



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:06 PM UTC

PDB ID : 7M4Q / pdb_00007m4q
EMDB ID : EMD-23664
Title : Multidrug Efflux pump AdeJ
Authors : Zhang, Z.
Deposited on : 2021-03-22
Resolution : 2.87 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 EMD 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

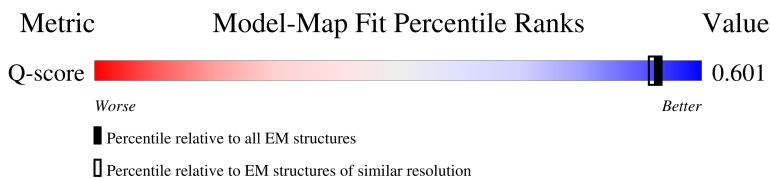
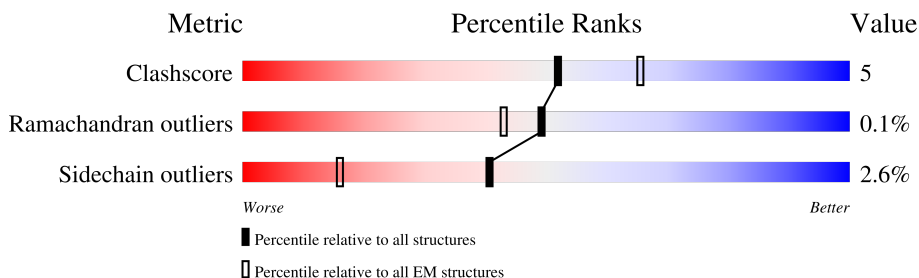
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	1058	 86% 13% ..
1	B	1058	 85% 13% ..
1	C	1058	 84% 14% ..

2 Entry composition [i](#)

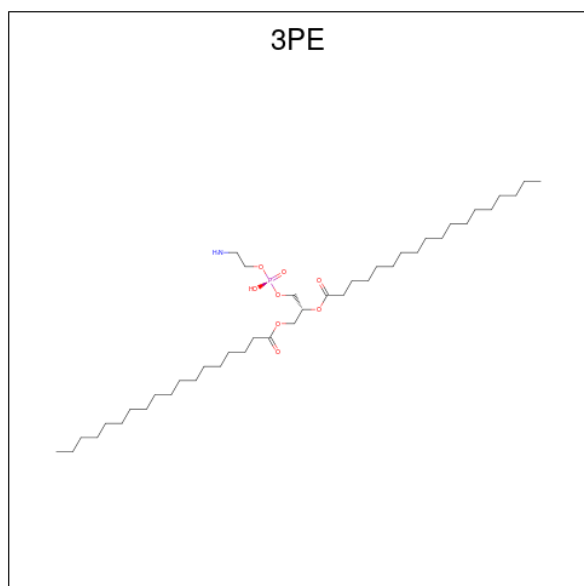
There are 2 unique types of molecules in this entry. The entry contains 48967 atoms, of which 24737 are hydrogens and 0 are deuteriums.

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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1049	Total	C	H	N	O	S	0	0
			16127	5146	8132	1327	1488	34		
1	B	1047	Total	C	H	N	O	S	0	0
			16090	5135	8111	1324	1486	34		
1	C	1046	Total	C	H	N	O	S	0	0
			16069	5129	8099	1322	1485	34		

- Molecule 2 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			58	17	31	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			64	19	35	1	8	1	

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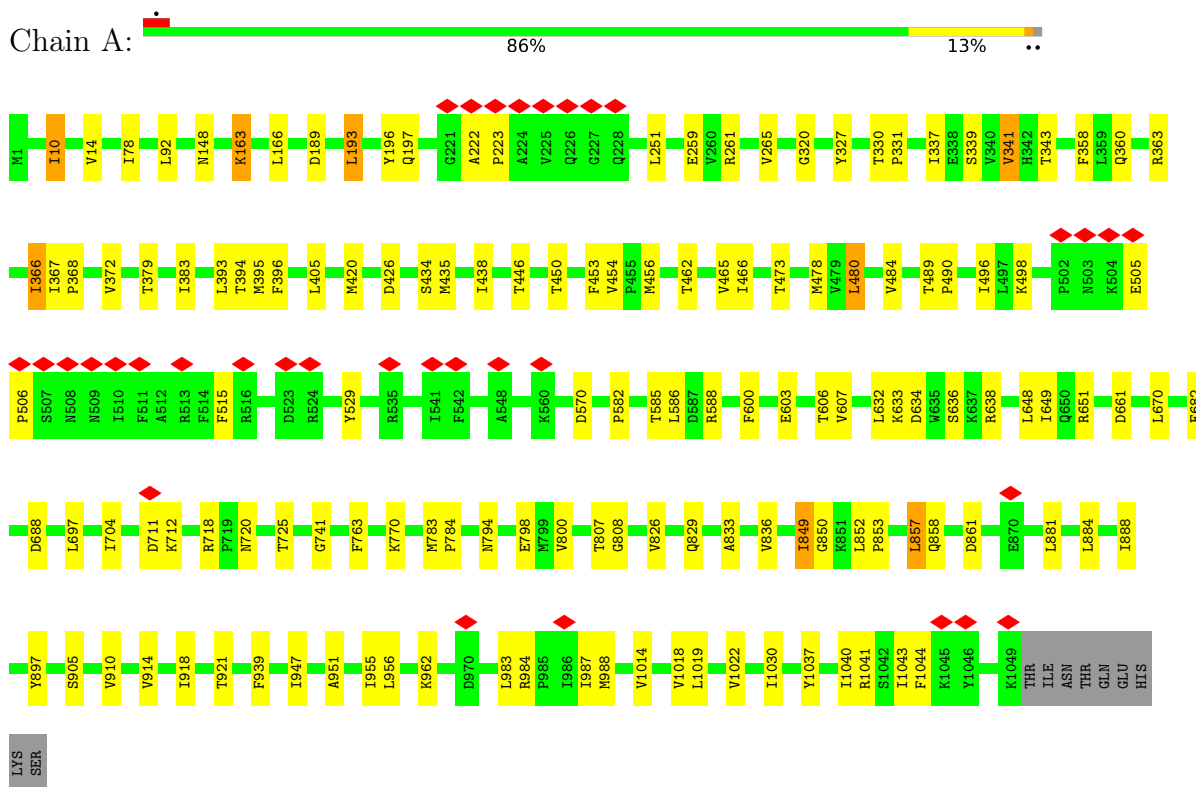
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Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	O	P		0
			82	26	47	8	1		
2	C	1	Total	C	H	O	P		0
			61	19	33	8	1		
2	C	1	Total	C	H	N	O	P	0
			95	29	56	1	8	1	
2	C	1	Total	C	H	O	P		0
			55	17	29	8	1		
2	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

