



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:27 AM UTC

PDB ID : 6PW5 / pdb_00006pw5
EMDB ID : EMD-20499
Title : Cryo-EM Structure of Thermo-Sensitive TRP Channel TRP1 from the Alga *Chlamydomonas reinhardtii* in Nanodiscs
Authors : McGoldrick, L.L.; Singh, A.K.; Sobolevsky, A.I.
Deposited on : 2019-07-22
Resolution : 3.45 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

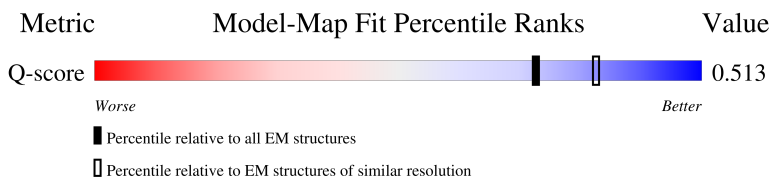
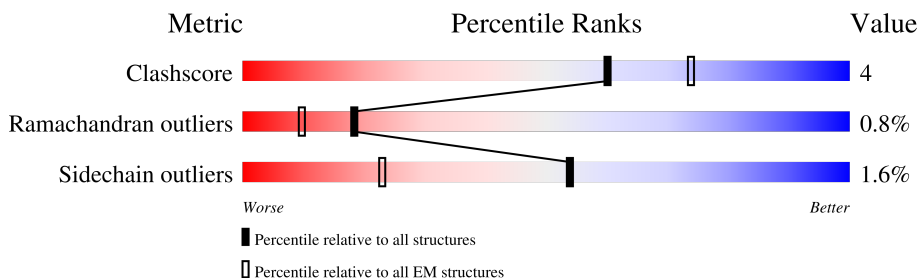
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	13836 (2.95 - 3.95)

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	901	
1	B	901	
1	C	901	
1	D	901	

2 Entry composition ⓘ

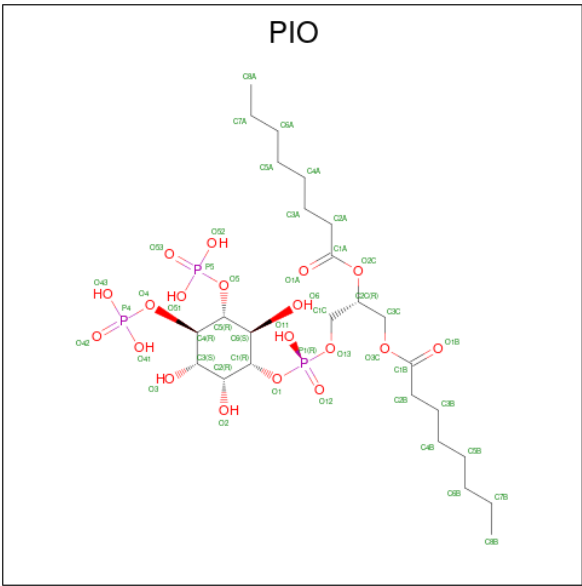
There are 4 unique types of molecules in this entry. The entry contains 24740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRP-like ion channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	734	Total 5858	3794	977	1040	47	0	0
1	B	782	Total 6197	3992	1039	1118	48	0	0
1	C	734	Total 5858	3794	977	1040	47	0	0
1	D	782	Total 6197	3992	1039	1118	48	0	0

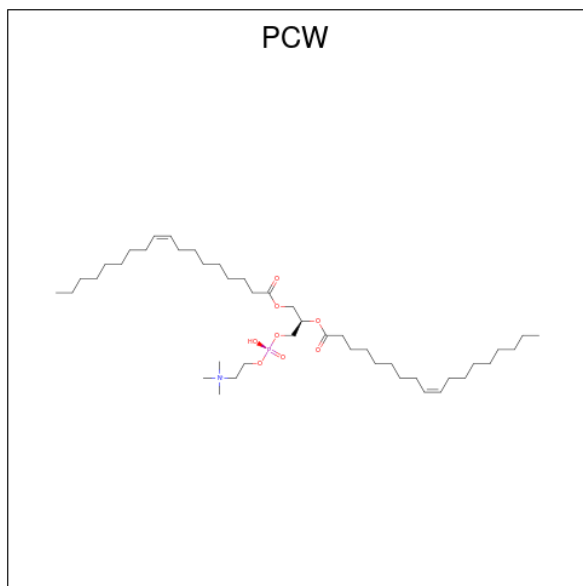
- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



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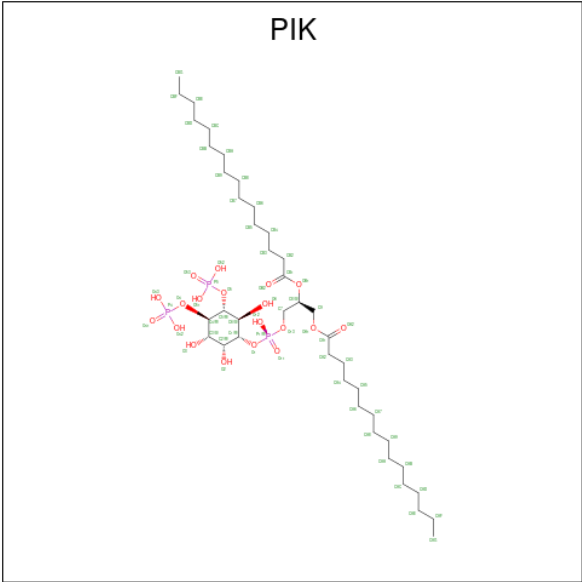
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			47	25	19	3	
2	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).

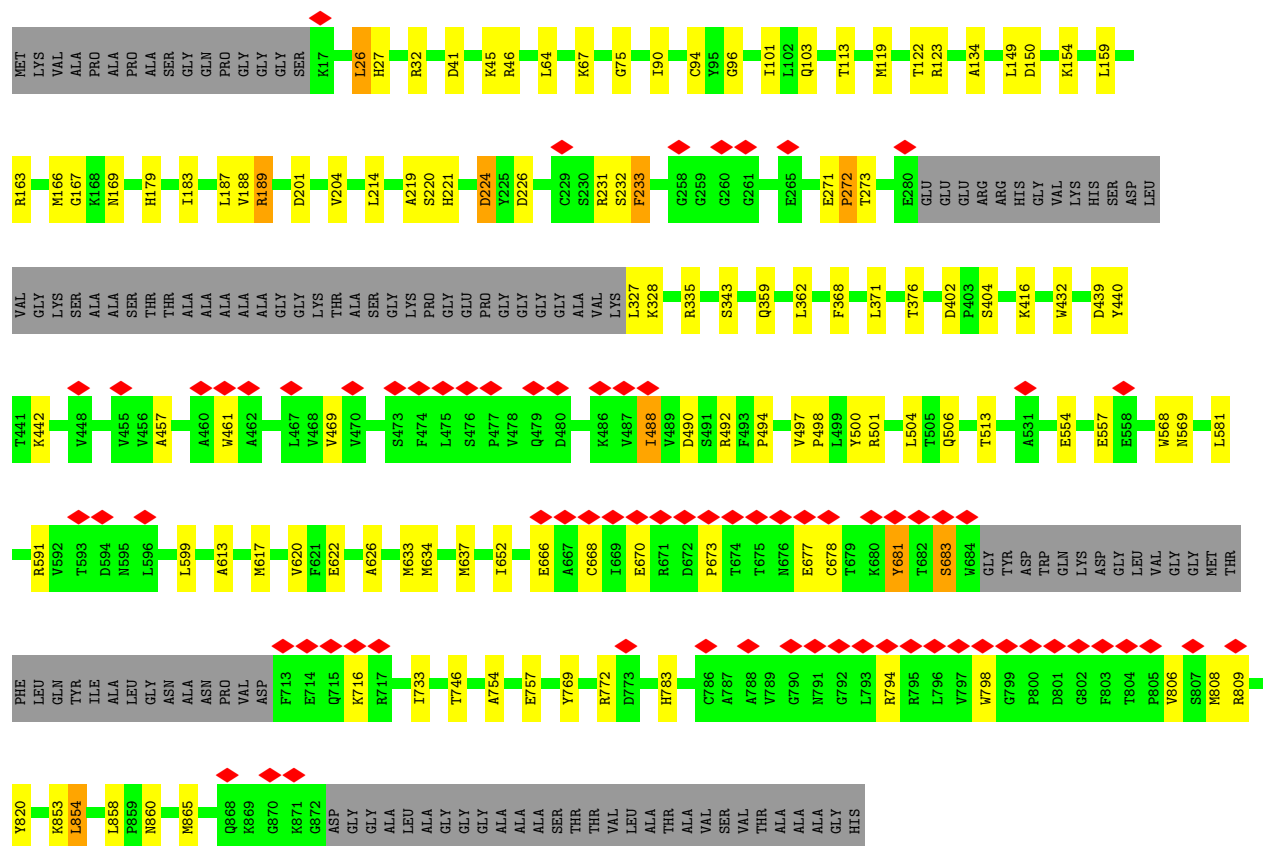


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
3	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 4 is (2S)-3-[[[(R)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dihexadecanoate (CCD ID: PIK) (formula: $C_{41}H_{81}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			63	41	19	3	
4	B	1	Total	C	O	P	0
			63	41	19	3	
4	C	1	Total	C	O	P	0
			63	41	19	3	
4	D	1	Total	C	O	P	0
			63	41	19	3	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	190.0, 190.0, 190.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PIO, PCW, PIK

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	0.51	0/5991	0.69	4/8133 (0.0%)
1	B	0.53	0/6336	0.75	6/8601 (0.1%)
1	C	0.52	0/5991	0.69	4/8133 (0.0%)
1	D	0.53	0/6336	0.75	6/8601 (0.1%)
All	All	0.52	0/24654	0.72	20/33468 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	7
1	C	0	3
1	D	0	7
All	All	0	20

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	VAL	N-CA-C	-6.44	105.89	113.42
1	C	380	VAL	N-CA-C	-6.44	105.89	113.42
1	A	75	GLY	CA-C-N	5.88	132.77	121.54
1	A	75	GLY	C-N-CA	5.88	132.77	121.54
1	C	75	GLY	CA-C-N	5.87	132.76	121.54
1	C	75	GLY	C-N-CA	5.87	132.76	121.54
1	B	683	SER	N-CA-C	5.74	119.81	112.12
1	D	683	SER	N-CA-C	5.71	119.78	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	ILE	CA-C-N	5.63	132.11	121.97
1	D	488	ILE	C-N-CA	5.63	132.11	121.97
1	C	777	PRO	N-CA-C	5.54	117.45	110.70
1	B	488	ILE	CA-C-N	5.52	131.90	121.97
1	B	488	ILE	C-N-CA	5.52	131.90	121.97
1	A	777	PRO	N-CA-C	5.50	117.41	110.70
1	B	159	LEU	CA-CB-CG	5.19	134.48	116.30
1	D	159	LEU	CA-CB-CG	5.19	134.47	116.30
1	D	96	GLY	CA-C-N	5.18	131.44	121.54
1	D	96	GLY	C-N-CA	5.18	131.44	121.54
1	B	96	GLY	CA-C-N	5.12	131.32	121.54
1	B	96	GLY	C-N-CA	5.12	131.32	121.54

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	ILE	Peptide
1	A	797	VAL	Peptide
1	A	820	TYR	Peptide
1	B	122	THR	Peptide
1	B	231	ARG	Peptide
1	B	271	GLU	Peptide
1	B	272	PRO	Peptide
1	B	681	TYR	Peptide
1	B	683	SER	Peptide
1	B	75	GLY	Peptide
1	C	488	ILE	Peptide
1	C	797	VAL	Peptide
1	C	820	TYR	Peptide
1	D	122	THR	Peptide
1	D	231	ARG	Peptide
1	D	271	GLU	Peptide
1	D	272	PRO	Peptide
1	D	681	TYR	Peptide
1	D	683	SER	Peptide
1	D	75	GLY	Peptide

