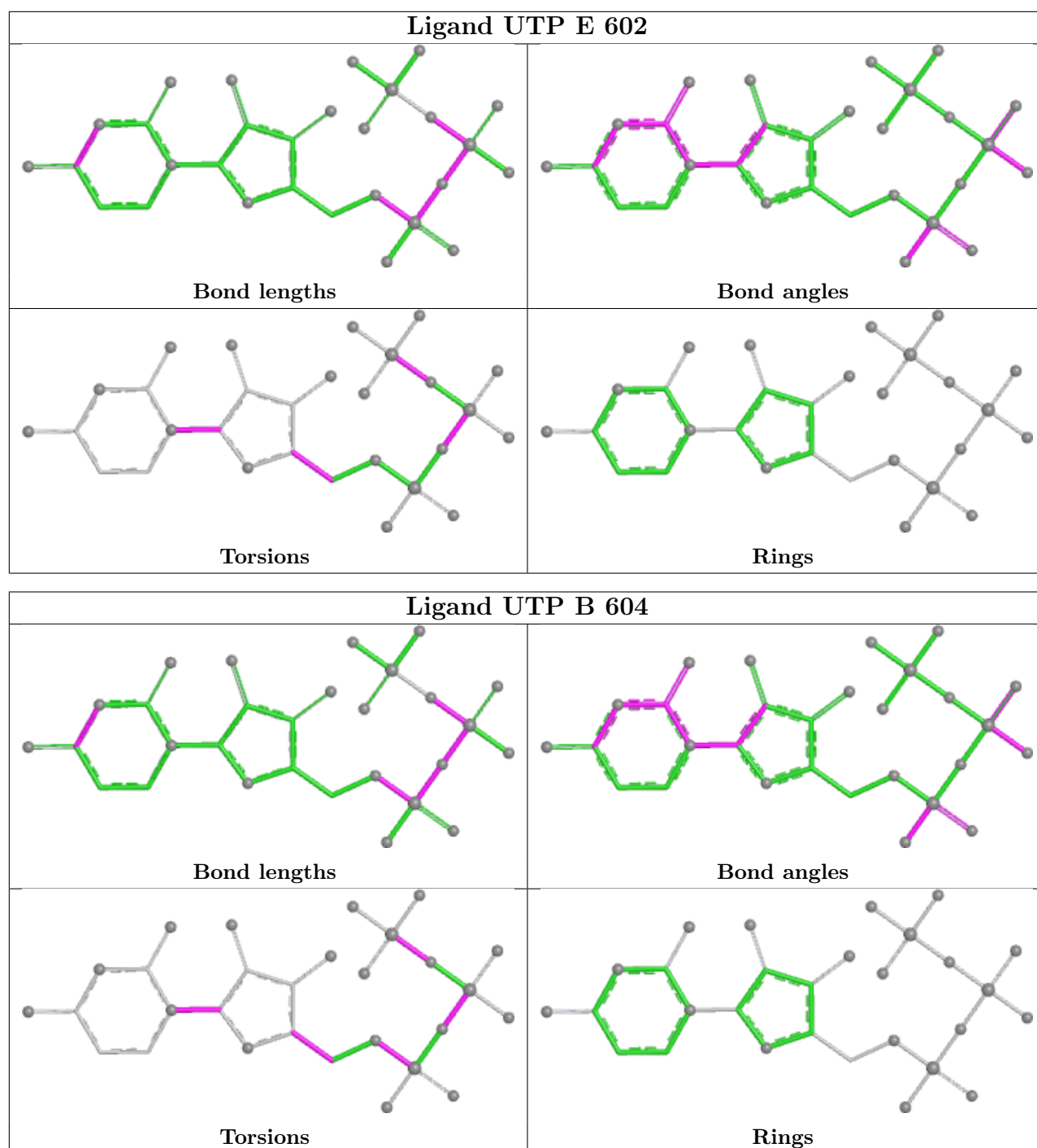
4 monomers are involved in 26 short contacts:

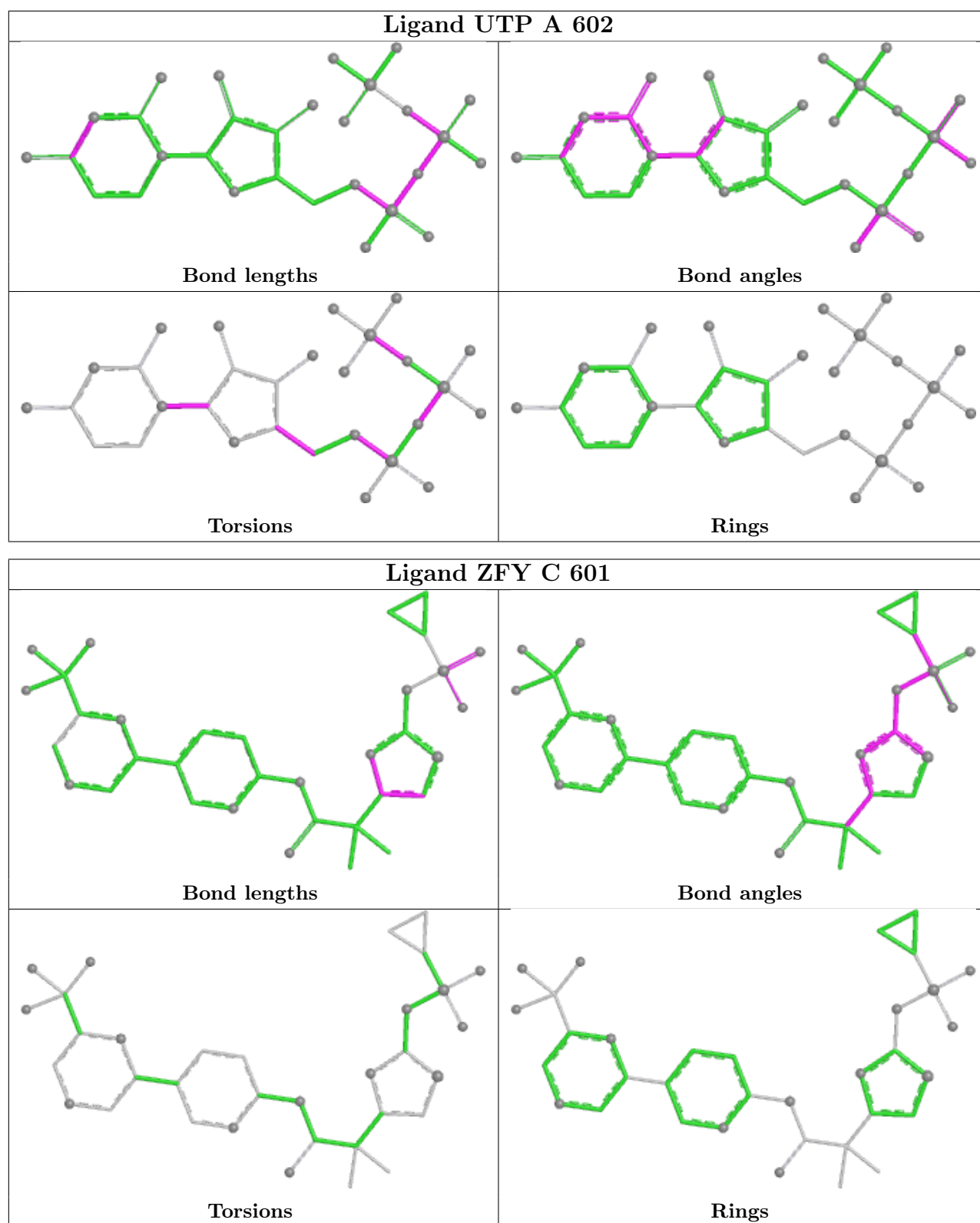
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GLN	7	0
3	E	604	GLN	7	0
3	A	604	GLN	6	0
3	C	602	GLN	6	0

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 ⓘ

There are no chain breaks in this entry.

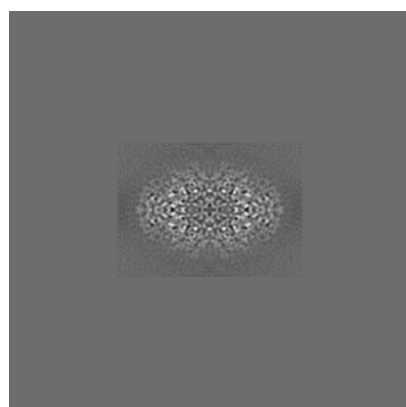
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23850. These allow visual inspection of the internal detail of the map and identification of artifacts.