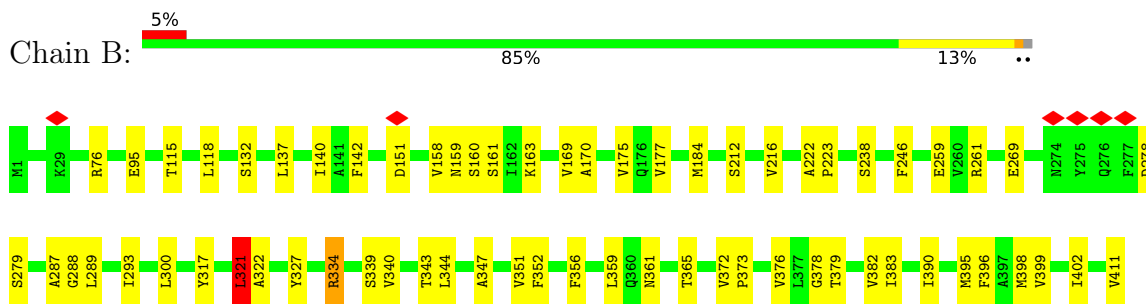
3 Residue-property plots

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: Efflux pump membrane transporter



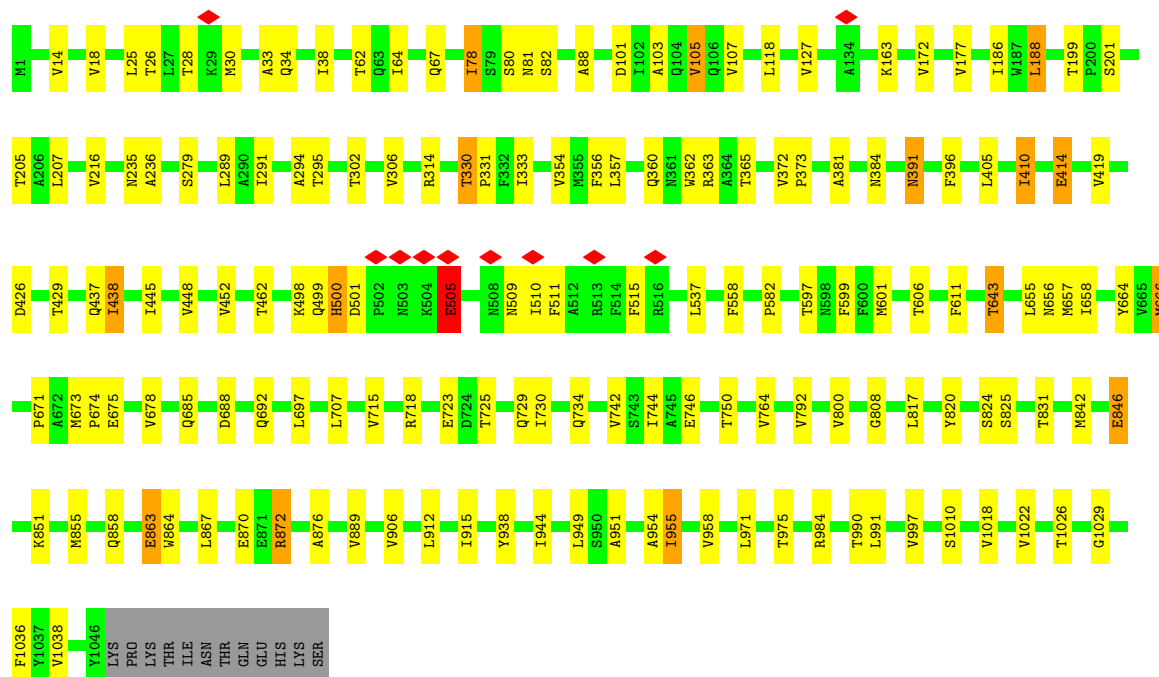
- Molecule 1: Efflux pump membrane transporter





- Molecule 1: Efflux pump membrane transporter

Chain C: 84% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.097	Depositor
Minimum map value	-1.688	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.203	Depositor
Recommended contour level	0.192	Depositor
Map size (Å)	143.64, 141.48001, 172.8	wwPDB
Map dimensions	160, 131, 133	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: 3PE

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	0.48	2/8154 (0.0%)	0.56	5/11087 (0.0%)
1	B	0.60	1/8137 (0.0%)	0.65	6/11064 (0.1%)
1	C	0.71	7/8128 (0.1%)	0.72	19/11053 (0.2%)
All	All	0.61	10/24419 (0.0%)	0.64	30/33204 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	915	ILE	C-O	-8.03	1.14	1.24
1	C	78	ILE	C-O	-6.90	1.16	1.24
1	C	419	VAL	C-O	-6.40	1.16	1.24
1	C	505	GLU	CA-C	5.77	1.60	1.52
1	C	685	GLN	C-O	-5.70	1.17	1.24
1	C	1036	PHE	CA-C	-5.61	1.45	1.52
1	B	830	GLY	C-O	-5.56	1.17	1.24
1	A	849	ILE	C-N	5.43	1.40	1.33
1	A	720	ASN	N-CA	-5.38	1.39	1.46
1	C	410	ILE	C-O	-5.21	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	ILE	N-CA-C	9.30	121.03	112.29
1	A	720	ASN	CA-C-N	7.24	127.73	122.16
1	A	720	ASN	C-N-CA	7.24	127.73	122.16
1	C	825	SER	N-CA-C	7.15	119.62	108.96
1	A	163	LYS	N-CA-C	6.79	118.34	111.07
1	B	463	THR	CA-C-N	6.70	127.42	119.98
1	B	463	THR	C-N-CA	6.70	127.42	119.98
1	C	501	ASP	N-CA-C	6.55	122.16	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	863	GLU	N-CA-C	6.24	123.76	114.09
1	C	80	SER	N-CA-C	6.13	118.73	109.23
1	C	666	MET	CB-CA-C	-6.10	103.14	110.15
1	C	396	PHE	N-CA-C	-5.95	104.88	111.36
1	C	78	ILE	CB-CA-C	-5.85	102.46	110.77
1	C	188	LEU	N-CA-C	5.69	118.90	110.48
1	C	445	ILE	CB-CA-C	-5.62	104.78	111.97
1	C	1029	GLY	N-CA-C	5.49	119.31	112.73
1	C	363	ARG	N-CA-C	-5.44	105.43	111.36
1	C	437	GLN	N-CA-C	5.36	118.29	111.69
1	B	321	LEU	N-CA-C	5.29	117.91	110.23
1	B	684	LEU	N-CA-C	5.26	117.39	109.23
1	C	1036	PHE	N-CA-C	-5.25	105.23	111.69
1	A	651	ARG	CA-C-N	5.21	126.84	120.22
1	A	651	ARG	C-N-CA	5.21	126.84	120.22
1	C	876	ALA	N-CA-C	5.21	116.95	111.28
1	C	419	VAL	CA-C-O	-5.20	115.66	121.17
1	B	575	MET	CA-C-N	5.08	130.95	122.73
1	B	575	MET	C-N-CA	5.08	130.95	122.73
1	C	500	HIS	CA-C-N	-5.06	116.93	123.16
1	C	500	HIS	C-N-CA	-5.06	116.93	123.16
1	C	846	GLU	N-CA-C	5.06	117.69	111.82

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	7995	8132	8132	85	0
1	B	7979	8111	8112	96	0
1	C	7970	8099	8099	87	0
2	B	142	195	183	0	0
2	C	144	200	189	0	0
All	All	24230	24737	24715	266	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 5.