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	5858	0	5916	59	0
1	B	6197	0	6215	64	0
1	C	5858	0	5916	63	0
1	D	6197	0	6215	68	0
2	A	47	0	44	2	0
2	B	47	0	44	2	0
2	C	47	0	44	1	0
2	D	47	0	44	2	0
3	A	54	0	82	2	0
3	B	41	0	53	3	0
3	C	54	0	82	2	0
3	D	41	0	53	3	0
4	A	63	0	77	1	0
4	B	63	0	75	1	0
4	C	63	0	77	0	0
4	D	63	0	75	1	0
All	All	24740	0	25012	224	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 (224) 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:53:LYS:N	1:A:58:THR:HG1	1.58	1.02
1:C:53:LYS:N	1:C:58:THR:HG1	1.60	1.00
1:A:625:SER:H	2:A:1001:PIO:H2	1.65	0.62
1:D:442:LYS:HZ1	2:D:1001:PIO:H3	1.65	0.62
1:B:440:TYR:HE2	3:B:1002:PCW:H32	1.65	0.61
1:B:27:HIS:HA	1:C:404:SER:HA	1.83	0.61
1:D:469:VAL:HG13	1:D:783:HIS:HB3	1.81	0.61
1:C:501:ARG:NH2	1:C:769:TYR:O	2.33	0.61
1:A:404:SER:HA	1:D:27:HIS:HA	1.83	0.60
1:D:440:TYR:HE2	3:D:1002:PCW:H32	1.65	0.60
1:B:469:VAL:HG13	1:B:783:HIS:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ARG:NH2	1:A:769:TYR:O	2.33	0.60
1:A:171:MET:HE1	1:A:183:ILE:HG23	1.83	0.60
1:C:171:MET:HE1	1:C:183:ILE:HG23	1.83	0.60
1:C:550:ASP:OD1	1:C:809:ARG:NH1	2.35	0.60
1:C:625:SER:H	2:C:1001:PIO:H2	1.66	0.60
1:D:501:ARG:NH2	1:D:772:ARG:O	2.35	0.59
1:A:529:VAL:HG23	1:A:530:PRO:HD3	1.84	0.59
1:D:568:TRP:NE1	1:D:622:GLU:OE2	2.35	0.59
1:A:734:LEU:HB3	1:B:634:MET:HE1	1.83	0.59
1:C:734:LEU:HB3	1:D:634:MET:HE1	1.83	0.59
1:B:568:TRP:NE1	1:B:622:GLU:OE2	2.35	0.59
1:B:201:ASP:HB3	1:B:204:VAL:HG22	1.84	0.59
1:A:550:ASP:OD1	1:A:809:ARG:NH1	2.35	0.58
1:B:219:ALA:O	1:B:221:HIS:ND1	2.36	0.58
1:B:501:ARG:NH2	1:B:772:ARG:O	2.35	0.58
1:D:201:ASP:HB3	1:D:204:VAL:HG22	1.84	0.58
1:D:219:ALA:O	1:D:221:HIS:ND1	2.36	0.58
1:C:529:VAL:HG23	1:C:530:PRO:HD3	1.84	0.58
1:D:45:LYS:HG3	1:D:46:ARG:HG3	1.85	0.57
1:A:352:MET:HE1	1:A:379:GLU:HB2	1.87	0.57
1:B:45:LYS:HG3	1:B:46:ARG:HG3	1.85	0.57
1:B:442:LYS:HZ1	2:B:1001:PIO:H3	1.69	0.57
1:C:61:GLU:OE2	1:D:492:ARG:NH2	2.38	0.56
1:A:72:LYS:HE2	1:A:78:ILE:HD12	1.87	0.56
1:C:72:LYS:HE2	1:C:78:ILE:HD12	1.87	0.56
1:B:26:LEU:HD12	1:C:404:SER:HB2	1.88	0.56
1:A:66:ASP:OD1	1:A:69:ARG:NH2	2.39	0.56
1:C:352:MET:HE1	1:C:379:GLU:HB2	1.87	0.56
1:A:61:GLU:OE2	1:B:492:ARG:NH2	2.39	0.56
1:C:169:ASN:H	1:C:172:MET:HB2	1.72	0.55
1:D:64:LEU:HD13	1:D:67:LYS:HD2	1.88	0.55
1:A:404:SER:HB2	1:D:26:LEU:HD12	1.88	0.55
1:B:64:LEU:HD13	1:B:67:LYS:HD2	1.88	0.55
1:C:500:TYR:HB3	3:C:1002:PCW:H19	1.88	0.55
1:A:169:ASN:H	1:A:172:MET:HB2	1.72	0.55
1:C:19:PRO:HB2	1:C:23:GLY:HA3	1.89	0.55
1:A:500:TYR:HB3	3:A:1002:PCW:H19	1.88	0.55
1:A:19:PRO:HB2	1:A:23:GLY:HA3	1.89	0.54
1:A:865:MET:HE2	1:B:865:MET:HE3	1.89	0.54
1:B:32:ARG:NH2	1:C:400:GLU:OE2	2.41	0.54
1:C:66:ASP:OD1	1:C:69:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:OE2	1:D:32:ARG:NH2	2.41	0.54
1:D:204:VAL:HG12	1:D:343:SER:HB3	1.90	0.54
1:B:204:VAL:HG12	1:B:343:SER:HB3	1.90	0.54
1:D:806:VAL:HG22	1:D:808:MET:H	1.73	0.54
1:C:23:GLY:HA2	1:C:27:HIS:HD2	1.74	0.53
1:C:457:ALA:HB1	3:C:1002:PCW:H211	1.89	0.53
1:A:457:ALA:HB1	3:A:1002:PCW:H211	1.89	0.53
1:B:806:VAL:HG22	1:B:808:MET:H	1.73	0.53
1:C:865:MET:HE2	1:D:865:MET:HE3	1.89	0.53
1:B:501:ARG:NH1	1:B:769:TYR:O	2.42	0.52
1:D:490:ASP:OD2	1:D:492:ARG:NE	2.40	0.52
1:B:90:ILE:HG13	1:B:119:MET:HG2	1.91	0.52
1:B:490:ASP:OD2	1:B:492:ARG:NE	2.39	0.52
1:D:501:ARG:NH1	1:D:769:TYR:O	2.42	0.52
1:A:23:GLY:HA2	1:A:27:HIS:HD2	1.74	0.52
1:A:168:LYS:NZ	1:B:439:ASP:OD2	2.43	0.52
1:A:851:ARG:HE	1:D:860:ASN:HD21	1.58	0.52
1:D:163:ARG:NH1	1:D:167:GLY:O	2.43	0.52
1:A:555:TYR:OH	1:A:560:ARG:NE	2.41	0.52
1:D:90:ILE:HG13	1:D:119:MET:HG2	1.91	0.52
1:B:416:LYS:NZ	1:B:757:GLU:OE2	2.38	0.51
1:B:513:THR:HG22	1:B:613:ALA:HB1	1.93	0.51
1:B:860:ASN:HD21	1:C:851:ARG:HE	1.58	0.51
1:C:168:LYS:NZ	1:D:439:ASP:OD2	2.43	0.51
1:D:513:THR:HG22	1:D:613:ALA:HB1	1.93	0.51
1:B:163:ARG:NH1	1:B:167:GLY:O	2.43	0.51
1:D:670:GLU:HB3	1:D:677:GLU:HB2	1.93	0.51
1:C:777:PRO:HA	1:C:780:ASN:HB2	1.93	0.51
1:C:534:ALA:HB3	1:C:537:ASN:H	1.76	0.51
1:A:534:ALA:HB3	1:A:537:ASN:H	1.76	0.50
1:B:670:GLU:HB3	1:B:677:GLU:HB2	1.93	0.50
1:C:534:ALA:H	1:C:538:THR:HG23	1.77	0.50
1:B:187:LEU:HD11	1:B:362:LEU:HD23	1.93	0.50
1:A:777:PRO:HA	1:A:780:ASN:HB2	1.93	0.50
1:C:555:TYR:OH	1:C:560:ARG:NE	2.41	0.50
1:C:513:THR:HG22	1:C:613:ALA:HB1	1.94	0.50
1:A:132:MET:O	1:A:136:TYR:N	2.39	0.49
1:A:534:ALA:H	1:A:538:THR:HG23	1.77	0.49
1:D:187:LEU:HD11	1:D:362:LEU:HD23	1.93	0.49
1:A:595:ASN:HD22	1:A:596:LEU:H	1.61	0.49
1:C:366:ARG:NH1	2:D:1001:PIO:O43	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:NH1	2:B:1001:PIO:O43	2.46	0.49
1:C:595:ASN:HD22	1:C:596:LEU:H	1.61	0.49
1:A:513:THR:HG22	1:A:613:ALA:HB1	1.94	0.48
1:B:666:GLU:HG2	1:B:681:TYR:H	1.78	0.48
1:C:53:LYS:N	1:C:58:THR:OG1	2.36	0.48
1:A:55:THR:HG23	1:A:58:THR:H	1.79	0.48
1:C:117:THR:HG22	1:C:155:PHE:HD1	1.79	0.48
1:C:132:MET:O	1:C:136:TYR:N	2.39	0.48
1:D:666:GLU:HG2	1:D:681:TYR:H	1.78	0.48
1:A:117:THR:HG22	1:A:155:PHE:HD1	1.79	0.47
1:A:188:VAL:HG21	1:A:214:LEU:HD22	1.96	0.47
1:B:668:CYS:HA	1:B:678:CYS:HA	1.97	0.47
1:D:633:MET:HE3	1:D:754:ALA:HA	1.96	0.47
1:A:633:MET:HE2	1:A:633:MET:HB3	1.82	0.47
1:B:506:GLN:HE21	1:B:620:VAL:HG12	1.80	0.47
1:D:103:GLN:NE2	1:D:224:ASP:OD1	2.48	0.47
1:A:737:ASN:HB3	1:B:637:MET:HE1	1.97	0.47
1:C:27:HIS:HA	1:D:404:SER:HA	1.97	0.47
1:A:426:GLN:HE21	1:D:179:HIS:HD2	1.63	0.47
1:C:55:THR:HG23	1:C:58:THR:H	1.79	0.47
1:D:188:VAL:HG21	1:D:214:LEU:HD12	1.97	0.47
1:A:667:ALA:HB3	1:B:599:LEU:HD21	1.98	0.46
1:B:103:GLN:NE2	1:B:224:ASP:OD1	2.48	0.46
1:B:633:MET:HE3	1:B:754:ALA:HA	1.96	0.46
1:A:395:ILE:HG22	1:A:834:GLN:HG3	1.97	0.46
1:B:188:VAL:HG21	1:B:214:LEU:HD12	1.97	0.46
1:C:667:ALA:HB3	1:D:599:LEU:HD21	1.98	0.46
1:A:124:CYS:SG	1:A:125:TRP:N	2.89	0.46
1:B:652:ILE:HA	1:C:615:PHE:HE1	1.81	0.46
1:C:82:ASP:OD1	1:C:82:ASP:N	2.49	0.46
1:B:179:HIS:HD2	1:C:426:GLN:HE21	1.63	0.46
1:A:27:HIS:HA	1:B:404:SER:HA	1.97	0.46
1:A:615:PHE:HE1	1:D:652:ILE:HA	1.81	0.46
1:D:668:CYS:HA	1:D:678:CYS:HA	1.97	0.46
1:C:188:VAL:HG21	1:C:214:LEU:HD22	1.96	0.46
1:C:737:ASN:HB3	1:D:637:MET:HE1	1.97	0.45
1:C:124:CYS:SG	1:C:125:TRP:N	2.89	0.45
1:A:727:PHE:HZ	4:B:1003:PIK:H26	1.82	0.45
1:B:494:PRO:HB3	1:B:500:TYR:HD2	1.82	0.45
1:D:150:ASP:OD2	1:D:189:ARG:NH2	2.49	0.45
1:D:506:GLN:HE21	1:D:620:VAL:HG12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:OD1	1:A:82:ASP:N	2.49	0.45
1:B:150:ASP:OD2	1:B:189:ARG:NH2	2.50	0.45
1:C:395:ILE:HG22	1:C:834:GLN:HG3	1.97	0.45
1:C:806:VAL:HG21	1:C:808:MET:HE2	1.98	0.45
1:C:117:THR:HG21	1:C:156:THR:HG22	1.99	0.45
1:A:806:VAL:HG21	1:A:808:MET:HE2	1.98	0.45
1:C:23:GLY:HA2	1:C:27:HIS:CD2	2.52	0.45
1:C:727:PHE:HZ	4:D:1003:PIK:H26	1.82	0.45
1:D:149:LEU:HD22	1:D:154:LYS:HG3	1.98	0.45
1:D:359:GLN:NE2	1:D:376:THR:OG1	2.50	0.45
1:A:117:THR:HG21	1:A:156:THR:HG22	1.99	0.44
1:A:596:LEU:HD13	1:A:597:ASN:H	1.82	0.44
1:B:149:LEU:HD22	1:B:154:LYS:HG3	1.98	0.44
1:D:327:LEU:HD12	1:D:328:LYS:HG2	1.98	0.44
1:D:494:PRO:HB3	1:D:500:TYR:HD2	1.82	0.44
1:B:327:LEU:HD12	1:B:328:LYS:HG2	1.98	0.44
1:B:359:GLN:NE2	1:B:376:THR:OG1	2.50	0.44
1:B:794:ARG:HA	1:B:798:TRP:HE3	1.83	0.44
1:C:137:GLN:HA	1:C:179:HIS:CE1	2.53	0.44
1:C:585:LEU:HD13	1:C:588:ILE:HD11	2.00	0.44
1:C:596:LEU:HD13	1:C:597:ASN:H	1.82	0.44
1:A:137:GLN:HA	1:A:179:HIS:CE1	2.53	0.43
1:B:457:ALA:O	1:B:461:TRP:N	2.50	0.43
1:B:716:LYS:HB2	1:C:600:LEU:HD12	2.00	0.43
1:D:119:MET:HE2	1:D:119:MET:HB3	1.89	0.43
1:B:46:ARG:HD2	1:C:488:ILE:HG22	2.01	0.43
1:C:78:ILE:O	1:C:89:SER:OG	2.35	0.43
1:B:335:ARG:HH12	1:B:853:LYS:HB2	1.84	0.43
1:B:854:LEU:HD22	1:D:858:LEU:HD21	2.00	0.43
1:D:335:ARG:HH12	1:D:853:LYS:HB2	1.83	0.43
1:B:94:CYS:HB2	1:B:134:ALA:HB2	2.01	0.43
1:D:416:LYS:NZ	1:D:757:GLU:OE2	2.39	0.43
1:C:143:MET:HE1	1:C:160:PHE:HE1	1.83	0.43
1:A:585:LEU:HD13	1:A:588:ILE:HD11	2.00	0.43
1:A:600:LEU:HD12	1:D:716:LYS:HB2	2.00	0.43
4:A:1003:PIK:H59	4:A:1003:PIK:H53	1.79	0.43
1:C:475:LEU:HD22	1:C:475:LEU:HA	1.86	0.43
1:D:794:ARG:HA	1:D:798:TRP:HE3	1.84	0.43
1:D:233:PHE:HD1	1:D:233:PHE:HA	1.70	0.43
1:A:23:GLY:HA2	1:A:27:HIS:CD2	2.52	0.42
1:C:87:TYR:HE2	3:D:1002:PCW:H63	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:HE2	3:B:1002:PCW:H63	1.84	0.42
1:B:55:THR:O	1:B:55:THR:OG1	2.37	0.42
1:B:554:GLU:OE2	1:B:569:ASN:ND2	2.52	0.42
1:C:594:ASP:OD1	1:C:594:ASP:N	2.51	0.42
1:D:554:GLU:OE2	1:D:569:ASN:ND2	2.52	0.42
1:A:488:ILE:HG22	1:D:46:ARG:HD2	2.01	0.42
3:B:1002:PCW:H381	3:B:1002:PCW:H412	1.88	0.42
1:B:168:LYS:NZ	1:C:439:ASP:OD2	2.47	0.42
1:B:432:TRP:CD1	1:B:498:PRO:HB2	2.55	0.42
1:D:637:MET:HE3	1:D:746:THR:HG21	2.02	0.42
1:A:143:MET:HE1	1:A:160:PHE:HE1	1.84	0.42
1:D:94:CYS:HB2	1:D:134:ALA:HB2	2.01	0.42
1:D:41:ASP:N	1:D:41:ASP:OD1	2.53	0.42
1:D:490:ASP:OD1	1:D:490:ASP:N	2.50	0.42
1:A:53:LYS:N	1:A:58:THR:OG1	2.36	0.41
1:D:402:ASP:OD1	1:D:402:ASP:N	2.51	0.41
1:D:432:TRP:CD1	1:D:498:PRO:HB2	2.55	0.41
1:B:119:MET:HE2	1:B:119:MET:HB3	1.89	0.41
1:D:457:ALA:O	1:D:461:TRP:N	2.50	0.41
1:A:752:THR:HG23	1:A:753:GLN:HG2	2.02	0.41
1:B:41:ASP:OD1	1:B:41:ASP:N	2.53	0.41
1:C:473:SER:HA	1:C:805:PRO:HG2	2.03	0.41
1:D:163:ARG:HD3	1:D:169:ASN:HB3	2.02	0.41
1:B:858:LEU:HD21	1:D:854:LEU:HD22	2.02	0.41
1:A:175:ALA:HA	1:A:183:ILE:HD11	2.03	0.41
1:C:768:SER:OG	1:C:810:LYS:NZ	2.54	0.41
1:B:55:THR:HG23	1:B:57:ILE:HG22	2.03	0.41
1:B:163:ARG:HD3	1:B:169:ASN:HB3	2.02	0.41
1:B:432:TRP:CH2	1:B:499:LEU:HD13	2.56	0.41
1:C:809:ARG:H	1:C:809:ARG:HG3	1.68	0.41
1:C:867:LYS:HB3	1:C:867:LYS:HE2	1.87	0.41
1:A:473:SER:HA	1:A:805:PRO:HG2	2.02	0.41
1:D:617:MET:HE2	1:D:617:MET:HB3	1.88	0.40
1:A:594:ASP:OD1	1:A:594:ASP:N	2.51	0.40
1:B:637:MET:HE3	1:B:746:THR:HG21	2.02	0.40
1:B:166:MET:HE3	1:B:166:MET:HB2	1.90	0.40
1:C:94:CYS:SG	1:C:130:SER:OG	2.68	0.40
1:D:183:ILE:HD13	1:D:183:ILE:HG21	1.92	0.40
1:D:557:GLU:OE2	1:D:809:ARG:N	2.54	0.40
3:D:1002:PCW:H41	3:D:1002:PCW:H73	1.91	0.40
1:C:644:ARG:HD2	1:D:626:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:PHE:HD1	1:D:371:LEU:HD12	1.87	0.40
1:D:497:VAL:HA	1:D:498:PRO:HD3	1.89	0.40
1:A:768:SER:OG	1:A:810:LYS:NZ	2.54	0.40
2:A:1001:PIO:H2AA	2:A:1001:PIO:H5A	1.91	0.40
1:B:557:GLU:OE2	1:B:809:ARG:N	2.54	0.40
1:B:561:ALA:O	1:B:565:SER:OG	2.36	0.40
1:D:166:MET:HE3	1:D:166:MET:HB2	1.90	0.40
1:D:226:ASP:N	1:D:226:ASP:OD1	2.53	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	726/901 (81%)	645 (89%)	79 (11%)	2 (0%)	36	67
1	B	776/901 (86%)	671 (86%)	95 (12%)	10 (1%)	9	39
1	C	726/901 (81%)	644 (89%)	80 (11%)	2 (0%)	36	67
1	D	776/901 (86%)	672 (87%)	95 (12%)	9 (1%)	10	41
All	All	3004/3604 (83%)	2632 (88%)	349 (12%)	23 (1%)	18	49