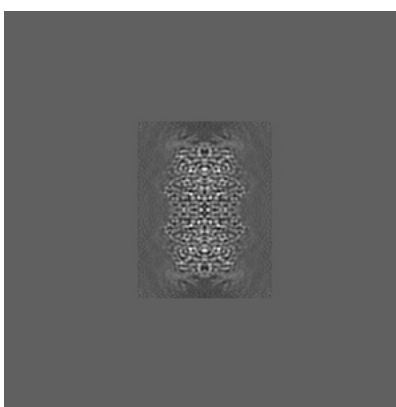
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

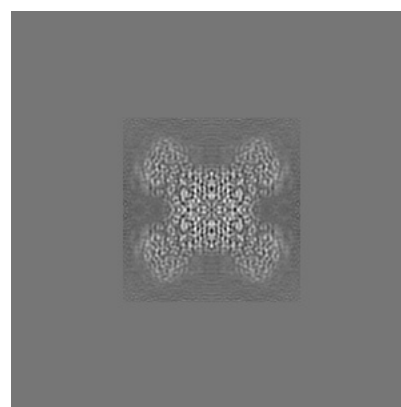
6.1.1 Primary map



X



Y

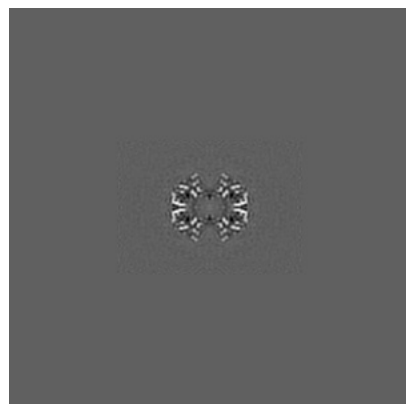


Z

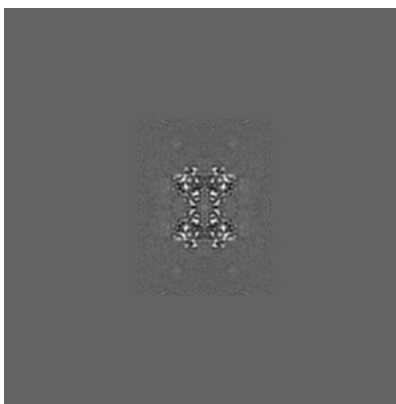
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

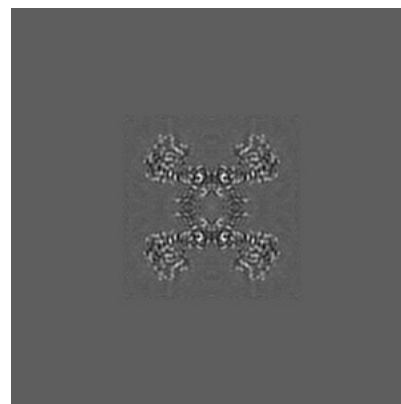
6.2.1 Primary map



X Index: 150



Y Index: 150

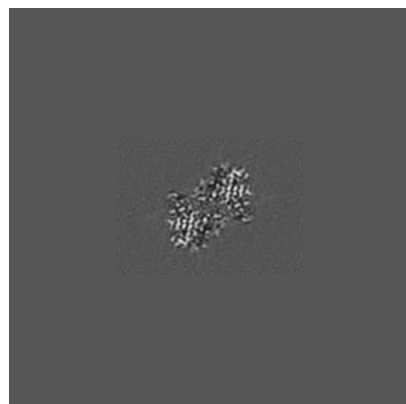


Z Index: 150

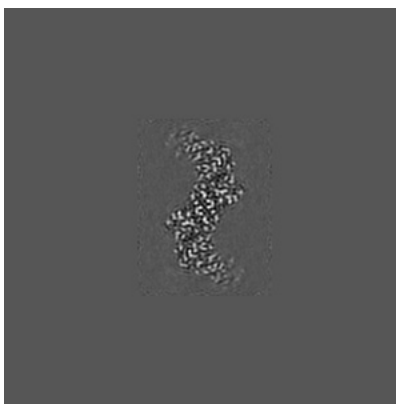
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