All (266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:LEU:HD13	1:B:676:LEU:C	1.71	1.16
1:B:676:LEU:HD13	1:B:676:LEU:O	1.46	1.13
1:B:997:VAL:HG21	1:B:1018:VAL:HG21	1.49	0.94
1:B:676:LEU:C	1:B:676:LEU:CD1	2.43	0.91
1:A:450:THR:O	1:A:454:VAL:HG23	1.75	0.86
1:B:321:LEU:HD13	1:B:322:ALA:N	1.95	0.81
1:C:64:ILE:HD11	1:C:118:LEU:HD23	1.61	0.81
1:C:707:LEU:HD11	1:C:855:MET:HE1	1.63	0.81
1:B:321:LEU:HD13	1:B:321:LEU:C	2.08	0.79
1:B:462:THR:HG21	1:B:676:LEU:HD23	1.67	0.77
1:B:344:LEU:HD22	1:B:402:ILE:HG21	1.65	0.76
1:C:666:MET:HE3	1:C:718:ARG:HD3	1.67	0.75
1:C:537:LEU:HD22	1:C:1038:VAL:HG11	1.67	0.75
1:B:462:THR:CG2	1:B:676:LEU:HD23	2.16	0.75
1:A:383:ILE:HG21	1:A:473:THR:HG22	1.68	0.74
1:B:327:TYR:CD2	1:B:573:VAL:HG11	2.23	0.74
1:B:673:MET:SD	1:B:674:PRO:HD2	2.27	0.74
1:A:603:GLU:O	1:A:607:VAL:HG22	1.88	0.72
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.71	0.72
1:A:394:THR:HG22	1:A:473:THR:HG21	1.71	0.72
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.73	0.69
1:C:163:LYS:HD3	1:C:177:VAL:HG21	1.74	0.69
1:C:582:PRO:HB3	1:C:725:THR:HG22	1.76	0.67
1:C:750:THR:HG21	1:C:792:VAL:HG22	1.76	0.67
1:A:453:PHE:CD2	1:A:478:MET:HE1	2.31	0.66
1:B:675:GLU:O	1:B:675:GLU:HG2	1.97	0.65
1:C:101:ASP:O	1:C:105:VAL:HG13	1.97	0.65
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.27	0.64
1:A:529:TYR:CZ	1:A:1030:ILE:HG22	2.34	0.63
1:C:723:GLU:O	1:C:725:THR:HG23	1.97	0.63
1:A:853:PRO:O	1:A:858:GLN:NE2	2.31	0.63
1:B:259:GLU:OE1	1:B:261:ARG:NH1	2.31	0.63
1:C:499:GLN:HA	1:C:499:GLN:OE1	1.99	0.62
1:A:259:GLU:OE1	1:A:261:ARG:NH1	2.33	0.62
1:B:885:SER:O	1:B:889:VAL:HG23	1.99	0.62
1:B:137:LEU:HD22	1:B:293:ILE:HG21	1.83	0.60
1:C:509:ASN:OD1	1:C:510:ILE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ILE:HD12	1:B:667:PRO:HB2	1.82	0.60
1:C:656:ASN:OD1	1:C:657:MET:N	2.33	0.60
1:B:1003:SER:O	1:B:1012:HIS:NE2	2.32	0.60
1:C:984:ARG:HH21	1:C:984:ARG:HG3	1.66	0.59
1:A:339:SER:O	1:A:343:THR:HG23	2.03	0.59
1:C:78:ILE:O	1:C:820:TYR:O	2.20	0.59
1:C:302:THR:O	1:C:306:VAL:HG23	2.03	0.59
1:C:664:TYR:CD1	1:C:666:MET:HG2	2.38	0.59
1:A:341:VAL:HG12	1:A:395:MET:HE2	1.84	0.59
1:B:321:LEU:C	1:B:321:LEU:CD1	2.76	0.59
1:C:505:GLU:HA	1:C:505:GLU:OE1	2.03	0.58
1:A:582:PRO:HB3	1:A:725:THR:HG22	1.85	0.58
1:A:600:PHE:O	1:A:607:VAL:HG21	2.03	0.58
1:C:62:THR:HG22	1:C:88:ALA:HB1	1.85	0.58
1:A:435:MET:HE2	1:A:435:MET:HA	1.85	0.58
1:A:897:TYR:O	1:A:962:LYS:NZ	2.37	0.58
1:A:10:ILE:O	1:A:14:VAL:HG23	2.03	0.58
1:C:25:LEU:O	1:C:28:THR:OG1	2.23	0.57
1:C:746:GLU:O	1:C:750:THR:HG22	2.03	0.57
1:B:356:PHE:O	1:B:359:LEU:O	2.22	0.57
1:B:379:THR:HG23	1:B:476:THR:HG23	1.87	0.57
1:A:396:PHE:CD2	1:A:1014:VAL:HG21	2.40	0.56
1:B:163:LYS:HD2	1:B:177:VAL:HG23	1.88	0.56
1:B:238:SER:O	1:C:734:GLN:NE2	2.37	0.56
1:B:554:LEU:HD13	1:B:915:ILE:HA	1.88	0.55
1:C:951:ALA:O	1:C:955:ILE:HG12	2.06	0.55
1:B:278:ASP:OD1	1:B:279:SER:N	2.39	0.55
1:B:678:VAL:HG22	1:B:678:VAL:O	2.07	0.54
1:C:38:ILE:HG23	1:C:462:THR:HG23	1.90	0.54
1:C:279:SER:OG	1:C:611:PHE:CZ	2.60	0.54
1:A:363:ARG:O	1:A:366:ILE:HG22	2.08	0.54
1:A:585:THR:HG22	1:A:586:LEU:N	2.23	0.54
1:B:607:VAL:HG12	1:B:608:GLU:O	2.07	0.54
1:A:807:THR:HG22	1:A:808:GLY:N	2.23	0.53
1:B:142:PHE:N	1:B:287:ALA:O	2.37	0.53
1:A:983:LEU:HD13	1:A:983:LEU:C	2.33	0.53
1:B:912:LEU:O	1:B:915:ILE:HG22	2.09	0.53
1:C:692:GLN:NE2	1:C:858:GLN:O	2.40	0.53
1:A:833:ALA:O	1:A:836:VAL:HG12	2.09	0.53
1:A:337:ILE:O	1:A:341:VAL:HG13	2.09	0.53
1:B:352:PHE:CD2	1:B:365:THR:HG22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:LEU:C	1:B:648:LEU:HD23	2.33	0.53
1:B:317:TYR:CD2	1:B:321:LEU:HD12	2.43	0.53
1:C:744:ILE:N	1:C:744:ILE:HD12	2.24	0.53
1:B:300:LEU:HD13	1:B:334:ARG:HD3	1.90	0.52
1:C:356:PHE:HD1	1:C:365:THR:HG21	1.74	0.52
1:A:910:VAL:HG13	1:A:947:ILE:HD13	1.90	0.52
1:B:998:LEU:HD23	1:B:998:LEU:O	2.09	0.52
1:C:997:VAL:HG11	1:C:1018:VAL:HG11	1.91	0.52
1:A:682:PHE:CD1	1:A:682:PHE:C	2.87	0.52
1:A:718:ARG:NH1	1:A:829:GLN:HG2	2.24	0.52
1:C:360:GLN:HG2	1:C:515:PHE:CG	2.44	0.52
1:C:177:VAL:HG22	1:C:289:LEU:CD2	2.39	0.52