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	THR
1	D	273	THR
1	B	220	SER
1	B	488	ILE
1	D	220	SER
1	D	488	ILE
1	A	673	PRO

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Mol	Chain	Res	Type
1	B	123	ARG
1	B	673	PRO
1	C	673	PRO
1	D	123	ARG
1	D	673	PRO
1	A	798	TRP
1	B	113	THR
1	C	798	TRP
1	D	113	THR
1	B	224	ASP
1	B	232	SER
1	D	224	ASP
1	D	232	SER
1	B	434	THR
1	B	272	PRO
1	D	272	PRO

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	638/740 (86%)	627 (98%)	11 (2%)	53	70
1	B	669/740 (90%)	659 (98%)	10 (2%)	57	72
1	C	638/740 (86%)	627 (98%)	11 (2%)	53	70
1	D	669/740 (90%)	659 (98%)	10 (2%)	57	72
All	All	2614/2960 (88%)	2572 (98%)	42 (2%)	54	71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	87	TYR
1	A	383	LEU
1	A	419	LEU
1	A	475	LEU

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Mol	Chain	Res	Type
1	A	488	ILE
1	A	529	VAL
1	A	596	LEU
1	A	630	LEU
1	A	814	VAL
1	A	858	LEU
1	B	26	LEU
1	B	101	ILE
1	B	189	ARG
1	B	233	PHE
1	B	504	LEU
1	B	581	LEU
1	B	591	ARG
1	B	733	ILE
1	B	820	TYR
1	B	854	LEU
1	C	71	LEU
1	C	87	TYR
1	C	383	LEU
1	C	419	LEU
1	C	475	LEU
1	C	488	ILE
1	C	529	VAL
1	C	596	LEU
1	C	630	LEU
1	C	814	VAL
1	C	858	LEU
1	D	26	LEU
1	D	101	ILE
1	D	189	ARG
1	D	233	PHE
1	D	504	LEU
1	D	581	LEU
1	D	591	ARG
1	D	733	ILE
1	D	820	TYR
1	D	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	97	ASN
1	A	179	HIS
1	A	331	HIS
1	A	338	GLN
1	A	374	GLN
1	A	426	GLN
1	A	595	ASN
1	A	855	ASN
1	A	868	GLN
1	B	103	GLN
1	B	177	GLN
1	B	179	HIS
1	B	359	GLN
1	B	374	GLN
1	B	479	GLN
1	B	506	GLN
1	B	843	ASN
1	B	860	ASN
1	C	27	HIS
1	C	86	HIS
1	C	97	ASN
1	C	179	HIS
1	C	331	HIS
1	C	338	GLN
1	C	374	GLN
1	C	595	ASN
1	C	632	GLN
1	C	737	ASN
1	C	855	ASN
1	C	868	GLN
1	D	103	GLN
1	D	177	GLN
1	D	359	GLN
1	D	374	GLN
1	D	479	GLN
1	D	506	GLN
1	D	843	ASN
1	D	860	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
3	PCW	A	1002	-	53,53,53	1.00	6 (11%)	59,61,61	1.22	6 (10%)
3	PCW	B	1002	-	40,40,53	1.18	5 (12%)	46,48,61	1.04	2 (4%)
2	PIO	C	1001	-	47,47,47	1.22	6 (12%)	62,65,65	1.23	6 (9%)
3	PCW	C	1002	-	53,53,53	1.00	6 (11%)	59,61,61	1.22	6 (10%)
3	PCW	D	1002	-	40,40,53	1.18	5 (12%)	46,48,61	1.04	2 (4%)
4	PIK	C	1003	-	63,63,63	1.06	5 (7%)	78,81,81	1.05	5 (6%)
4	PIK	D	1003	-	63,63,63	1.08	6 (9%)	78,81,81	1.09	4 (5%)
2	PIO	D	1001	-	47,47,47	1.23	5 (10%)	62,65,65	1.16	4 (6%)
2	PIO	A	1001	-	47,47,47	1.21	6 (12%)	62,65,65	1.23	6 (9%)
4	PIK	A	1003	-	63,63,63	1.06	5 (7%)	78,81,81	1.04	5 (6%)
2	PIO	B	1001	-	47,47,47	1.22	5 (10%)	62,65,65	1.16	4 (6%)
4	PIK	B	1003	-	63,63,63	1.09	6 (9%)	78,81,81	1.09	4 (5%)

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
3	PCW	A	1002	-	-	28/57/57/57	-
3	PCW	B	1002	-	-	21/44/44/57	-
2	PIO	C	1001	-	-	16/44/68/68	0/1/1/1
3	PCW	C	1002	-	-	28/57/57/57	-
3	PCW	D	1002	-	-	21/44/44/57	-
4	PIK	C	1003	-	-	24/60/84/84	0/1/1/1
4	PIK	D	1003	-	-	27/60/84/84	0/1/1/1
2	PIO	D	1001	-	-	17/44/68/68	0/1/1/1
2	PIO	A	1001	-	-	16/44/68/68	0/1/1/1
4	PIK	A	1003	-	-	21/60/84/84	0/1/1/1
2	PIO	B	1001	-	-	17/44/68/68	0/1/1/1
4	PIK	B	1003	-	-	27/60/84/84	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	PIO	P4-O4	3.54	1.65	1.59
2	D	1001	PIO	P4-O4	3.54	1.65	1.59
4	B	1003	PIK	P4-O4	3.42	1.65	1.59
4	A	1003	PIK	P5-O5	3.37	1.65	1.59
4	D	1003	PIK	P4-O4	3.36	1.65	1.59
4	C	1003	PIK	P5-O5	3.34	1.65	1.59
4	D	1003	PIK	P5-O5	3.28	1.65	1.59
4	B	1003	PIK	P5-O5	3.26	1.65	1.59
2	C	1001	PIO	P4-O4	3.19	1.65	1.59
2	A	1001	PIO	P4-O4	3.15	1.65	1.59
2	B	1001	PIO	P5-O5	3.07	1.64	1.59
4	C	1003	PIK	P4-O4	3.06	1.64	1.59
2	D	1001	PIO	P5-O5	3.03	1.64	1.59
4	A	1003	PIK	P4-O4	3.01	1.64	1.59
3	D	1002	PCW	O2-C2	-3.00	1.39	1.46
3	B	1002	PCW	O2-C2	-2.98	1.39	1.46
2	C	1001	PIO	P5-O5	2.92	1.64	1.59
2	A	1001	PIO	P5-O5	2.90	1.64	1.59
4	D	1003	PIK	OB1-C8	-2.77	1.40	1.46
4	B	1003	PIK	OB1-C8	-2.76	1.40	1.46
2	B	1001	PIO	O2C-C2C	-2.66	1.40	1.46
2	D	1001	PIO	O2C-C2C	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	PIK	OB1-C8	-2.63	1.40	1.46
4	A	1003	PIK	OB1-C8	-2.62	1.40	1.46
2	C	1001	PIO	O3C-C3C	-2.60	1.39	1.45
2	A	1001	PIO	O3C-C3C	-2.60	1.39	1.45
4	B	1003	PIK	P1-O1	2.50	1.66	1.59
2	A	1001	PIO	O2C-C2C	-2.49	1.40	1.46
2	C	1001	PIO	O2C-C2C	-2.49	1.40	1.46
4	D	1003	PIK	P1-O1	2.47	1.66	1.59
4	C	1003	PIK	OA1-CA1	2.47	1.40	1.33
2	C	1001	PIO	O2C-C1A	2.46	1.41	1.34
4	A	1003	PIK	OA1-CA1	2.45	1.40	1.33
3	A	1002	PCW	O3-C3	-2.45	1.39	1.45
2	B	1001	PIO	O3C-C3C	-2.44	1.39	1.45
2	D	1001	PIO	O3C-C3C	-2.44	1.39	1.45
3	C	1002	PCW	O3-C3	-2.43	1.39	1.45
2	A	1001	PIO	O2C-C1A	2.43	1.41	1.34
4	B	1003	PIK	OA1-CA1	2.42	1.40	1.33
4	D	1003	PIK	OA1-CA1	2.42	1.40	1.33
3	B	1002	PCW	O3-C11	2.38	1.40	1.33
4	A	1003	PIK	OB1-CB1	2.35	1.40	1.34
4	C	1003	PIK	OB1-CB1	2.35	1.40	1.34
3	D	1002	PCW	O3-C11	2.34	1.40	1.33
3	C	1002	PCW	C5-N	-2.32	1.44	1.51
3	B	1002	PCW	C5-N	-2.30	1.44	1.51
3	D	1002	PCW	C5-N	-2.29	1.44	1.51
3	A	1002	PCW	C5-N	-2.28	1.44	1.51
3	D	1002	PCW	O3-C3	-2.28	1.40	1.45
3	C	1002	PCW	C6-N	-2.28	1.43	1.50
2	D	1001	PIO	O2C-C1A	2.28	1.40	1.34
3	B	1002	PCW	O3-C3	-2.27	1.40	1.45
3	A	1002	PCW	C6-N	-2.26	1.43	1.50
2	B	1001	PIO	O2C-C1A	2.24	1.40	1.34
3	D	1002	PCW	C6-N	-2.21	1.43	1.50
2	A	1001	PIO	O3C-C1B	2.19	1.39	1.33
2	C	1001	PIO	O3C-C1B	2.19	1.39	1.33
3	C	1002	PCW	O3-C11	2.18	1.39	1.33
3	B	1002	PCW	C6-N	-2.18	1.43	1.50
3	A	1002	PCW	O3-C11	2.16	1.39	1.33
3	A	1002	PCW	O2-C2	-2.14	1.41	1.46
3	C	1002	PCW	O2-C2	-2.14	1.41	1.46
3	A	1002	PCW	O2-C31	2.11	1.40	1.34
3	C	1002	PCW	O2-C31	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	PIK	OB1-CB1	2.07	1.40	1.34
4	D	1003	PIK	OB1-CB1	2.07	1.40	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PIO	O2C-C1A-C2A	4.88	122.03	111.48
2	D	1001	PIO	O2C-C1A-C2A	4.88	122.03	111.48
2	A	1001	PIO	O2C-C1A-C2A	4.11	120.38	111.48
2	C	1001	PIO	O2C-C1A-C2A	4.11	120.37	111.48
3	D	1002	PCW	O2-C31-C32	4.03	120.19	111.48
3	B	1002	PCW	O2-C31-C32	4.03	120.19	111.48
4	D	1003	PIK	OB1-CB1-CB2	3.85	119.81	111.48
4	B	1003	PIK	OB1-CB1-CB2	3.84	119.78	111.48
4	C	1003	PIK	OB1-CB1-CB2	3.38	118.80	111.48
4	A	1003	PIK	OB1-CB1-CB2	3.37	118.77	111.48
3	A	1002	PCW	O3-C3-C2	3.31	117.95	108.40
3	C	1002	PCW	O3-C3-C2	3.30	117.92	108.40
2	C	1001	PIO	O3C-C1B-C2B	3.25	121.76	111.83
2	A	1001	PIO	O3C-C1B-C2B	3.25	121.74	111.83
3	C	1002	PCW	C2-O2-C31	3.20	125.44	117.80
3	A	1002	PCW	C2-O2-C31	3.19	125.43	117.80
3	A	1002	PCW	O2-C31-C32	3.17	118.33	111.48
3	C	1002	PCW	O2-C31-C32	3.14	118.28	111.48
4	D	1003	PIK	OA1-CA1-CA2	3.08	121.22	111.83
2	A	1001	PIO	C3-C2-C1	3.07	116.66	109.68
2	C	1001	PIO	C3-C2-C1	3.06	116.63	109.68
4	B	1003	PIK	OA1-CA1-CA2	3.06	121.16	111.83
2	C	1001	PIO	C2-C3-C4	3.05	116.60	109.68
2	A	1001	PIO	C2-C3-C4	3.03	116.57	109.68
4	C	1003	PIK	OA1-CA1-CA2	2.85	120.53	111.83
4	A	1003	PIK	OA1-CA1-CA2	2.84	120.49	111.83
2	B	1001	PIO	O3C-C1B-C2B	2.81	120.39	111.83
2	D	1001	PIO	O3C-C1B-C2B	2.78	120.31	111.83
3	B	1002	PCW	O3-C11-C12	2.73	120.17	111.83
3	D	1002	PCW	O3-C11-C12	2.73	120.16	111.83
3	C	1002	PCW	C33-C32-C31	-2.72	103.73	113.69
3	A	1002	PCW	C33-C32-C31	-2.72	103.73	113.69
4	A	1003	PIK	O1-C1-C6	2.68	114.40	108.73
3	C	1002	PCW	O3-C11-C12	2.66	119.94	111.83
3	A	1002	PCW	O3-C11-C12	2.64	119.89	111.83
2	B	1001	PIO	P5-O5-C5	-2.60	116.50	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	PIO	P5-O5-C5	-2.59	116.52	123.43
4	A	1003	PIK	C9-C8-C7	-2.46	106.06	111.78
4	C	1003	PIK	O1-C1-C6	2.43	113.87	108.73
4	D	1003	PIK	P4-O4-C4	-2.40	117.02	123.43
4	B	1003	PIK	P4-O4-C4	-2.40	117.03	123.43
4	C	1003	PIK	C9-C8-C7	-2.39	106.21	111.78
3	A	1002	PCW	O2-C2-C3	2.36	116.82	108.34
3	C	1002	PCW	O2-C2-C3	2.36	116.80	108.34
4	D	1003	PIK	P5-O5-C5	-2.35	117.17	123.43
4	B	1003	PIK	P5-O5-C5	-2.33	117.20	123.43
2	D	1001	PIO	O2C-C1A-O1A	-2.20	118.57	123.70
2	B	1001	PIO	O2C-C1A-O1A	-2.18	118.60	123.70
4	C	1003	PIK	C6-C1-C2	2.14	113.84	110.86
2	C	1001	PIO	C6-C1-C2	2.14	113.82	110.86
2	A	1001	PIO	C6-C1-C2	2.12	113.81	110.86
2	A	1001	PIO	C3C-C2C-C1C	-2.08	106.94	111.78
2	C	1001	PIO	C3C-C2C-C1C	-2.08	106.95	111.78
4	A	1003	PIK	P4-O4-C4	-2.03	118.00	123.43