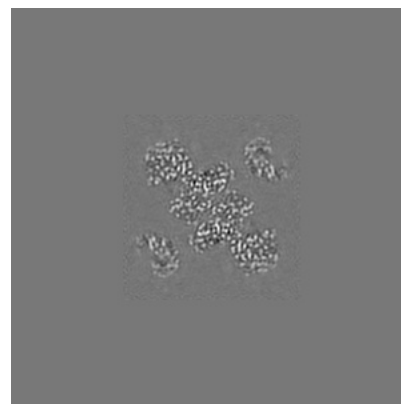
6.3.1 Primary map



X Index: 138



Y Index: 126

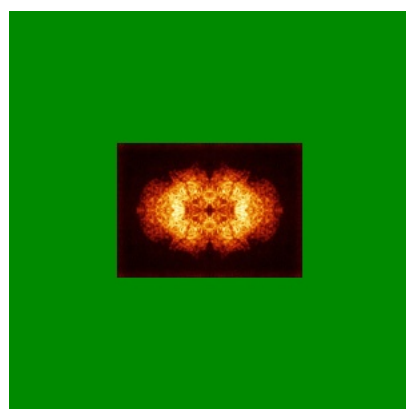


Z Index: 158

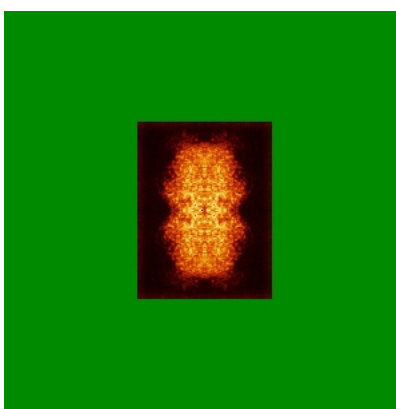
The images above show the largest variance slices of the map in three orthogonal directions.

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

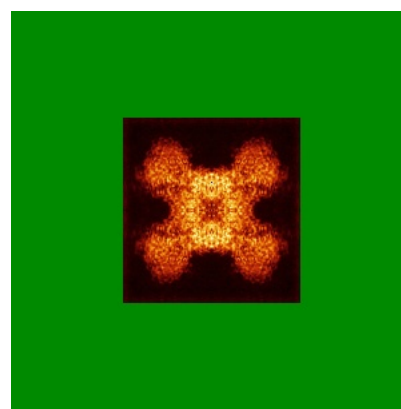
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