1:A:529:TYR:CE1	1:A:1030:ILE:HG22	2.45	0.52
1:C:448:VAL:O	1:C:452:VAL:HG23	2.10	0.51
1:B:807:THR:HG22	1:B:808:GLY:H	1.75	0.51
1:A:372:VAL:HG22	1:A:405:LEU:HD11	1.92	0.51
1:B:398:MET:O	1:B:402:ILE:HG23	2.11	0.51
1:A:951:ALA:O	1:A:955:ILE:HG12	2.10	0.51
1:A:704:ILE:HD11	1:A:852:LEU:HD11	1.91	0.51
1:B:676:LEU:O	1:B:676:LEU:CD1	2.38	0.51
1:B:1026:THR:HG23	1:B:1027:PHE:N	2.26	0.51
1:A:921:THR:HG21	1:A:939:PHE:CE1	2.46	0.51
1:A:505:GLU:N	1:A:506:PRO:CD	2.74	0.51
1:B:845:MET:HA	1:B:845:MET:HE2	1.92	0.51
1:B:137:LEU:HD22	1:B:293:ILE:CG2	2.39	0.51
1:A:857:LEU:HD22	1:A:857:LEU:N	2.25	0.50
1:B:682:PHE:CD1	1:B:682:PHE:C	2.88	0.50
1:B:321:LEU:HD13	1:B:322:ALA:CA	2.41	0.50
1:C:62:THR:HG21	1:C:82:SER:OG	2.12	0.50
1:C:954:ALA:O	1:C:958:VAL:HG22	2.11	0.50
1:B:845:MET:HE2	1:B:845:MET:CA	2.41	0.50
1:C:201:SER:O	1:C:205:THR:HG23	2.11	0.50
1:C:177:VAL:HG22	1:C:289:LEU:HD23	1.94	0.50
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.93	0.50
1:B:997:VAL:HG21	1:B:1018:VAL:CG2	2.30	0.50
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.94	0.50
1:B:862:TYR:CD1	1:B:862:TYR:C	2.89	0.49
1:A:910:VAL:HG13	1:A:947:ILE:CD1	2.42	0.49
1:B:558:PHE:CD2	1:B:918:ILE:HD11	2.47	0.49
1:A:462:THR:O	1:A:465:VAL:HG22	2.12	0.49
1:B:786:ASP:N	1:B:786:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:THR:OG1	1:C:643:THR:HG22	2.12	0.49
1:A:570:ASP:OD2	1:A:638:ARG:NH2	2.44	0.49
1:C:537:LEU:CD2	1:C:1038:VAL:HG11	2.39	0.49
1:C:664:TYR:HD1	1:C:666:MET:HG2	1.77	0.49
1:A:849:ILE:HG22	1:A:849:ILE:O	2.13	0.49
1:C:216:VAL:HG21	1:C:236:ALA:HB2	1.95	0.48
1:C:715:VAL:HG23	1:C:831:THR:HB	1.93	0.48
1:A:496:ILE:O	1:A:496:ILE:HG22	2.13	0.48
1:B:344:LEU:HD23	1:B:402:ILE:HD13	1.95	0.48
1:B:902:ILE:HD11	1:B:1041:ARG:NH2	2.29	0.48
1:C:103:ALA:O	1:C:107:VAL:HG23	2.14	0.48
1:A:711:ASP:OD1	1:A:712:LYS:N	2.46	0.48
1:C:744:ILE:HD12	1:C:744:ILE:H	1.78	0.48
1:B:608:GLU:HG3	1:B:609:SER:H	1.79	0.48
1:C:64:ILE:HD11	1:C:118:LEU:CD2	2.36	0.48
1:A:358:PHE:HB2	1:A:988:MET:HE3	1.95	0.48
1:A:456:MET:HG3	1:A:881:LEU:HD21	1.96	0.48
1:A:480:LEU:O	1:A:484:VAL:HG23	2.13	0.48
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.44	0.48
1:B:339:SER:O	1:B:343:THR:HG23	2.14	0.48
1:C:216:VAL:HG12	1:C:216:VAL:O	2.14	0.48
1:A:794:ASN:OD1	1:A:798:GLU:N	2.46	0.48
1:B:649:ILE:HG23	1:B:667:PRO:HB2	1.94	0.48
1:A:446:THR:O	1:A:450:THR:HG23	2.14	0.47
1:B:659:ILE:HG23	1:B:659:ILE:O	2.14	0.47
1:A:914:VAL:HG12	1:A:918:ILE:HD12	1.96	0.47
1:B:656:ASN:ND2	1:B:665:VAL:HG21	2.29	0.47
1:B:343:THR:HG21	1:B:1000:LEU:HD11	1.96	0.47
1:C:452:VAL:HG22	1:C:889:VAL:HG21	1.97	0.47
1:C:656:ASN:OD1	1:C:656:ASN:C	2.56	0.47
1:A:420:MET:HE1	1:A:498:LYS:O	2.15	0.47
1:A:633:LYS:O	1:A:638:ARG:NH1	2.42	0.47
1:B:576:THR:C	1:B:577:LEU:HD12	2.39	0.47
1:B:939:PHE:CZ	1:B:943:ILE:HD11	2.50	0.47
1:A:897:TYR:OH	1:A:955:ILE:HD12	2.14	0.47
1:B:216:VAL:HG12	1:B:216:VAL:O	2.15	0.47
1:B:222:ALA:HB3	1:B:223:PRO:HD3	1.96	0.47
1:B:580:LEU:CD1	1:B:589:THR:HG23	2.44	0.47
1:B:580:LEU:HD12	1:B:589:THR:HG23	1.96	0.46
1:B:916:GLY:HA3	1:B:1024:SER:HB3	1.97	0.46
1:C:655:LEU:HA	1:C:658:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:HB2	1:C:333:ILE:HG23	1.98	0.46
1:B:76:ARG:NH1	1:B:873:GLU:OE2	2.49	0.46
1:C:410:ILE:O	1:C:414:GLU:HB3	2.16	0.46
1:B:922:TYR:CE1	1:B:926:ILE:HD13	2.50	0.46
1:A:606:THR:HG22	1:A:632:LEU:HD22	1.97	0.46
1:C:38:ILE:HG21	1:C:673:MET:HE1	1.98	0.46
1:C:971:LEU:O	1:C:975:THR:HG22	2.16	0.46
1:A:196:TYR:O	1:A:197:GLN:HG2	2.15	0.45
1:C:426:ASP:OD1	1:C:429:THR:OG1	2.32	0.45
1:A:921:THR:HG21	1:A:939:PHE:HE1	1.80	0.45
1:C:842:MET:HE3	1:C:864:TRP:CE2	2.50	0.45
1:B:383:ILE:CG2	1:B:476:THR:HG21	2.47	0.45
1:B:655:LEU:O	1:B:659:ILE:HG22	2.17	0.45
1:B:985:PRO:O	1:B:989:THR:HG23	2.16	0.45
1:C:984:ARG:HG3	1:C:984:ARG:NH2	2.31	0.45
1:C:14:VAL:O	1:C:18:VAL:HG23	2.17	0.45
1:C:864:TRP:HA	1:C:864:TRP:CE3	2.51	0.45
1:B:916:GLY:HA3	1:B:1024:SER:CB	2.47	0.45
1:B:376:VAL:HG13	1:B:398:MET:CE	2.47	0.45
1:A:1043:ILE:HG23	1:A:1044:PHE:CD2	2.51	0.45
1:A:163:LYS:HB3	1:A:163:LYS:HE2	1.77	0.44