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PIO	C1-O1-P1-O13
2	A	1001	PIO	C1C-O13-P1-O1
2	A	1001	PIO	C1C-O13-P1-O11
2	A	1001	PIO	C1C-O13-P1-O12
2	A	1001	PIO	C2A-C1A-O2C-C2C
2	B	1001	PIO	C2-C1-O1-P1
2	B	1001	PIO	C6-C1-O1-P1
2	B	1001	PIO	C1C-O13-P1-O1
2	B	1001	PIO	O1A-C1A-O2C-C2C
2	B	1001	PIO	C2A-C1A-O2C-C2C
2	C	1001	PIO	C1-O1-P1-O13
2	C	1001	PIO	C1C-O13-P1-O1
2	C	1001	PIO	C1C-O13-P1-O11
2	C	1001	PIO	C1C-O13-P1-O12
2	C	1001	PIO	C2A-C1A-O2C-C2C
2	D	1001	PIO	C2-C1-O1-P1
2	D	1001	PIO	C6-C1-O1-P1
2	D	1001	PIO	C1C-O13-P1-O1
2	D	1001	PIO	O1A-C1A-O2C-C2C

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Mol	Chain	Res	Type	Atoms
2	D	1001	PIO	C2A-C1A-O2C-C2C
3	A	1002	PCW	O4P-C4-C5-N
3	A	1002	PCW	C1-O3P-P-O2P
3	A	1002	PCW	C1-O3P-P-O4P
3	B	1002	PCW	O4P-C4-C5-N
3	B	1002	PCW	C4O-C41-C42-C43
3	B	1002	PCW	C1-O3P-P-O4P
3	B	1002	PCW	C4-O4P-P-O1P
3	B	1002	PCW	C4-O4P-P-O2P
3	B	1002	PCW	C4-O4P-P-O3P
3	C	1002	PCW	O4P-C4-C5-N
3	C	1002	PCW	C1-O3P-P-O2P
3	C	1002	PCW	C1-O3P-P-O4P
3	D	1002	PCW	O4P-C4-C5-N
3	D	1002	PCW	C4O-C41-C42-C43
3	D	1002	PCW	C1-O3P-P-O4P
3	D	1002	PCW	C4-O4P-P-O1P
3	D	1002	PCW	C4-O4P-P-O2P
3	D	1002	PCW	C4-O4P-P-O3P
4	A	1003	PIK	C6-C1-O1-P1
4	A	1003	PIK	CA2-CA1-OA1-C9
4	B	1003	PIK	C7-O13-P1-O12
4	B	1003	PIK	C7-O13-P1-O1
4	B	1003	PIK	C8-C7-O13-P1
4	C	1003	PIK	C6-C1-O1-P1
4	C	1003	PIK	CA2-CA1-OA1-C9
4	D	1003	PIK	C7-O13-P1-O12
4	D	1003	PIK	C7-O13-P1-O1
4	D	1003	PIK	C8-C7-O13-P1
4	A	1003	PIK	OA2-CA1-OA1-C9
4	C	1003	PIK	OA2-CA1-OA1-C9
3	B	1002	PCW	C12-C11-O3-C3
3	D	1002	PCW	C12-C11-O3-C3
2	A	1001	PIO	O1A-C1A-O2C-C2C
2	C	1001	PIO	O1A-C1A-O2C-C2C
3	B	1002	PCW	O11-C11-O3-C3
3	D	1002	PCW	O11-C11-O3-C3
2	A	1001	PIO	C2C-C1C-O13-P1
2	C	1001	PIO	C2C-C1C-O13-P1
2	B	1001	PIO	C2B-C1B-O3C-C3C
2	D	1001	PIO	C2B-C1B-O3C-C3C
2	B	1001	PIO	O1B-C1B-O3C-C3C

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Mol	Chain	Res	Type	Atoms
2	D	1001	PIO	O1B-C1B-O3C-C3C
4	B	1003	PIK	CA2-CA1-OA1-C9
4	D	1003	PIK	CA2-CA1-OA1-C9
4	C	1003	PIK	CB1-CB2-CB3-CB4
4	A	1003	PIK	CB1-CB2-CB3-CB4
3	A	1002	PCW	C11-C12-C13-C14
3	C	1002	PCW	C11-C12-C13-C14
4	B	1003	PIK	OA2-CA1-OA1-C9
4	D	1003	PIK	OA2-CA1-OA1-C9
2	A	1001	PIO	C1B-C2B-C3B-C4B
2	C	1001	PIO	C1B-C2B-C3B-C4B
2	B	1001	PIO	C1A-C2A-C3A-C4A
2	D	1001	PIO	C1A-C2A-C3A-C4A
2	A	1001	PIO	C2B-C1B-O3C-C3C
2	C	1001	PIO	C2B-C1B-O3C-C3C
4	B	1003	PIK	CB1-CB2-CB3-CB4
4	D	1003	PIK	CB1-CB2-CB3-CB4
3	A	1002	PCW	C12-C13-C14-C15
3	C	1002	PCW	C12-C13-C14-C15
4	C	1003	PIK	CB6-CB7-CB8-CB9
3	B	1002	PCW	C12-C13-C14-C15
3	D	1002	PCW	C12-C13-C14-C15
4	A	1003	PIK	CB6-CB7-CB8-CB9
3	C	1002	PCW	C33-C34-C35-C36
3	A	1002	PCW	C33-C34-C35-C36
4	B	1003	PIK	CB2-CB3-CB4-CB5
4	D	1003	PIK	CB2-CB3-CB4-CB5
4	A	1003	PIK	CA5-CA6-CA7-CA8
4	B	1003	PIK	CB6-CB7-CB8-CB9
4	D	1003	PIK	CB6-CB7-CB8-CB9
2	A	1001	PIO	O1B-C1B-O3C-C3C
2	C	1001	PIO	O1B-C1B-O3C-C3C
3	B	1002	PCW	C13-C14-C15-C16
3	D	1002	PCW	C13-C14-C15-C16
3	A	1002	PCW	C12-C11-O3-C3
3	C	1002	PCW	C12-C11-O3-C3
3	B	1002	PCW	C32-C33-C34-C35
3	D	1002	PCW	C32-C33-C34-C35
4	C	1003	PIK	CB7-CB8-CB9-CBA
4	C	1003	PIK	CA5-CA6-CA7-CA8
3	A	1002	PCW	C34-C35-C36-C37
3	C	1002	PCW	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
4	B	1003	PIK	CA2-CA3-CA4-CA5
4	D	1003	PIK	CA2-CA3-CA4-CA5
4	D	1003	PIK	CA5-CA6-CA7-CA8
4	B	1003	PIK	CA5-CA6-CA7-CA8
2	A	1001	PIO	C3B-C4B-C5B-C6B
2	C	1001	PIO	C3B-C4B-C5B-C6B
3	A	1002	PCW	C32-C33-C34-C35
3	C	1002	PCW	C32-C33-C34-C35
4	B	1003	PIK	CB8-CB9-CBA-CBB
4	D	1003	PIK	CB8-CB9-CBA-CBB
4	A	1003	PIK	CB2-CB1-OB1-C8
4	C	1003	PIK	CB2-CB1-OB1-C8
4	C	1003	PIK	CB4-CB5-CB6-CB7
4	A	1003	PIK	OB2-CB1-OB1-C8
3	A	1002	PCW	C31-C32-C33-C34
3	C	1002	PCW	C31-C32-C33-C34
4	B	1003	PIK	CA1-CA2-CA3-CA4
4	D	1003	PIK	CA1-CA2-CA3-CA4
4	C	1003	PIK	OB2-CB1-OB1-C8
3	B	1002	PCW	O3P-C1-C2-O2
3	D	1002	PCW	O3P-C1-C2-O2
3	A	1002	PCW	O11-C11-O3-C3
3	C	1002	PCW	O11-C11-O3-C3
4	B	1003	PIK	CB3-CB4-CB5-CB6
4	D	1003	PIK	CB3-CB4-CB5-CB6
4	A	1003	PIK	CB4-CB5-CB6-CB7
3	B	1002	PCW	C31-C32-C33-C34
3	D	1002	PCW	C31-C32-C33-C34
4	A	1003	PIK	CA1-CA2-CA3-CA4
4	B	1003	PIK	CBA-CBB-CBC-CBD
4	D	1003	PIK	CBA-CBB-CBC-CBD
2	D	1001	PIO	C3A-C4A-C5A-C6A
4	A	1003	PIK	CB7-CB8-CB9-CBA
2	B	1001	PIO	C3A-C4A-C5A-C6A
4	A	1003	PIK	CB5-CB6-CB7-CB8
3	D	1002	PCW	C34-C35-C36-C37
2	D	1001	PIO	C3B-C4B-C5B-C6B
3	B	1002	PCW	C34-C35-C36-C37
2	B	1001	PIO	C3B-C4B-C5B-C6B
4	B	1003	PIK	CBB-CBC-CBD-CBE
4	D	1003	PIK	CBB-CBC-CBD-CBE
4	B	1003	PIK	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
4	D	1003	PIK	CA4-CA5-CA6-CA7
3	A	1002	PCW	C20-C21-C22-C23
3	C	1002	PCW	C20-C21-C22-C23
4	C	1003	PIK	CB5-CB6-CB7-CB8
3	B	1002	PCW	O3P-C1-C2-C3
3	D	1002	PCW	O3P-C1-C2-C3
4	A	1003	PIK	O13-C7-C8-C9
4	C	1003	PIK	O13-C7-C8-C9
4	D	1003	PIK	O13-C7-C8-C9
4	B	1003	PIK	CBC-CBD-CBE-CBF
4	D	1003	PIK	CBC-CBD-CBE-CBF
3	B	1002	PCW	C33-C34-C35-C36
3	A	1002	PCW	C1-C2-C3-O3
3	C	1002	PCW	C1-C2-C3-O3
3	B	1002	PCW	C35-C36-C37-C38
3	D	1002	PCW	C33-C34-C35-C36
3	D	1002	PCW	C35-C36-C37-C38
3	A	1002	PCW	C36-C37-C38-C39
3	C	1002	PCW	C36-C37-C38-C39
3	A	1002	PCW	O2-C2-C3-O3
3	C	1002	PCW	O2-C2-C3-O3
4	B	1003	PIK	O13-C7-C8-C9
4	C	1003	PIK	CA1-CA2-CA3-CA4
3	A	1002	PCW	C23-C24-C25-C26
3	C	1002	PCW	C23-C24-C25-C26
4	A	1003	PIK	O13-C7-C8-OB1
4	C	1003	PIK	O13-C7-C8-OB1
2	B	1001	PIO	C1-O1-P1-O12
2	D	1001	PIO	C1-O1-P1-O12
4	A	1003	PIK	CA7-CA8-CA9-CAA
4	B	1003	PIK	CA8-CA9-CAA-CAB
4	D	1003	PIK	CA8-CA9-CAA-CAB
4	B	1003	PIK	O13-C7-C8-OB1
4	D	1003	PIK	O13-C7-C8-OB1
4	B	1003	PIK	CAB-CAC-CAD-CAE
4	D	1003	PIK	CAB-CAC-CAD-CAE
4	C	1003	PIK	CAB-CAC-CAD-CAE
2	B	1001	PIO	C1C-O13-P1-O12
2	D	1001	PIO	C1C-O13-P1-O12
3	A	1002	PCW	C4-O4P-P-O1P
3	A	1002	PCW	C4-O4P-P-O2P
3	A	1002	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	B	1002	PCW	C1-O3P-P-O2P
3	C	1002	PCW	C4-O4P-P-O1P
3	C	1002	PCW	C4-O4P-P-O2P
3	C	1002	PCW	C4-O4P-P-O3P
3	D	1002	PCW	C1-O3P-P-O2P
4	B	1003	PIK	C7-O13-P1-O11
4	D	1003	PIK	C7-O13-P1-O11
4	B	1003	PIK	OA1-CA1-CA2-CA3
4	D	1003	PIK	OA1-CA1-CA2-CA3
4	A	1003	PIK	CB8-CB9-CBA-CBB
4	A	1003	PIK	CA3-CA4-CA5-CA6
4	C	1003	PIK	CA9-CAA-CAB-CAC
4	C	1003	PIK	CBB-CBC-CBD-CBE
4	C	1003	PIK	CB8-CB9-CBA-CBB
4	B	1003	PIK	C2-C1-O1-P1
4	D	1003	PIK	C2-C1-O1-P1
4	C	1003	PIK	CBA-CBB-CBC-CBD
3	A	1002	PCW	C44-C45-C46-C47
3	C	1002	PCW	C44-C45-C46-C47
3	C	1002	PCW	C43-C44-C45-C46
3	A	1002	PCW	C43-C44-C45-C46
2	A	1001	PIO	C4-O4-P4-O42
2	C	1001	PIO	C4-O4-P4-O42
4	C	1003	PIK	CA3-CA4-CA5-CA6
4	A	1003	PIK	CBA-CBB-CBC-CBD
2	D	1001	PIO	C1B-C2B-C3B-C4B
3	A	1002	PCW	C14-C15-C16-C17
3	C	1002	PCW	C14-C15-C16-C17
2	B	1001	PIO	C1B-C2B-C3B-C4B
4	A	1003	PIK	CB9-CBA-CBB-CBC
2	B	1001	PIO	C4B-C5B-C6B-C7B
2	D	1001	PIO	C4B-C5B-C6B-C7B
3	A	1002	PCW	C39-C40-C41-C42
3	C	1002	PCW	C39-C40-C41-C42
3	C	1002	PCW	C16-C17-C18-C19
3	A	1002	PCW	C16-C17-C18-C19
2	B	1001	PIO	O3C-C1B-C2B-C3B
3	B	1002	PCW	O31-C31-O2-C2
3	D	1002	PCW	O31-C31-O2-C2
4	C	1003	PIK	CBC-CBD-CBE-CBF
2	D	1001	PIO	O3C-C1B-C2B-C3B
2	A	1001	PIO	C1-O1-P1-O11

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Mol	Chain	Res	Type	Atoms
2	A	1001	PIO	C1-O1-P1-O12
2	C	1001	PIO	C1-O1-P1-O11
2	C	1001	PIO	C1-O1-P1-O12
4	A	1003	PIK	C1-O1-P1-O12
4	C	1003	PIK	C1-O1-P1-O12
4	C	1003	PIK	CA7-CA8-CA9-CAA
2	A	1001	PIO	O2C-C1A-C2A-C3A
2	C	1001	PIO	O2C-C1A-C2A-C3A
3	A	1002	PCW	O2-C31-C32-C33
3	C	1002	PCW	O2-C31-C32-C33
4	B	1003	PIK	C4-O4-P4-O43
4	D	1003	PIK	C4-O4-P4-O43
2	D	1001	PIO	O2C-C1A-C2A-C3A
2	B	1001	PIO	O2C-C1A-C2A-C3A
3	B	1002	PCW	C15-C16-C17-C18
3	D	1002	PCW	C15-C16-C17-C18
4	A	1003	PIK	CBC-CBD-CBE-CBF
2	B	1001	PIO	O1A-C1A-C2A-C3A
2	D	1001	PIO	O1A-C1A-C2A-C3A
4	B	1003	PIK	CA3-CA4-CA5-CA6
4	D	1003	PIK	CA3-CA4-CA5-CA6
2	A	1001	PIO	O1A-C1A-C2A-C3A
3	A	1002	PCW	O31-C31-C32-C33
3	C	1002	PCW	O31-C31-C32-C33
3	A	1002	PCW	C22-C23-C24-C25
2	C	1001	PIO	O1A-C1A-C2A-C3A
3	A	1002	PCW	C40-C41-C42-C43
3	C	1002	PCW	C22-C23-C24-C25
4	B	1003	PIK	OB1-CB1-CB2-CB3
4	D	1003	PIK	OB1-CB1-CB2-CB3
3	B	1002	PCW	C32-C31-O2-C2
3	D	1002	PCW	C32-C31-O2-C2
3	C	1002	PCW	C40-C41-C42-C43
4	C	1003	PIK	OA1-CA1-CA2-CA3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