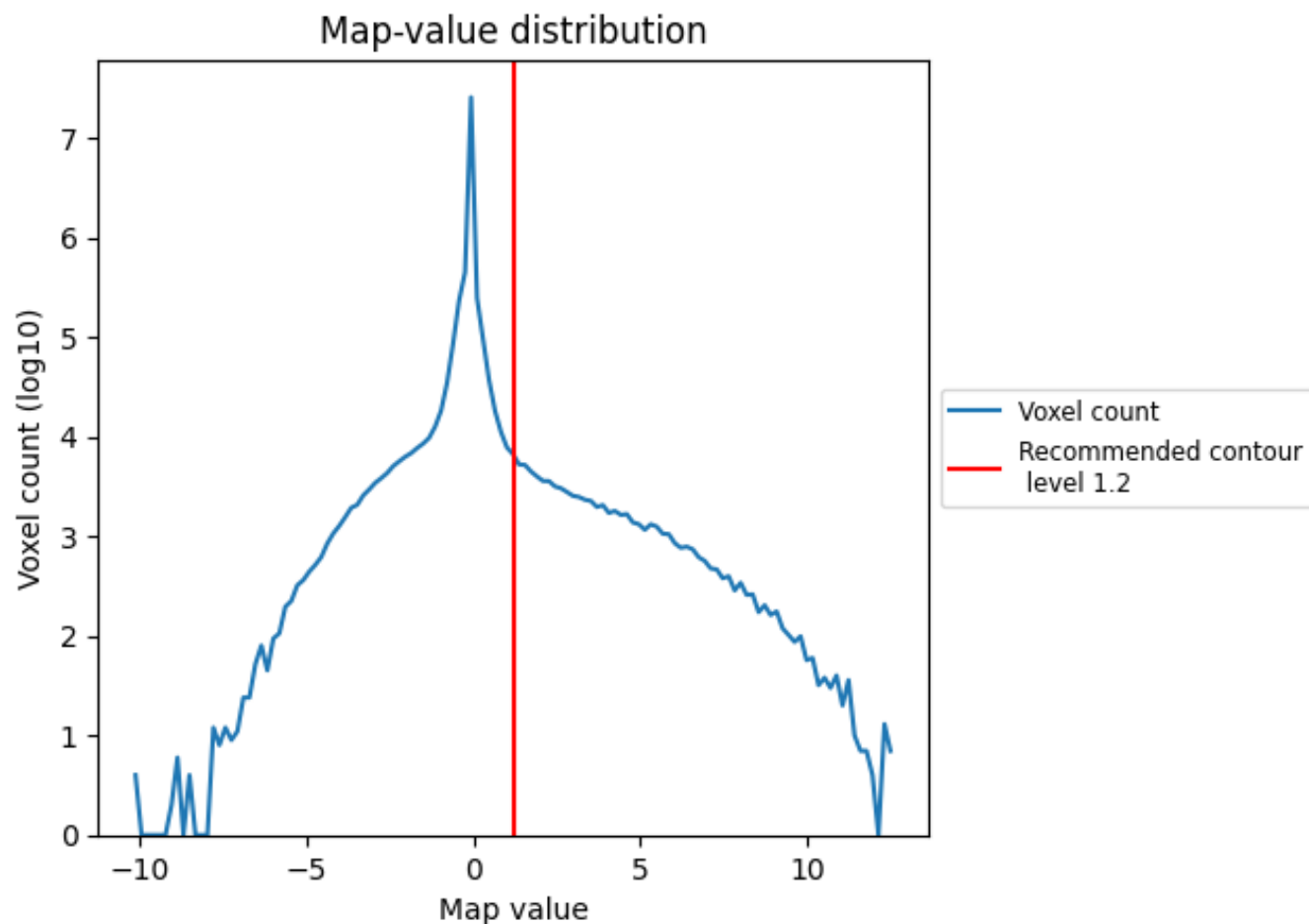
6.6 Mask visualisation

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

7 Map analysis [i](#)

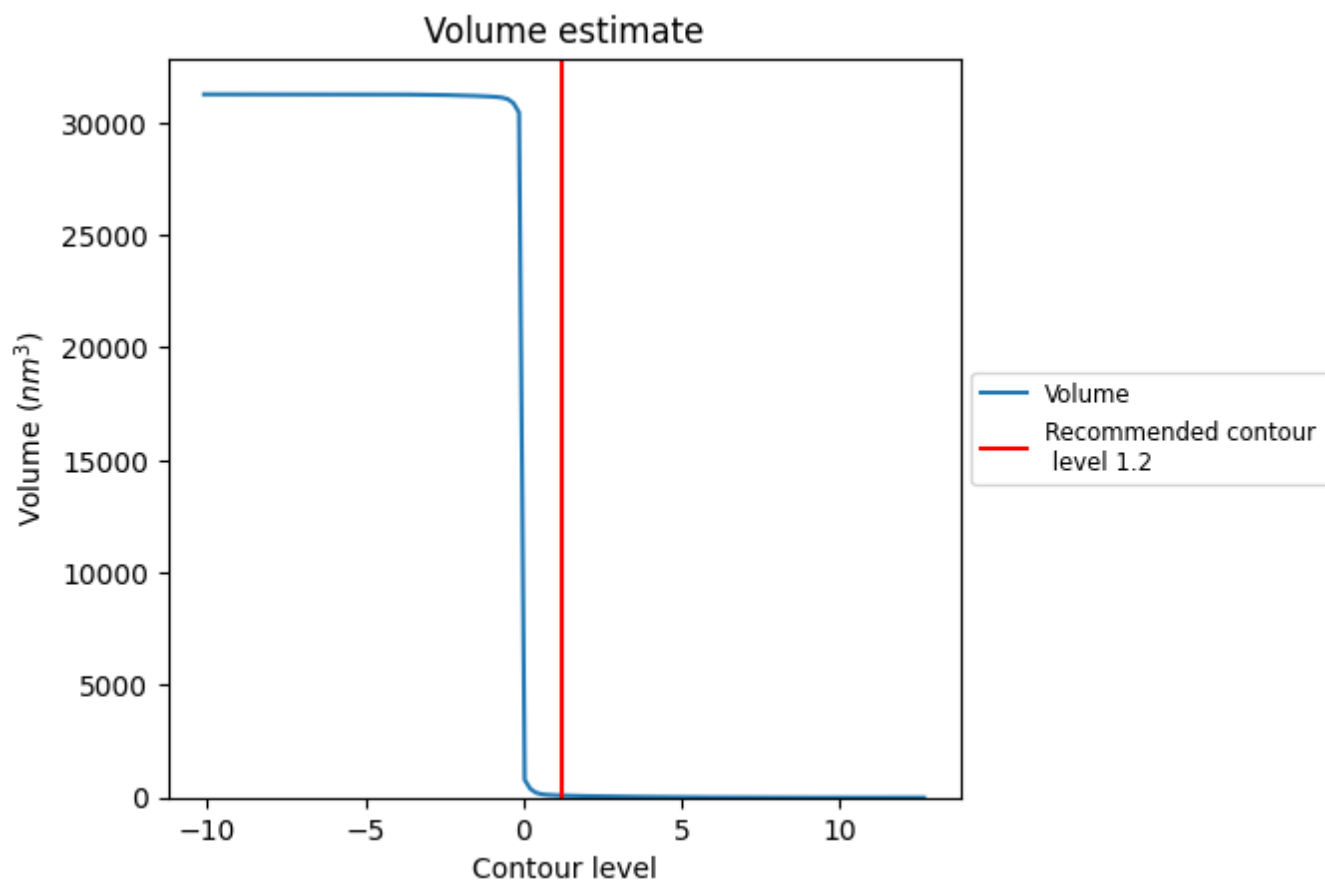
This section contains the results of statistical analysis of the map.