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.87	0.44
1:A:688:ASP:HB2	1:A:697:LEU:HD13	1.98	0.44
1:B:997:VAL:O	1:B:997:VAL:HG22	2.18	0.44
1:C:671:PRO:HG2	1:C:674:PRO:HA	2.00	0.44
1:A:763:PHE:CE1	1:A:770:LYS:HB2	2.53	0.44
1:A:905:SER:N	1:A:1040:ILE:HD13	2.32	0.44
1:A:426:ASP:OD1	1:A:426:ASP:N	2.51	0.44
1:A:1037:TYR:OH	1:A:1041:ARG:NH1	2.51	0.44
1:B:175:VAL:HG12	1:B:289:LEU:HD22	2.00	0.44
1:A:1019:LEU:O	1:A:1022:VAL:HG12	2.17	0.43
1:C:729:GLN:O	1:C:808:GLY:HA2	2.18	0.43
1:C:33:ALA:O	1:C:391:ASN:HA	2.18	0.43
1:C:199:THR:HG22	1:C:201:SER:H	1.83	0.43
1:C:675:GLU:OE1	1:C:675:GLU:N	2.47	0.43
1:C:742:VAL:HG21	1:C:800:VAL:HG21	1.99	0.43
1:B:344:LEU:CD2	1:B:402:ILE:HD13	2.48	0.43
1:C:362:TRP:HA	1:C:365:THR:HG22	1.99	0.43
1:A:78:ILE:HG12	1:A:92:LEU:HD23	2.01	0.43
1:B:587:ASP:O	1:B:591:LYS:HG2	2.19	0.43
1:A:434:SER:O	1:A:438:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD23	1:C:207:LEU:HA	1.87	0.43
1:A:330:THR:N	1:A:331:PRO:CD	2.82	0.43
1:B:115:THR:HA	1:B:118:LEU:HD12	2.01	0.43
1:B:378:GLY:O	1:B:382:VAL:HG23	2.19	0.43
1:C:688:ASP:HB2	1:C:697:LEU:HD13	2.01	0.43
1:C:906:VAL:HG21	1:C:955:ILE:CD1	2.49	0.43
1:C:330:THR:N	1:C:331:PRO:CD	2.82	0.42
1:B:151:ASP:OD1	1:B:151:ASP:N	2.52	0.42
1:B:582:PRO:O	1:B:583:ASN:HB2	2.19	0.42
1:B:762:ASP:OD1	1:B:762:ASP:N	2.52	0.42
1:B:1014:VAL:O	1:B:1018:VAL:HG22	2.19	0.42
1:C:872:ARG:HD3	1:C:872:ARG:HA	1.67	0.42
1:A:783:MET:HE3	1:A:784:PRO:HD2	2.00	0.42
1:A:884:LEU:O	1:A:888:ILE:HG12	2.19	0.42
1:A:850:GLY:O	1:A:853:PRO:HD2	2.19	0.42
1:C:870:GLU:OE2	1:C:870:GLU:HA	2.20	0.42
1:B:347:ALA:O	1:B:351:VAL:HG23	2.19	0.42
1:B:462:THR:HG22	1:B:676:LEU:HD23	1.99	0.42
1:B:645:ILE:O	1:B:649:ILE:HG12	2.20	0.42
1:A:489:THR:OG1	1:A:490:PRO:HD3	2.19	0.42
1:B:915:ILE:O	1:B:919:VAL:HG23	2.20	0.42
1:C:26:THR:HG21	1:C:381:ALA:HA	2.01	0.42
1:C:30:MET:HE2	1:C:384:ASN:HB2	2.01	0.42
1:C:1026:THR:O	1:C:1026:THR:HG22	2.19	0.42
1:A:741:GLY:O	1:A:794:ASN:HB2	2.19	0.42
1:A:148:ASN:OD1	1:A:320:GLY:HA3	2.20	0.42
1:A:189:ASP:OD1	1:A:189:ASP:C	2.63	0.42
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.02	0.42
1:B:169:VAL:HG12	1:B:170:ALA:N	2.35	0.42
1:C:597:THR:HG22	1:C:601:MET:HE2	2.01	0.42
1:A:379:THR:O	1:A:383:ILE:HG12	2.20	0.42
1:C:354:VAL:O	1:C:357:LEU:HB3	2.20	0.42
1:C:938:TYR:CE2	1:C:1010:SER:HB3	2.55	0.42
1:C:990:THR:HG22	1:C:1022:VAL:HG13	2.02	0.42
1:A:984:ARG:O	1:A:987:ILE:HG22	2.19	0.41
1:C:599:PHE:CD2	1:C:655:LEU:HD13	2.55	0.41
1:A:634:ASP:O	1:A:638:ARG:HG3	2.20	0.41
1:A:956:LEU:N	1:A:956:LEU:HD23	2.34	0.41
1:C:294:ALA:O	1:C:295:THR:C	2.62	0.41
1:B:396:PHE:O	1:B:399:VAL:HG22	2.20	0.41
1:A:222:ALA:HB3	1:A:223:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:CE2	1:A:478:MET:HE1	2.55	0.41
1:B:140:ILE:O	1:B:288:GLY:HA2	2.21	0.41
1:C:851:LYS:HB3	1:C:855:MET:HE3	2.03	0.41
1:C:955:ILE:N	1:C:955:ILE:HD13	2.35	0.41
1:B:390:ILE:HG23	1:B:395:MET:HE2	2.03	0.41
1:C:163:LYS:CD	1:C:177:VAL:HG21	2.47	0.41
1:A:193:LEU:HD12	1:A:265:VAL:HB	2.02	0.41
1:A:327:TYR:OH	1:A:670:LEU:HD11	2.21	0.41
1:A:358:PHE:O	1:A:360:GLN:NE2	2.53	0.41
1:B:158:VAL:HG13	1:B:159:ASN:N	2.36	0.41
1:B:372:VAL:O	1:B:376:VAL:HG23	2.21	0.41
1:C:81:ASN:HA	1:C:817:LEU:O	2.21	0.41
1:B:184:MET:HE3	1:B:246:PHE:CD2	2.56	0.41
1:C:500:HIS:O	1:C:500:HIS:CG	2.70	0.41
1:A:588:ARG:NH1	1:A:661:ASP:OD1	2.54	0.40
1:B:212:SER:HB2	1:C:744:ILE:HG22	2.03	0.40
1:B:581:PRO:HD3	1:B:663:SER:OG	2.21	0.40
1:B:635:TRP:CG	1:B:1006:ALA:HB2	2.56	0.40
1:B:160:SER:OG	1:B:161:SER:N	2.54	0.40
1:C:655:LEU:O	1:C:658:ILE:HG22	2.20	0.40
1:A:360:GLN:OE1	1:A:515:PHE:HD2	2.03	0.40
1:A:396:PHE:CE2	1:A:1014:VAL:HG21	2.57	0.40
1:A:405:LEU:C	1:A:405:LEU:HD12	2.46	0.40
1:B:969:GLU:HB2	1:B:974:ALA:HB2	2.02	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	1047/1058 (99%)	1024 (98%)	23 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1045/1058 (99%)	1011 (97%)	33 (3%)	1 (0%)	48 74
1	C	1044/1058 (99%)	1024 (98%)	19 (2%)	1 (0%)	48 74
All	All	3136/3174 (99%)	3059 (98%)	75 (2%)	2 (0%)	49 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	691	GLY
1	C	505	GLU