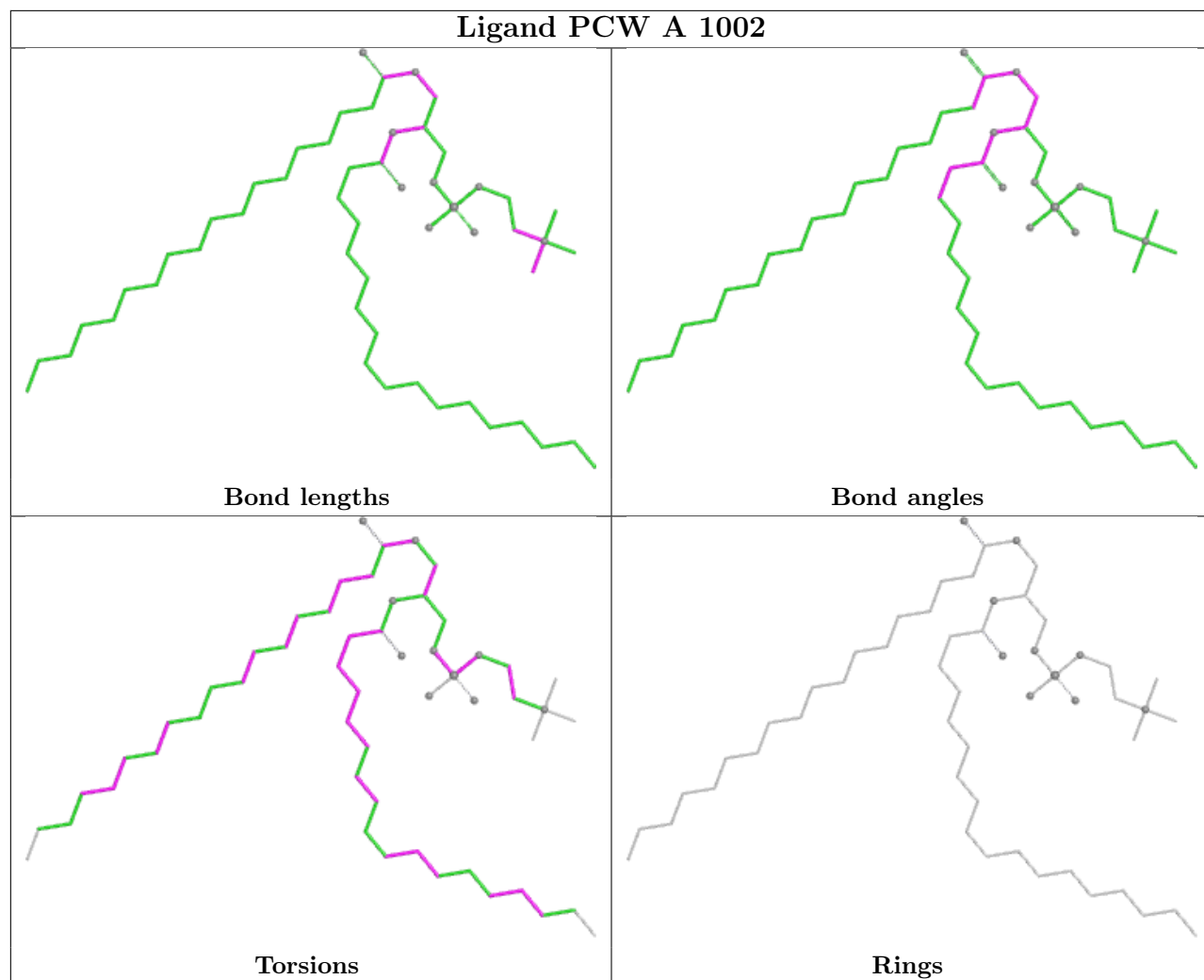
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PCW	2	0
3	B	1002	PCW	3	0
2	C	1001	PIO	1	0

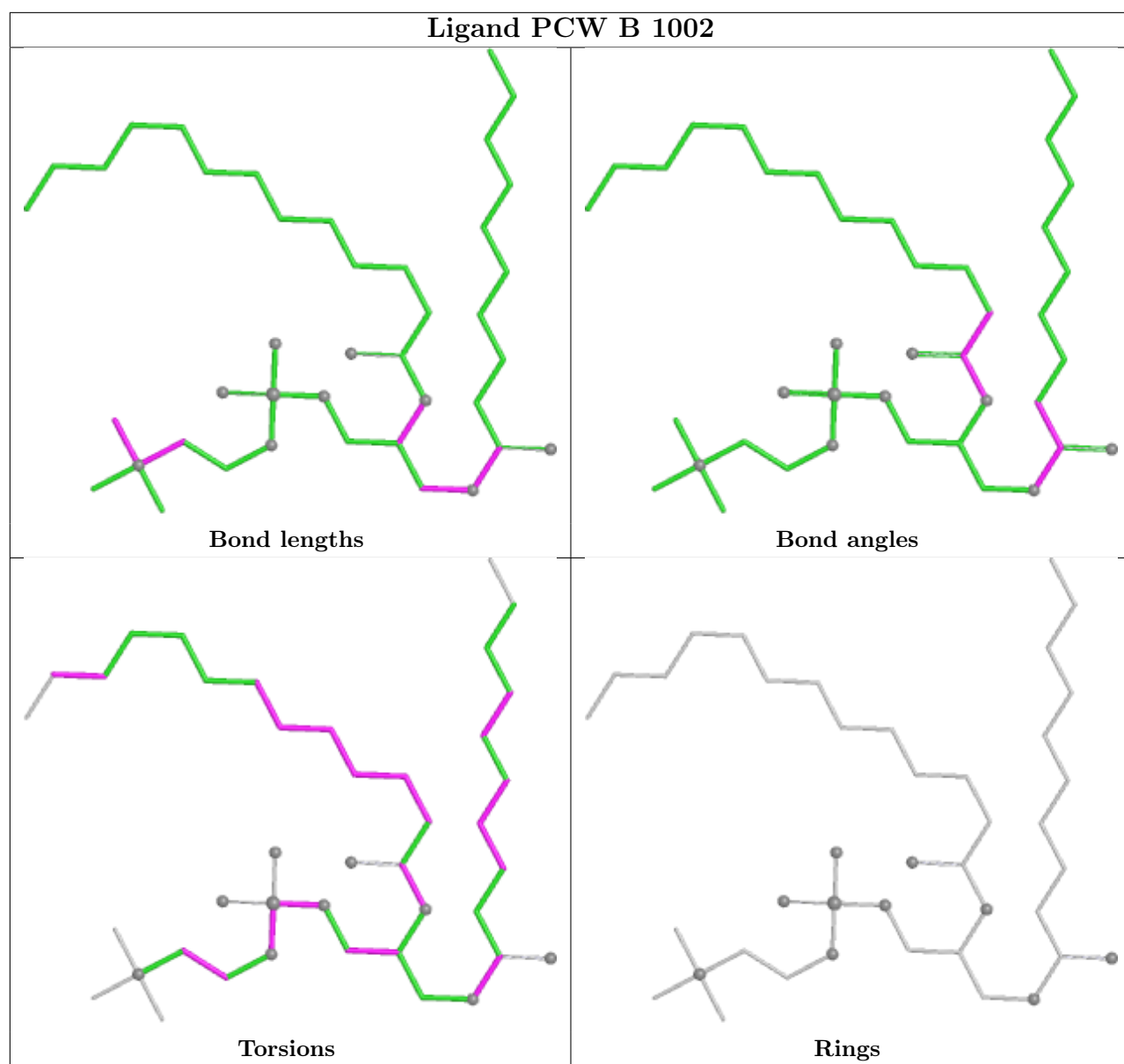
Continued on next page...

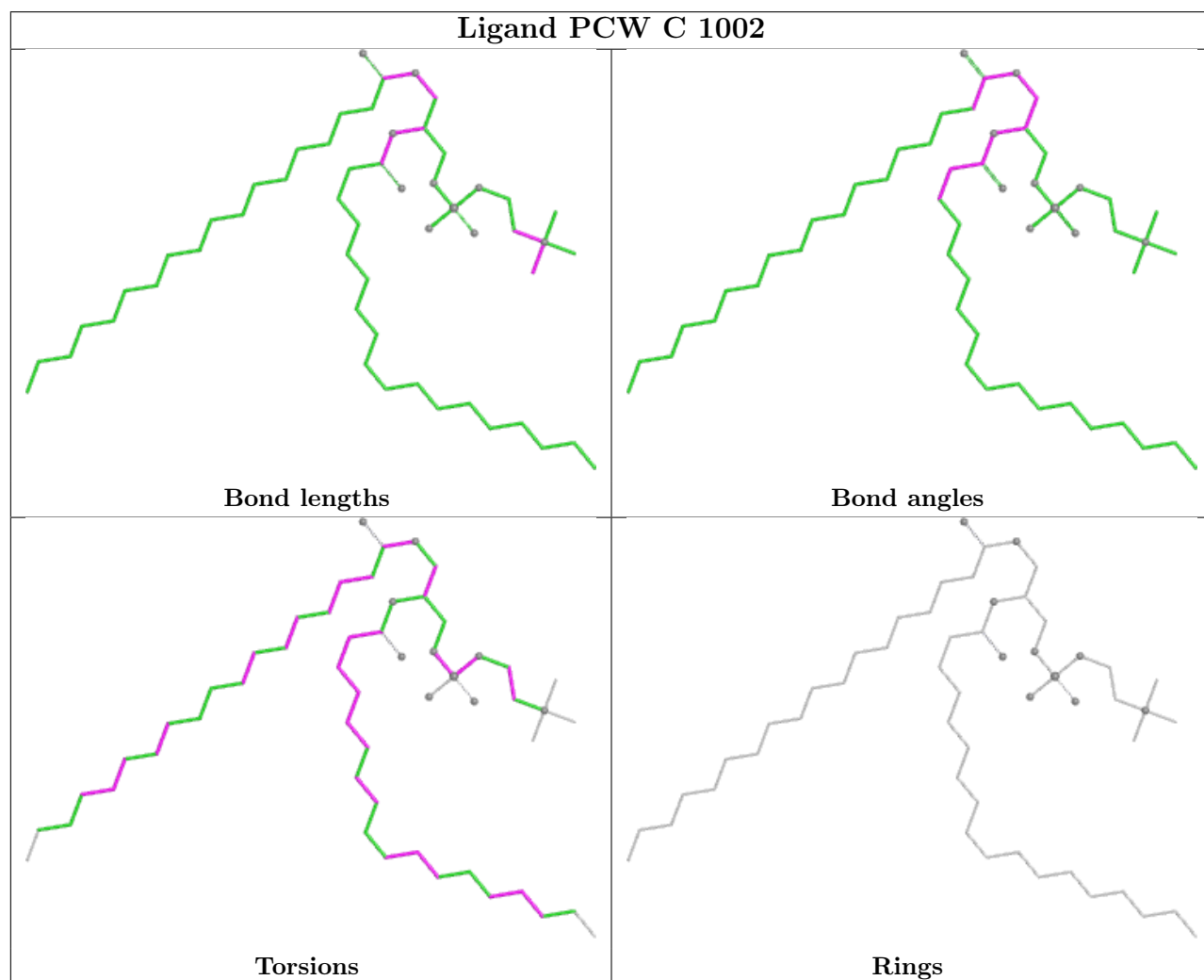
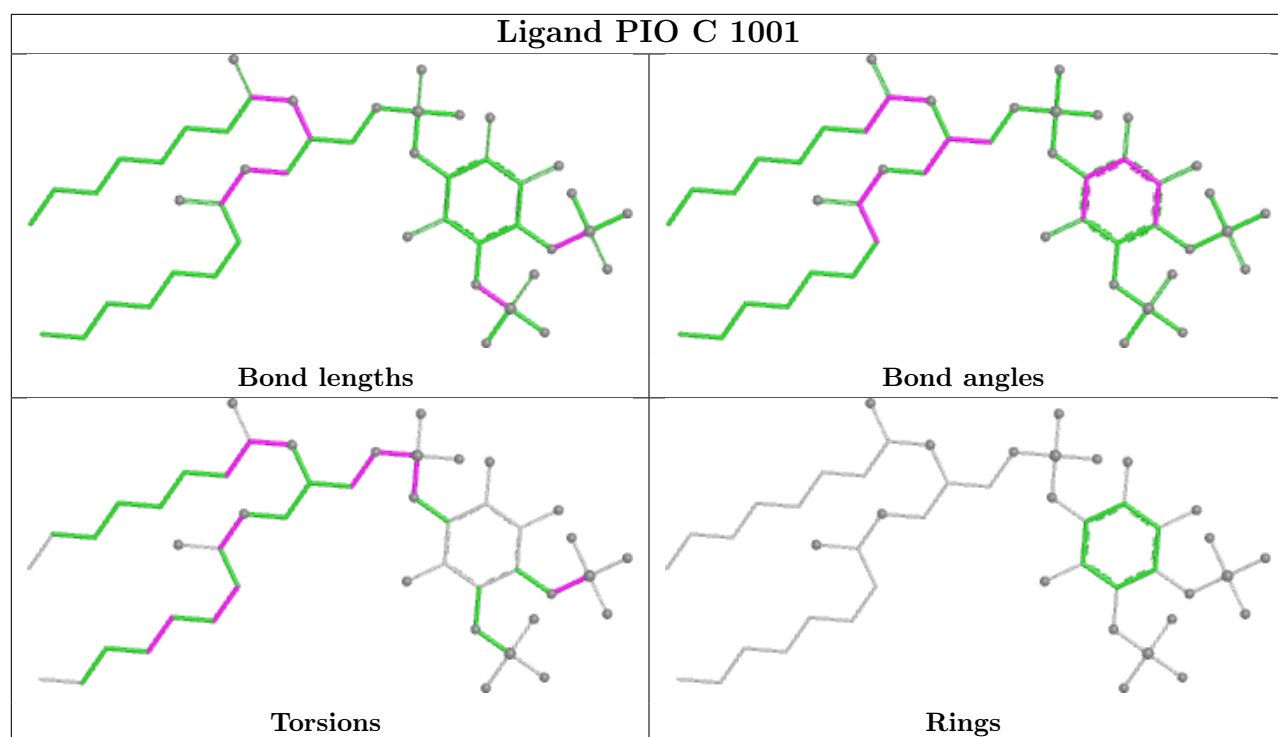
Continued from previous page...