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.

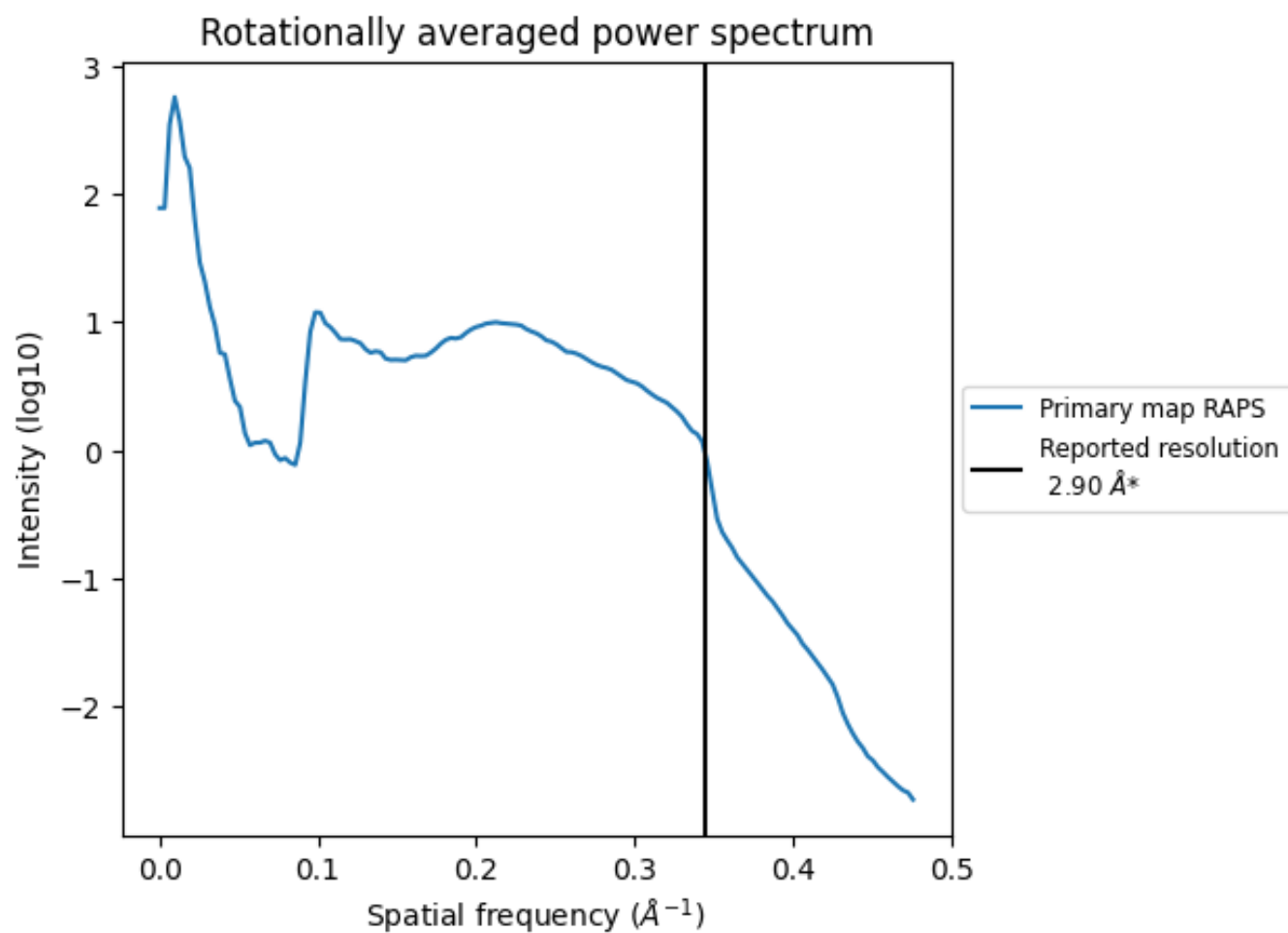
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 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 0.345 Å⁻¹