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	865/874 (99%)	851 (98%)	14 (2%)	55 81
1	B	863/874 (99%)	838 (97%)	25 (3%)	37 68
1	C	862/874 (99%)	833 (97%)	29 (3%)	32 64
All	All	2590/2622 (99%)	2522 (97%)	68 (3%)	41 71

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	193	LEU
1	A	251	LEU
1	A	341	VAL
1	A	366	ILE
1	A	480	LEU
1	A	636	SER
1	A	648	LEU
1	A	649	ILE
1	A	800	VAL
1	A	826	VAL
1	A	857	LEU

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Mol	Chain	Res	Type
1	A	861	ASP
1	A	1018	VAL
1	B	95	GLU
1	B	132	SER
1	B	269	GLU
1	B	321	LEU
1	B	334	ARG
1	B	361	ASN
1	B	411	VAL
1	B	462	THR
1	B	573	VAL
1	B	575	MET
1	B	612	THR
1	B	616	PHE
1	B	657	MET
1	B	676	LEU
1	B	684	LEU
1	B	687	LYS
1	B	690	SER
1	B	698	ILE
1	B	769	VAL
1	B	786	ASP
1	B	800	VAL
1	B	870	GLU
1	B	918	ILE
1	B	937	ILE
1	B	1023	LEU
1	C	67	GLN
1	C	105	VAL
1	C	127	VAL
1	C	186	ILE
1	C	188	LEU
1	C	235	ASN
1	C	314	ARG
1	C	330	THR
1	C	391	ASN
1	C	405	LEU
1	C	414	GLU
1	C	438	ILE
1	C	498	LYS
1	C	511	PHE
1	C	558	PHE

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Mol	Chain	Res	Type
1	C	643	THR
1	C	678	VAL
1	C	730	ILE
1	C	764	VAL
1	C	824	SER
1	C	846	GLU
1	C	863	GLU
1	C	867	LEU
1	C	872	ARG
1	C	912	LEU
1	C	944	ILE
1	C	949	LEU
1	C	955	ILE
1	C	991	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	159	ASN
1	A	342	HIS
1	A	583	ASN
1	A	692	GLN
1	B	104	GLN
1	B	210	GLN
1	B	213	GLN
1	B	237	GLN
1	B	361	ASN
1	B	656	ASN
1	B	694	HIS
1	B	731	ASN
1	B	858	GLN
1	B	936	ASN
1	C	3	GLN
1	C	93	ASN
1	C	342	HIS
1	C	391	ASN
1	C	720	ASN
1	C	729	GLN
1	C	827	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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$
2	3PE	B	1101	-	26,26,50	1.25	2 (7%)	29,31,55	1.41	3 (10%)
2	3PE	C	1104	-	50,50,50	0.96	2 (4%)	53,55,55	0.97	2 (3%)
2	3PE	C	1102	-	38,38,50	1.00	4 (10%)	41,43,55	1.14	2 (4%)
2	3PE	B	1102	-	50,50,50	0.89	4 (8%)	53,55,55	1.08	2 (3%)
2	3PE	C	1103	-	25,25,50	1.24	4 (16%)	28,30,55	1.18	2 (7%)
2	3PE	C	1101	-	27,27,50	1.20	5 (18%)	30,32,55	1.38	2 (6%)
2	3PE	B	1104	-	34,34,50	1.11	2 (5%)	37,39,55	0.99	2 (5%)
2	3PE	B	1103	-	28,28,50	1.15	3 (10%)	31,33,55	1.33	2 (6%)