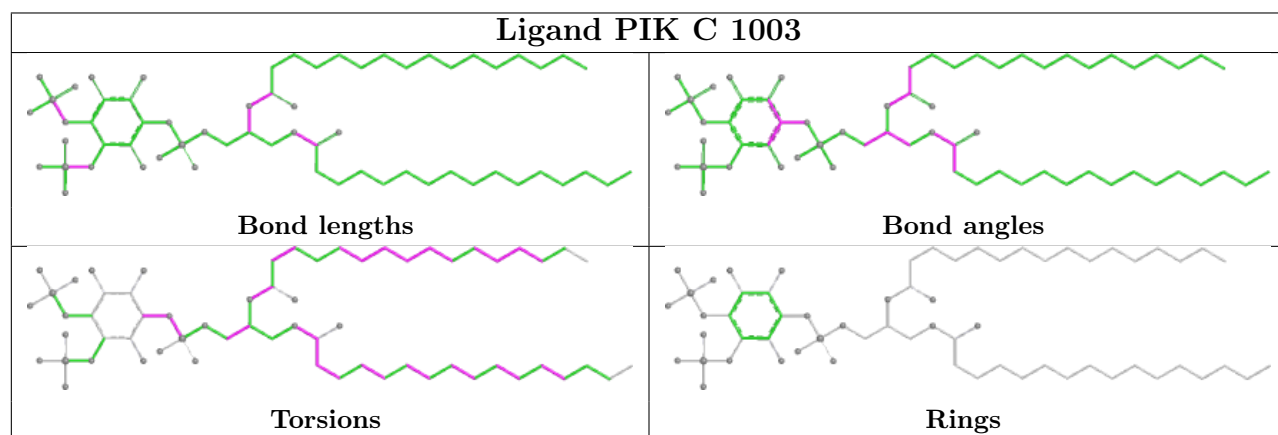
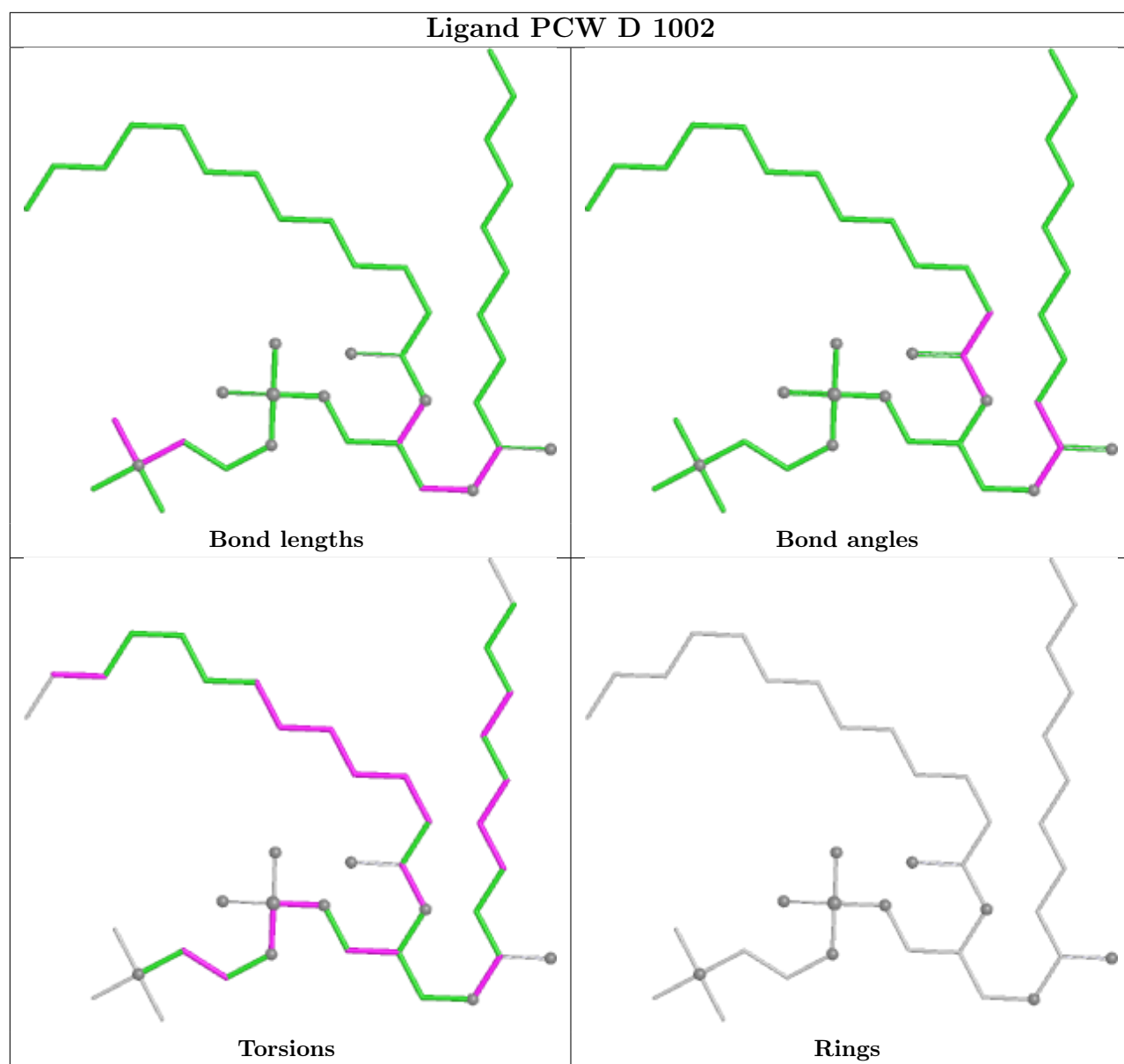
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	PCW	2	0
3	D	1002	PCW	3	0
4	D	1003	PIK	1	0
2	D	1001	PIO	2	0
2	A	1001	PIO	2	0
4	A	1003	PIK	1	0
2	B	1001	PIO	2	0
4	B	1003	PIK	1	0

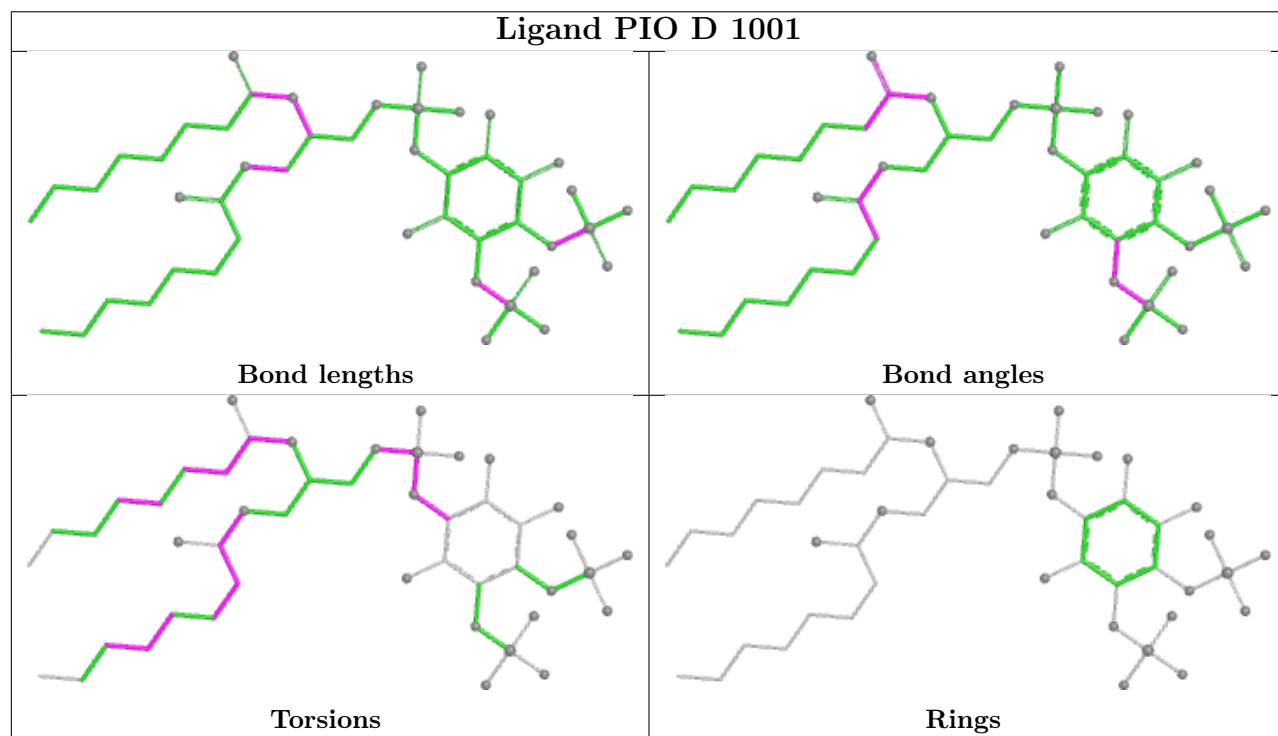
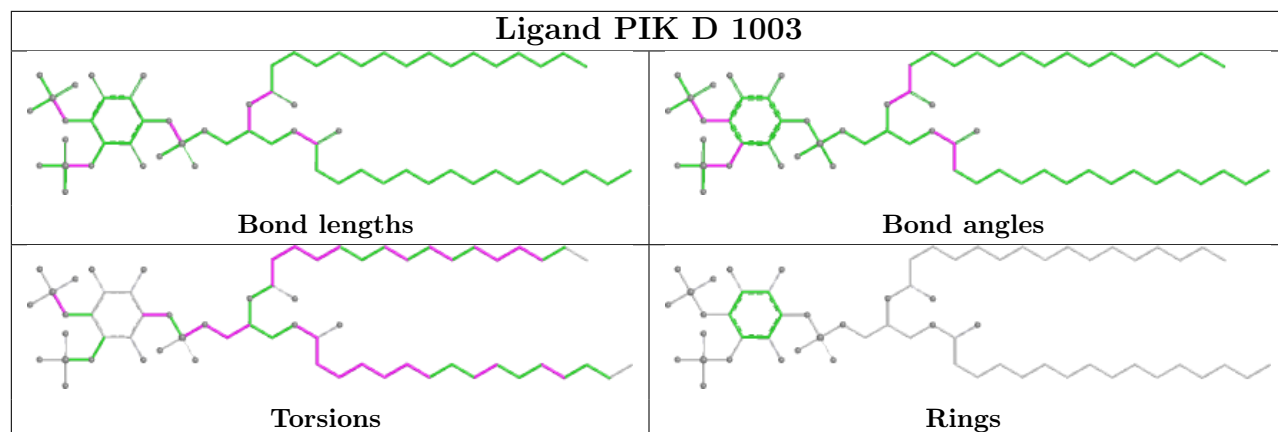
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

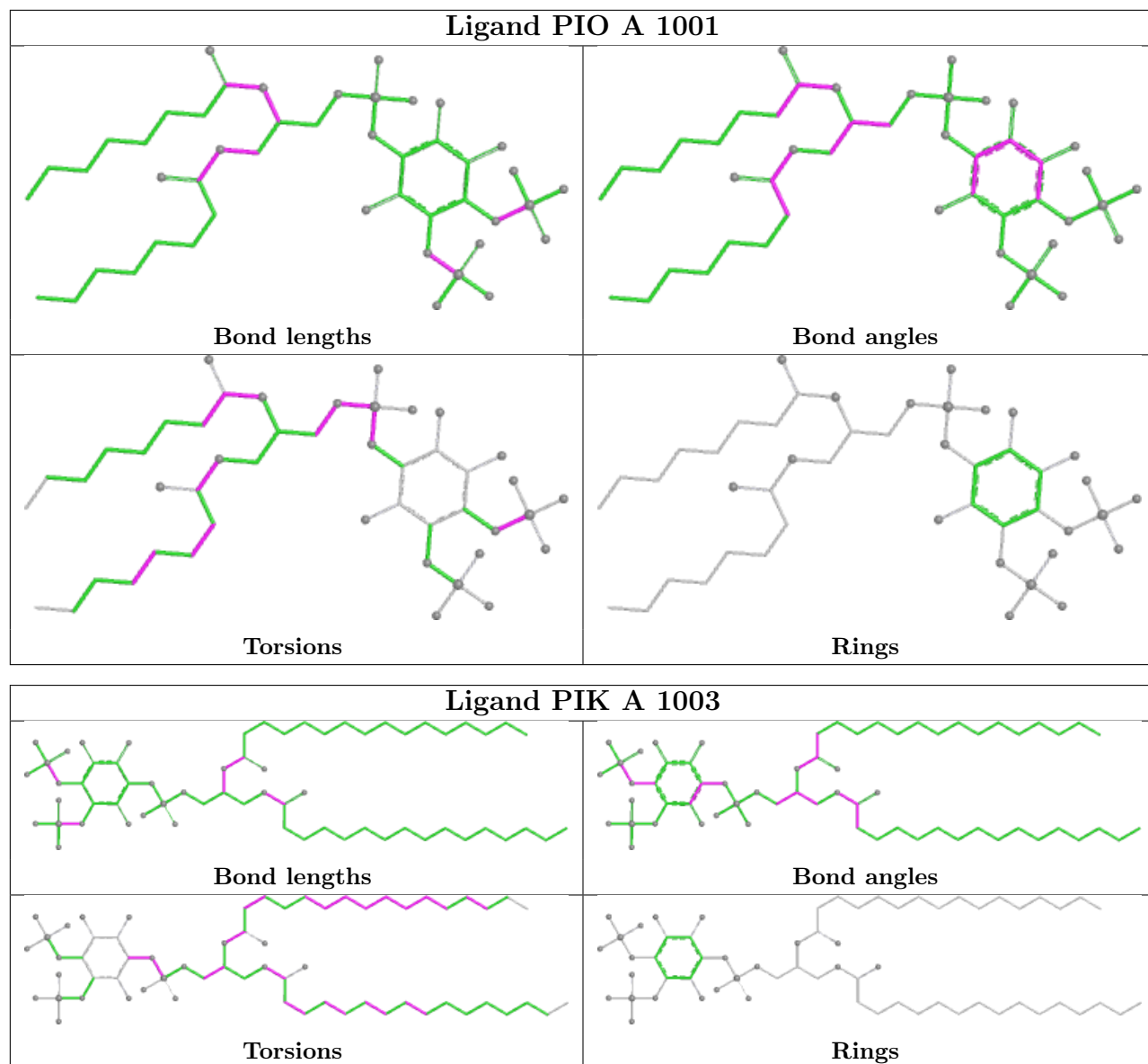


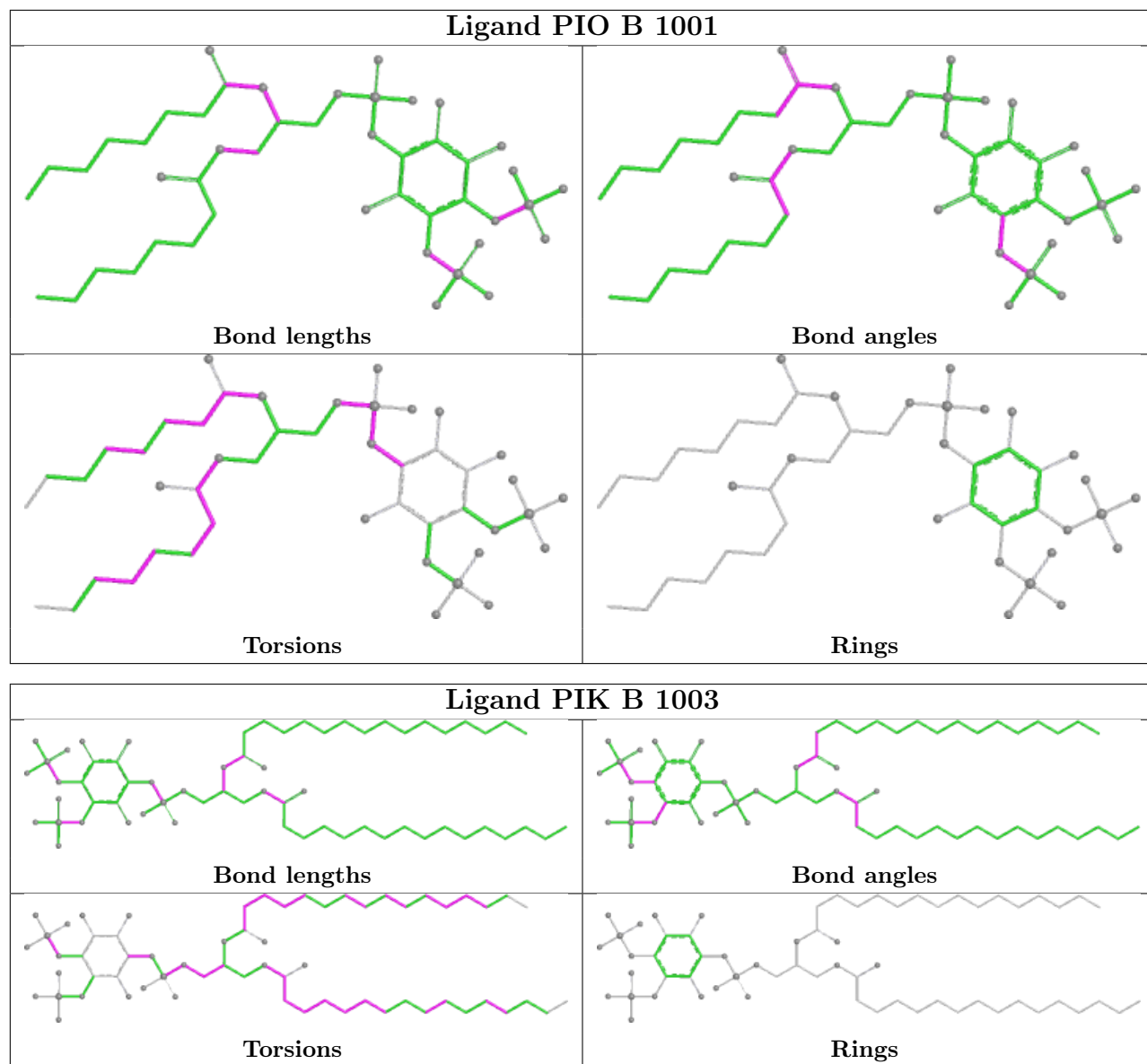












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

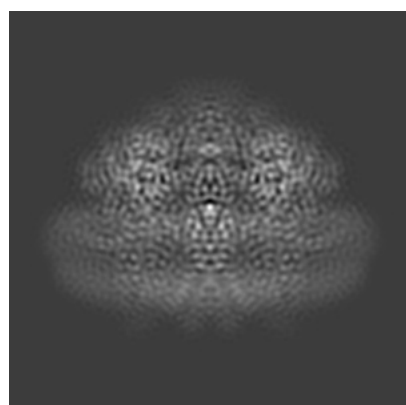
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20499. These allow visual inspection of the internal detail of the map and identification of artifacts.