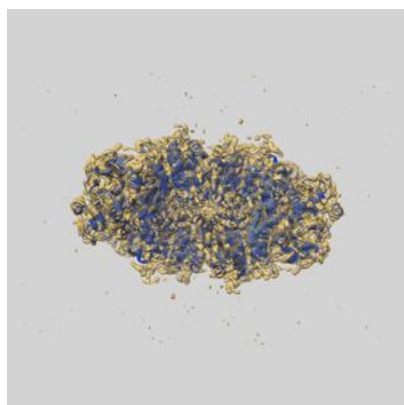
8 Fourier-Shell correlation

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

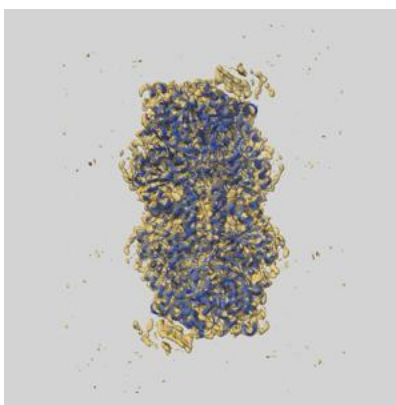
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23850 and PDB model 7MIG. Per-residue inclusion information can be found in section 3 on page 7.

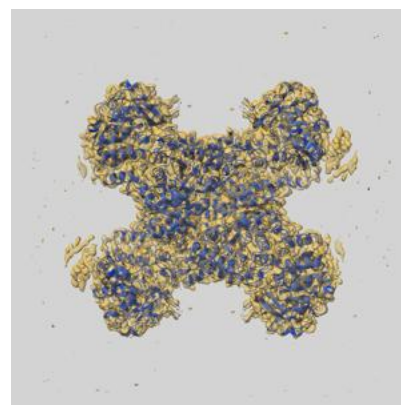
9.1 Map-model overlay [i](#)



X



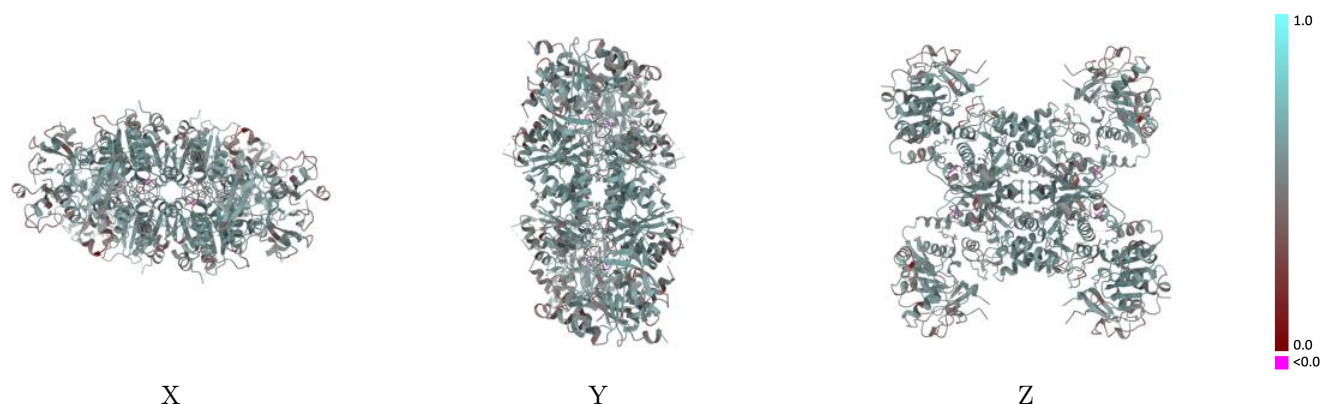
Y



Z

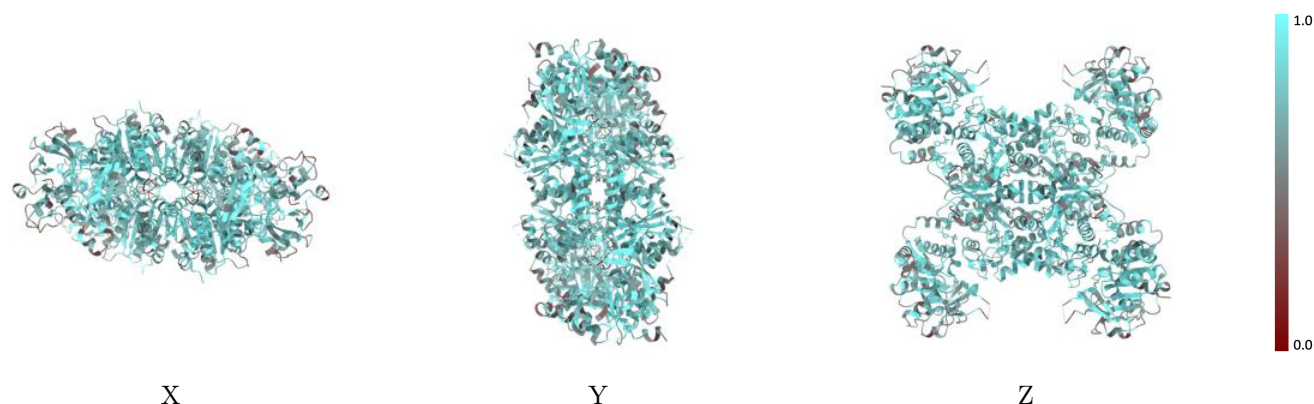
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