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
2	3PE	B	1101	-	-	11/30/30/54	-
2	3PE	C	1104	-	-	11/54/54/54	-
2	3PE	C	1102	-	-	14/42/42/54	-
2	3PE	B	1102	-	-	11/54/54/54	-
2	3PE	C	1103	-	-	9/29/29/54	-
2	3PE	C	1101	-	-	7/29/29/54	-
2	3PE	B	1104	-	-	13/38/38/54	-
2	3PE	B	1103	-	-	11/32/32/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1104	3PE	O21-C21	4.52	1.47	1.34
2	B	1104	3PE	O31-C31	4.26	1.45	1.33
2	C	1104	3PE	O31-C31	4.19	1.45	1.33
2	B	1101	3PE	O21-C21	4.17	1.46	1.34
2	B	1104	3PE	O21-C21	4.13	1.46	1.34
2	B	1101	3PE	O31-C31	3.88	1.44	1.33
2	C	1102	3PE	O21-C2	-2.72	1.40	1.46
2	B	1103	3PE	O21-C2	-2.69	1.40	1.46
2	C	1101	3PE	P-O13	2.61	1.64	1.54
2	C	1103	3PE	O31-C31	2.60	1.40	1.33
2	C	1103	3PE	O21-C2	-2.57	1.40	1.46
2	B	1103	3PE	O31-C31	2.53	1.40	1.33
2	B	1102	3PE	O21-C2	-2.45	1.40	1.46
2	C	1101	3PE	O31-C3	-2.44	1.39	1.45
2	C	1102	3PE	O31-C31	2.40	1.40	1.33
2	B	1102	3PE	O31-C31	2.38	1.40	1.33
2	C	1101	3PE	O21-C2	-2.32	1.41	1.46
2	C	1103	3PE	O21-C21	2.32	1.40	1.34
2	C	1101	3PE	O31-C31	2.28	1.40	1.33
2	B	1102	3PE	O21-C21	2.28	1.40	1.34
2	C	1101	3PE	O21-C21	2.18	1.40	1.34
2	C	1102	3PE	O31-C3	-2.18	1.40	1.45
2	C	1102	3PE	O21-C21	2.14	1.40	1.34
2	C	1103	3PE	O31-C3	-2.07	1.40	1.45
2	B	1102	3PE	O31-C3	-2.05	1.40	1.45
2	B	1103	3PE	O21-C21	2.04	1.40	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	3PE	O21-C21-C22	5.26	122.86	111.48
2	C	1101	3PE	O21-C21-C22	4.81	121.89	111.48
2	B	1103	3PE	O21-C21-C22	4.71	121.66	111.48
2	C	1102	3PE	O21-C21-C22	4.21	120.60	111.48
2	C	1104	3PE	O21-C21-C22	4.18	120.53	111.48
2	B	1102	3PE	O21-C21-C22	4.08	120.31	111.48
2	C	1103	3PE	O21-C21-C22	3.94	120.00	111.48
2	B	1104	3PE	O21-C21-C22	3.61	119.29	111.48
2	B	1102	3PE	O31-C31-C32	3.39	122.17	111.83
2	B	1103	3PE	O31-C31-C32	2.95	120.83	111.83
2	C	1102	3PE	O31-C31-C32	2.87	120.59	111.83
2	B	1101	3PE	O31-C31-C32	2.72	120.12	111.83
2	C	1101	3PE	O31-C31-C32	2.70	120.08	111.83
2	B	1101	3PE	O31-C31-O32	-2.59	117.15	123.63
2	C	1103	3PE	O31-C31-C32	2.52	119.52	111.83
2	C	1104	3PE	O31-C31-C32	2.51	119.49	111.83
2	B	1104	3PE	O31-C31-C32	2.36	119.02	111.83

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	3PE	C1-O11-P-O12
2	B	1101	3PE	C11-O13-P-O11
2	B	1101	3PE	C2-C1-O11-P
2	B	1101	3PE	O21-C2-C3-O31
2	B	1103	3PE	C1-O11-P-O12
2	B	1103	3PE	C11-O13-P-O11
2	B	1103	3PE	C11-O13-P-O12
2	B	1103	3PE	C11-O13-P-O14
2	C	1102	3PE	C1-O11-P-O12
2	C	1102	3PE	C1-O11-P-O13
2	C	1102	3PE	C1-O11-P-O14
2	C	1103	3PE	C11-O13-P-O12
2	C	1103	3PE	C11-O13-P-O14
2	C	1104	3PE	C2-C1-O11-P
2	C	1104	3PE	C32-C31-O31-C3
2	C	1104	3PE	O32-C31-O31-C3
2	C	1104	3PE	C39-C3A-C3B-C3C
2	B	1102	3PE	C26-C27-C28-C29
2	C	1104	3PE	C3D-C3E-C3F-C3G
2	B	1104	3PE	C36-C37-C38-C39
2	C	1104	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
2	B	1101	3PE	C32-C31-O31-C3
2	B	1101	3PE	C24-C25-C26-C27
2	B	1104	3PE	C22-C21-O21-C2
2	B	1104	3PE	C23-C24-C25-C26
2	C	1104	3PE	C37-C38-C39-C3A
2	C	1103	3PE	C32-C33-C34-C35
2	B	1102	3PE	C32-C31-O31-C3
2	B	1104	3PE	O11-C1-C2-O21
2	C	1101	3PE	C32-C31-O31-C3
2	B	1104	3PE	O22-C21-O21-C2
2	B	1101	3PE	C1-C2-C3-O31
2	B	1101	3PE	O32-C31-O31-C3
2	C	1101	3PE	O32-C31-O31-C3
2	B	1102	3PE	O32-C31-O31-C3
2	C	1101	3PE	C28-C29-C2A-C2B
2	B	1103	3PE	O31-C31-C32-C33
2	B	1104	3PE	O11-C1-C2-C3
2	B	1102	3PE	C33-C34-C35-C36
2	C	1101	3PE	O21-C2-C3-O31
2	C	1102	3PE	C31-C32-C33-C34
2	B	1104	3PE	C3-C2-O21-C21
2	B	1103	3PE	O11-C1-C2-O21
2	C	1101	3PE	C1-C2-C3-O31
2	B	1104	3PE	C26-C27-C28-C29
2	B	1103	3PE	O11-C1-C2-C3
2	B	1101	3PE	O21-C21-C22-C23
2	B	1102	3PE	C2E-C2F-C2G-C2H
2	C	1104	3PE	C23-C24-C25-C26
2	B	1101	3PE	C1-O11-P-O13
2	B	1101	3PE	C11-O13-P-O14
2	B	1103	3PE	C1-O11-P-O13
2	B	1103	3PE	C1-O11-P-O14
2	C	1103	3PE	C1-O11-P-O12
2	C	1103	3PE	C1-O11-P-O13
2	C	1103	3PE	C1-O11-P-O14
2	C	1104	3PE	C1-O11-P-O12
2	C	1104	3PE	C1-O11-P-O13
2	C	1104	3PE	C1-O11-P-O14
2	C	1102	3PE	C23-C24-C25-C26
2	B	1102	3PE	C29-C2A-C2B-C2C
2	C	1102	3PE	C28-C29-C2A-C2B
2	C	1101	3PE	C31-C32-C33-C34