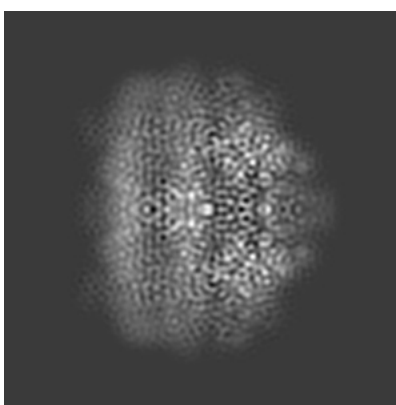
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

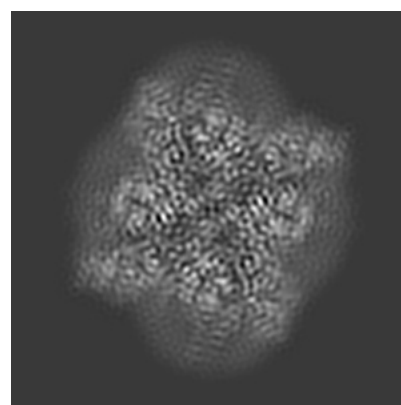
6.1.1 Primary map



X



Y

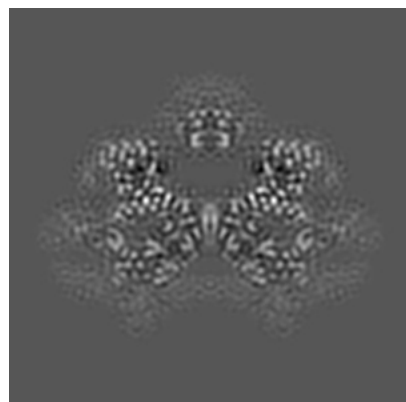


Z

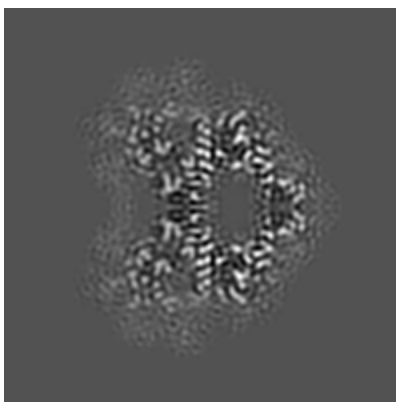
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

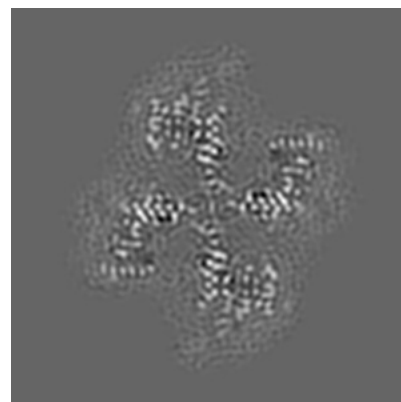
6.2.1 Primary map



X Index: 100



Y Index: 100

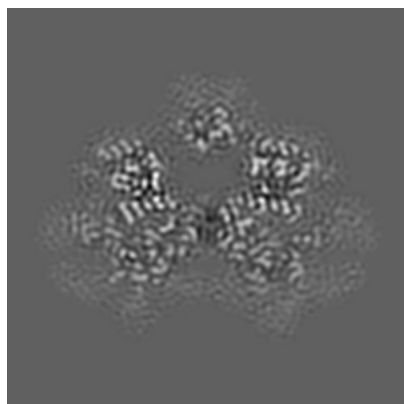


Z Index: 100

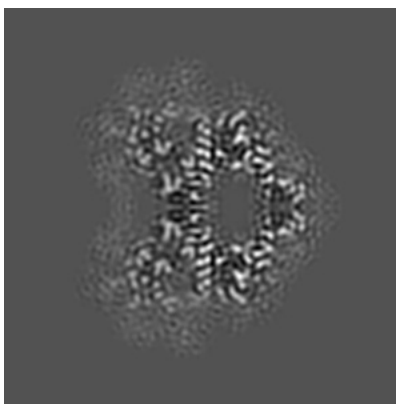
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

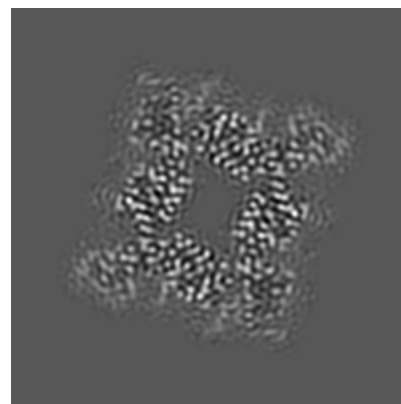
6.3.1 Primary map



X Index: 102



Y Index: 100

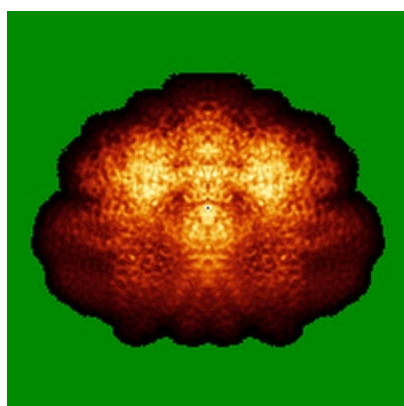


Z Index: 118

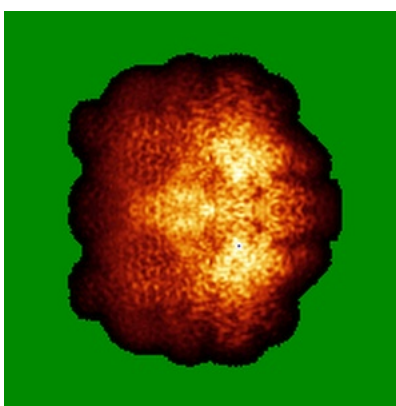
The images above show the largest variance slices of the map in three orthogonal directions.

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

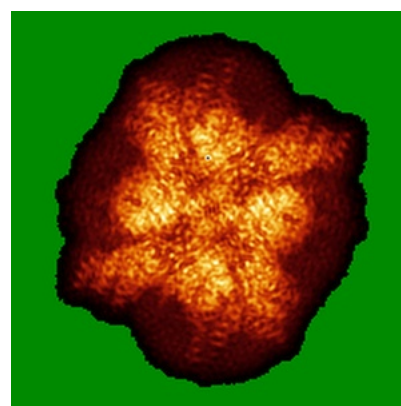
6.4.1 Primary map



X



Y

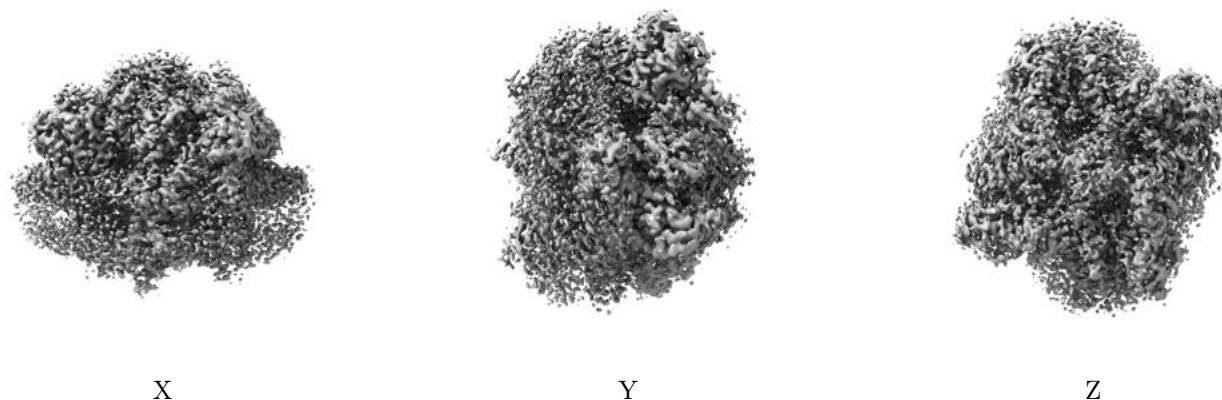


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0169. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

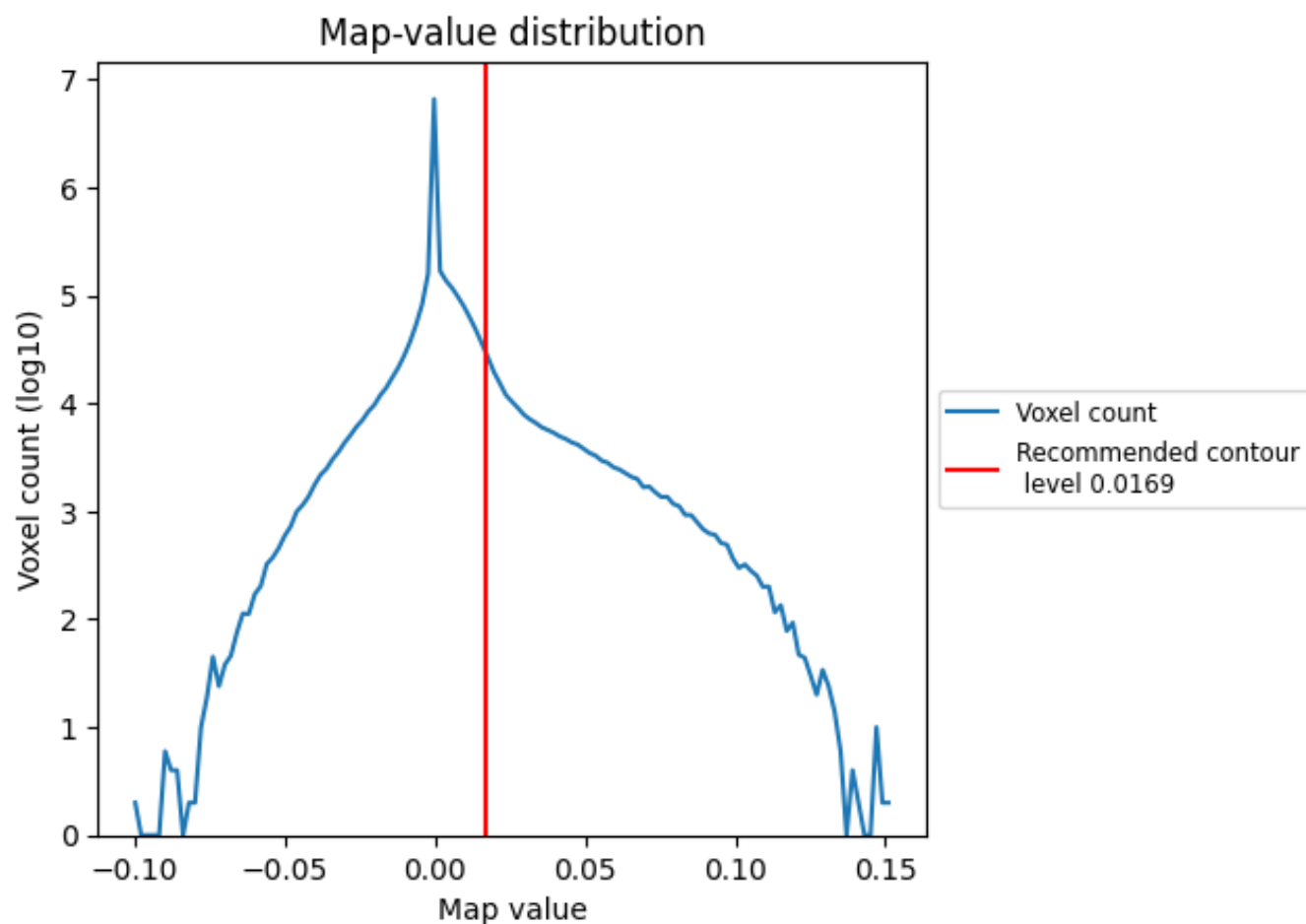
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