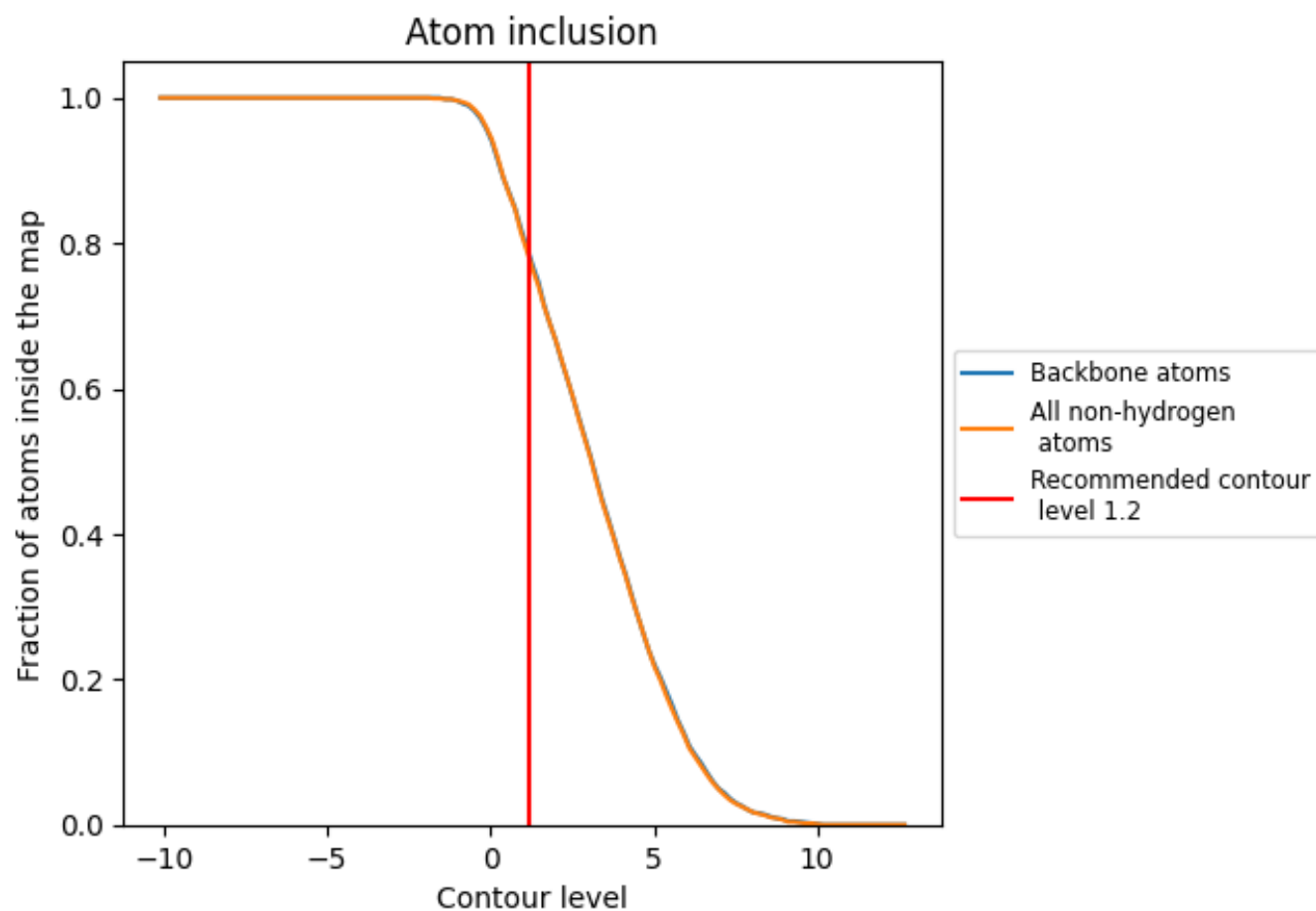
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.5380
A	0.7770	0.5380
B	0.7770	0.5380
C	0.7760	0.5380
E	0.7770	0.5390