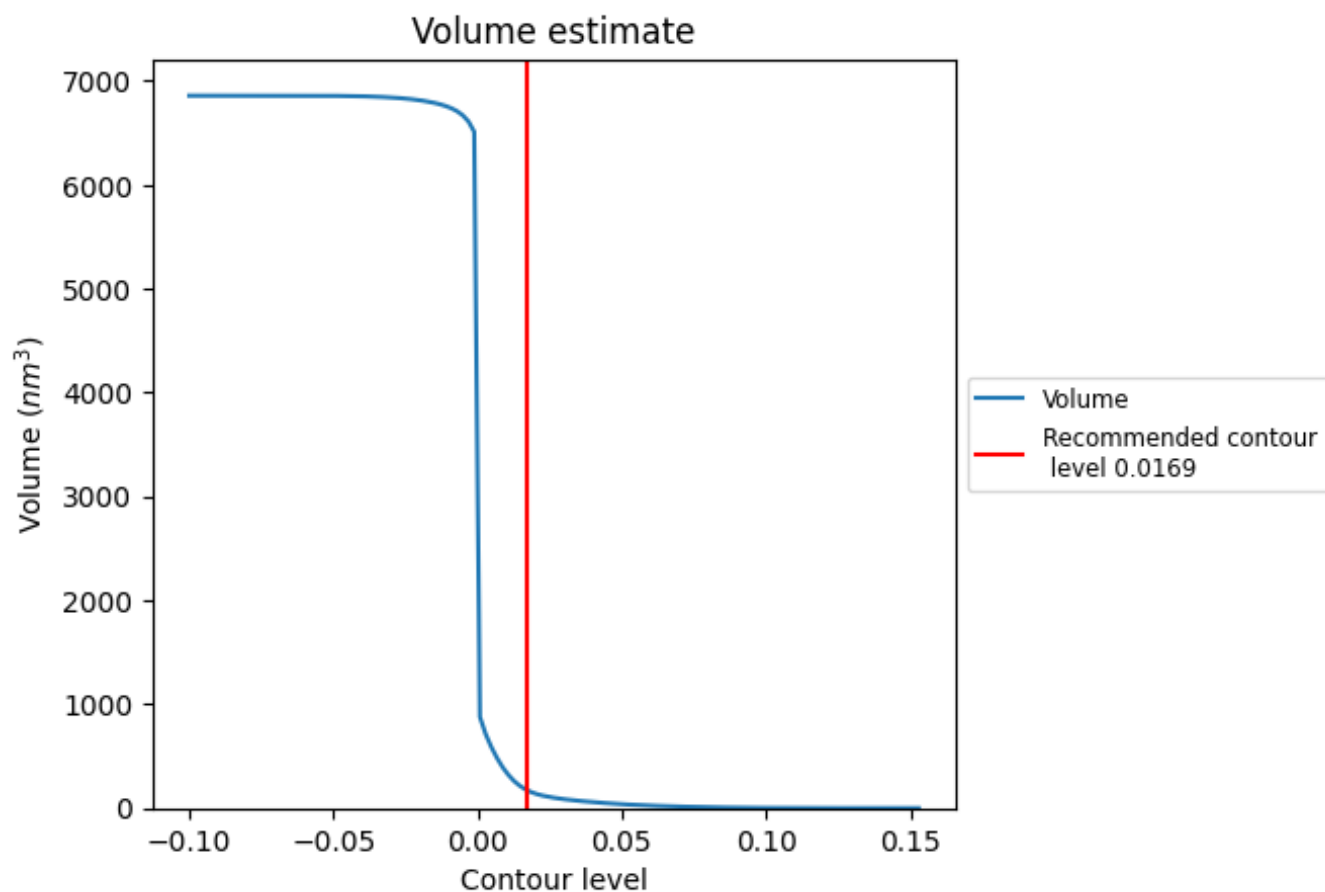
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

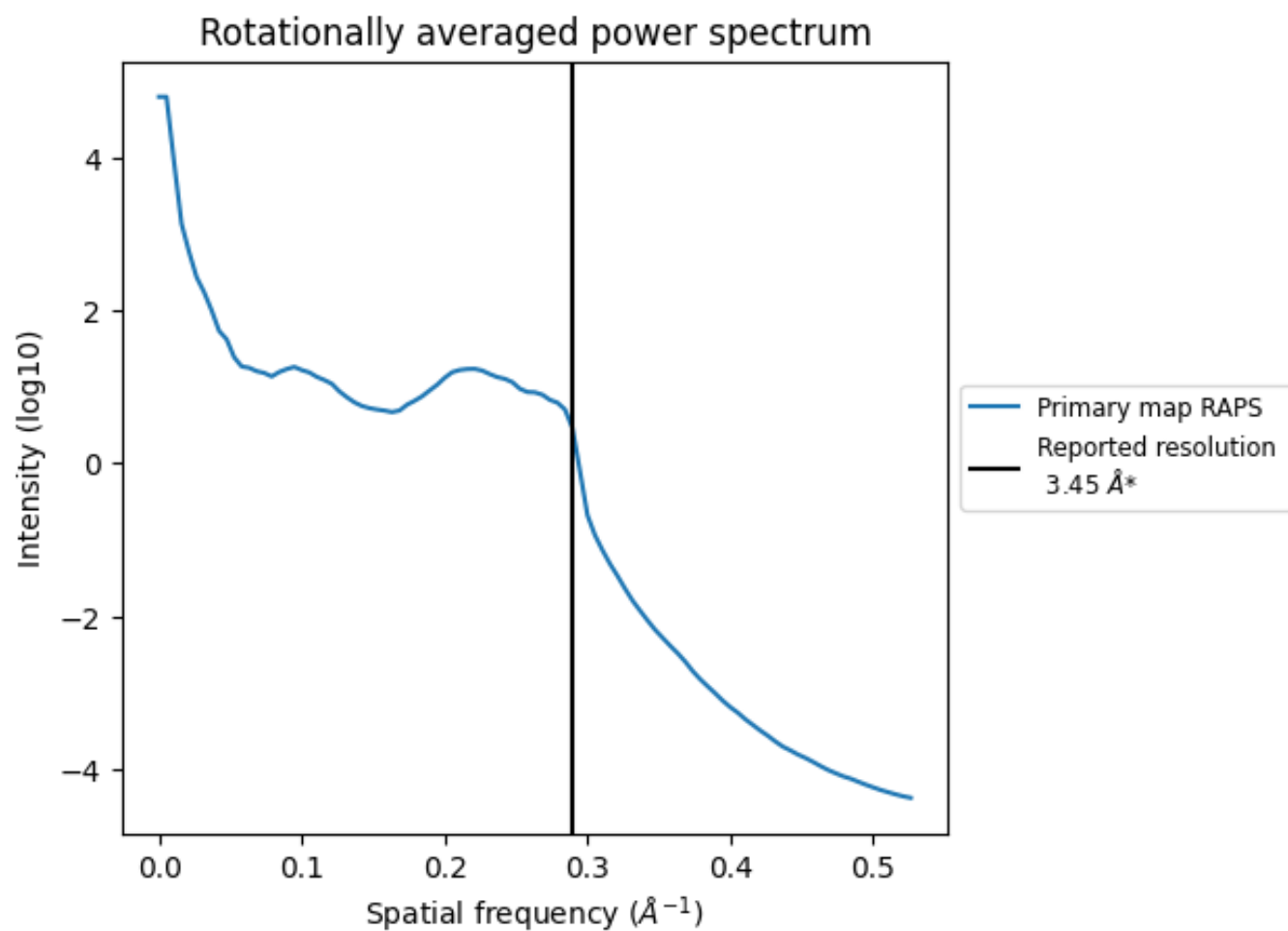
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 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 0.290 $\text{\AA}^{-1}$

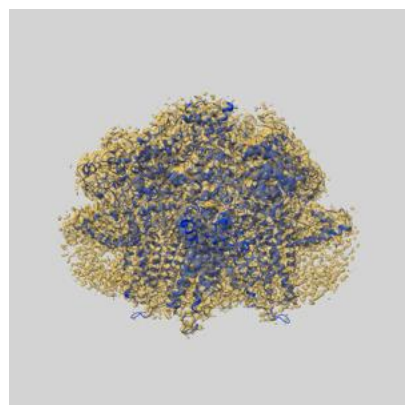
8 Fourier-Shell correlation

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

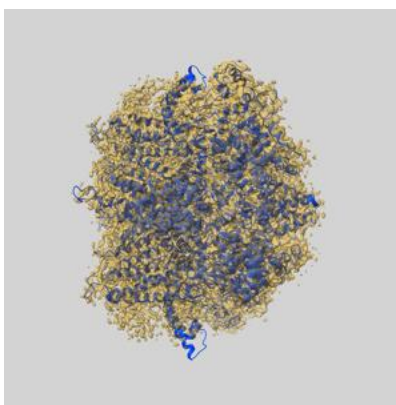
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20499 and PDB model 6PW5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

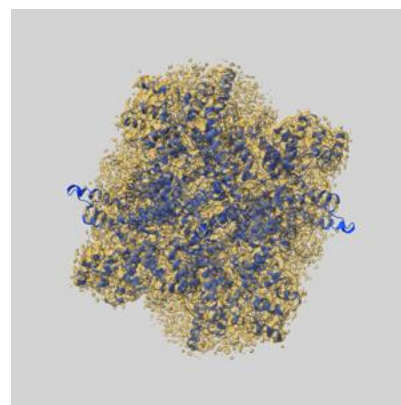
9.1 Map-model overlay [i](#)



X



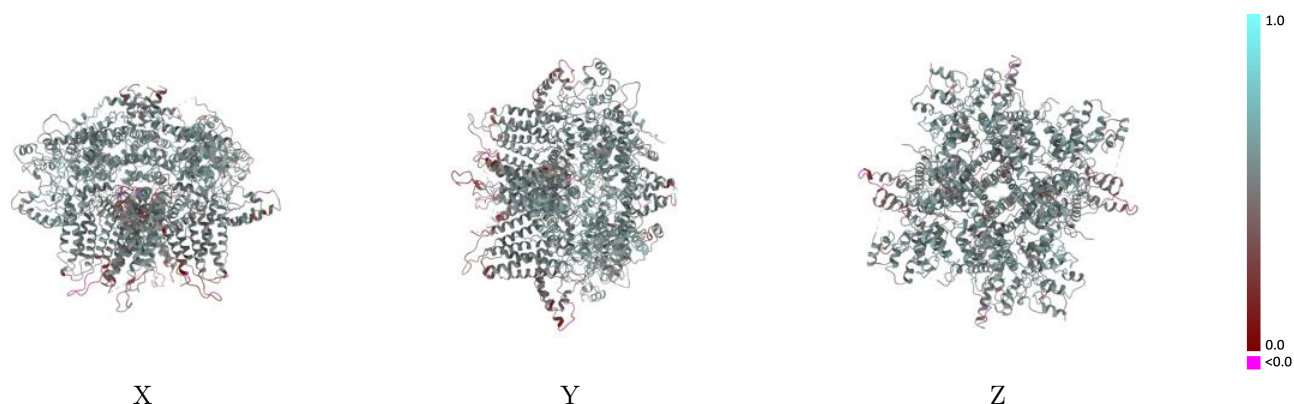
Y



Z

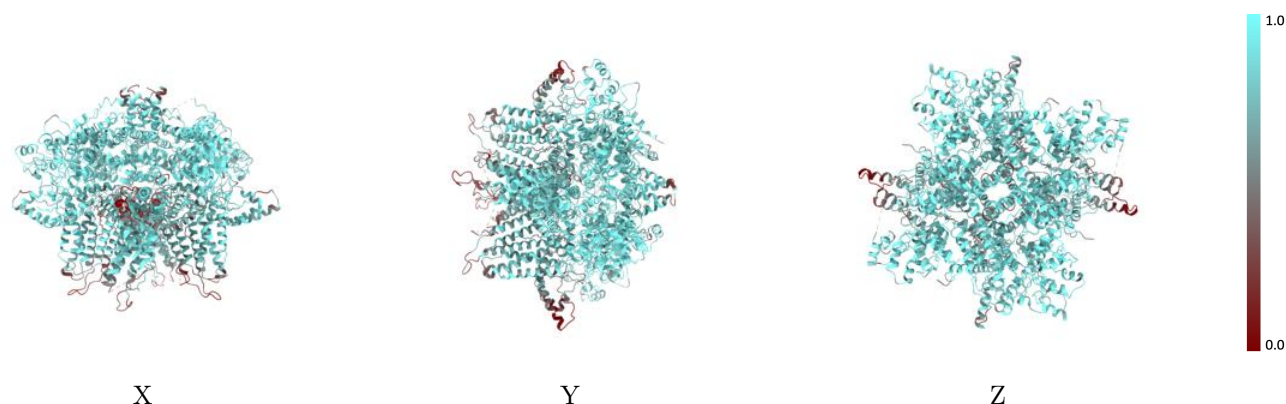
The images above show the 3D surface view of the map at the recommended contour level 0.0169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



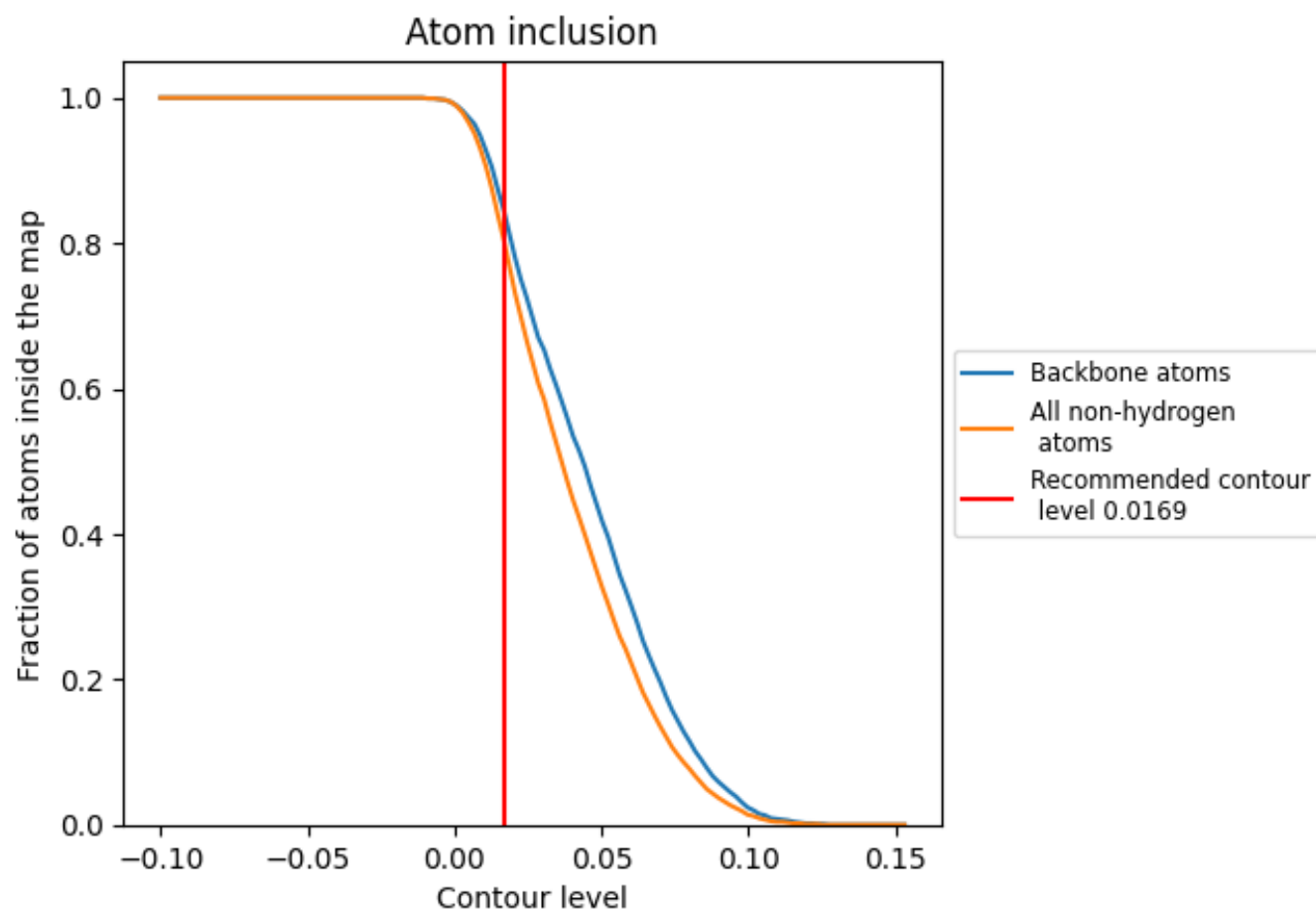
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0169).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.0169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5130
A	0.8290	0.5240
B	0.7770	0.5020
C	0.8290	0.5250
D	0.7770	0.5020