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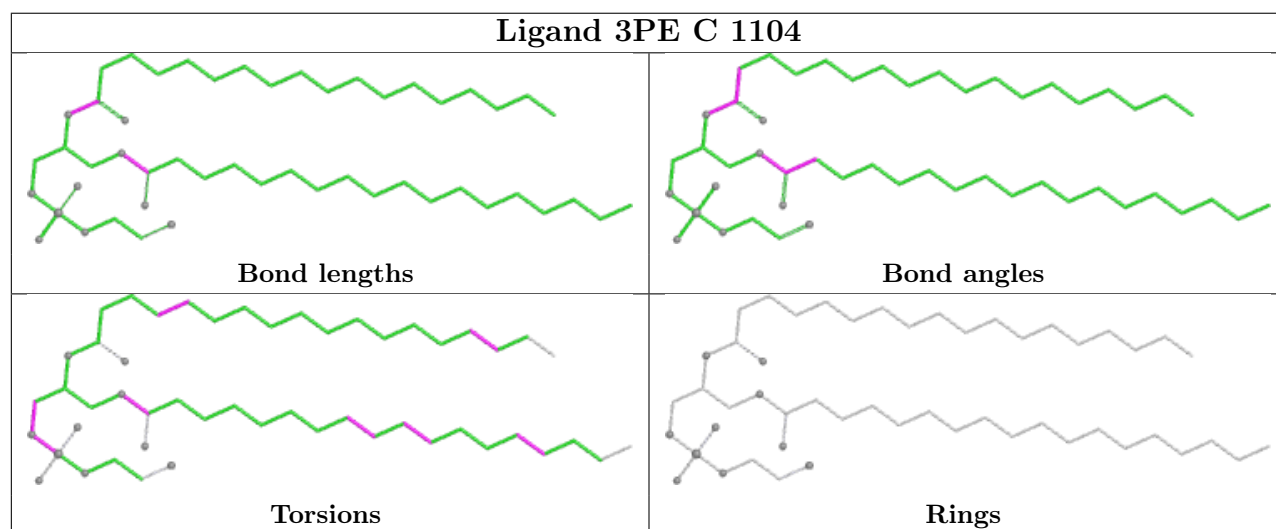
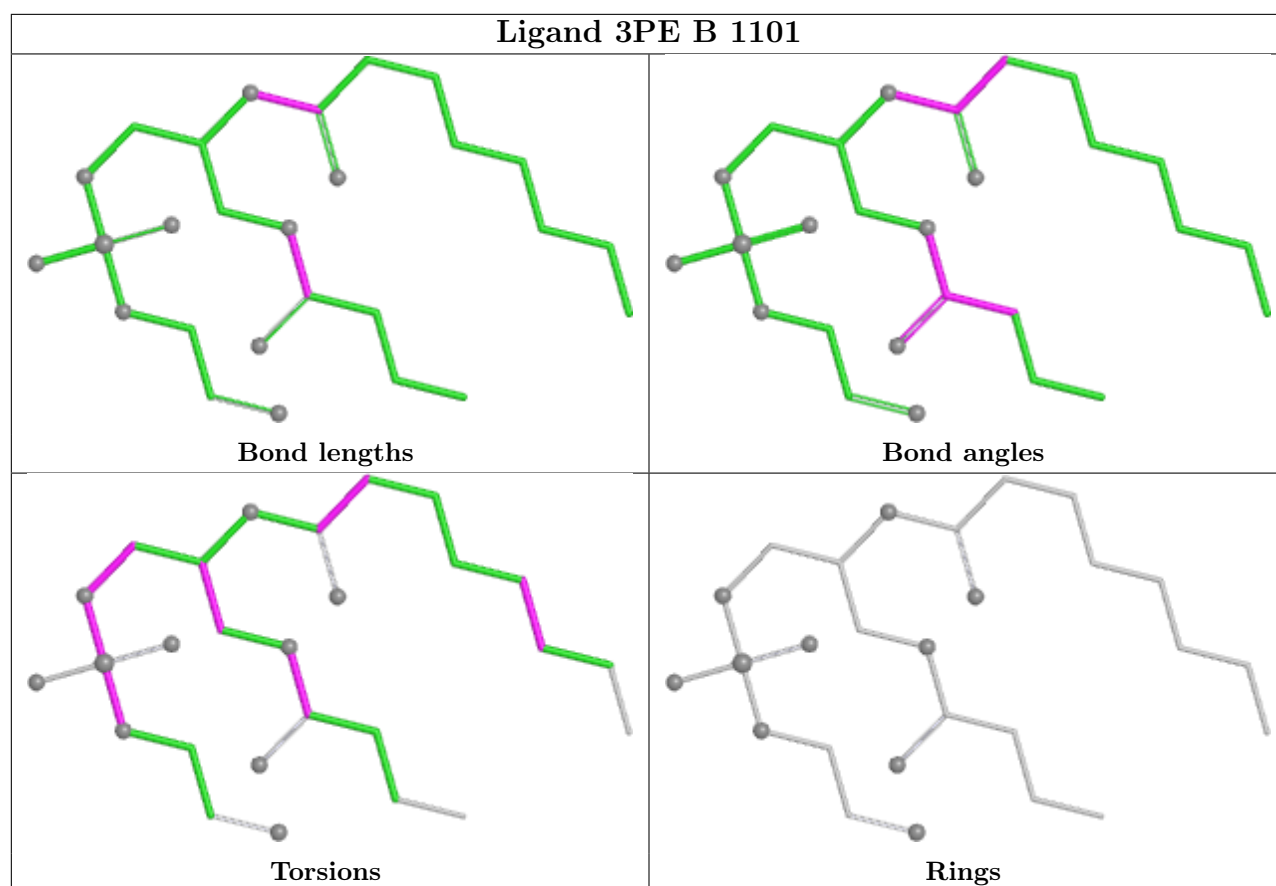
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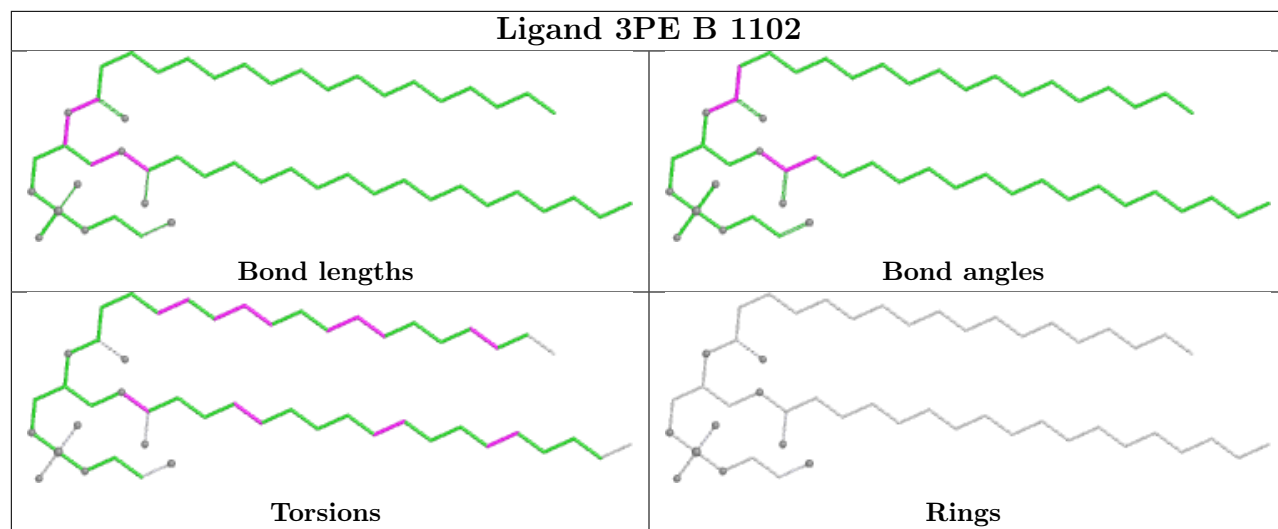
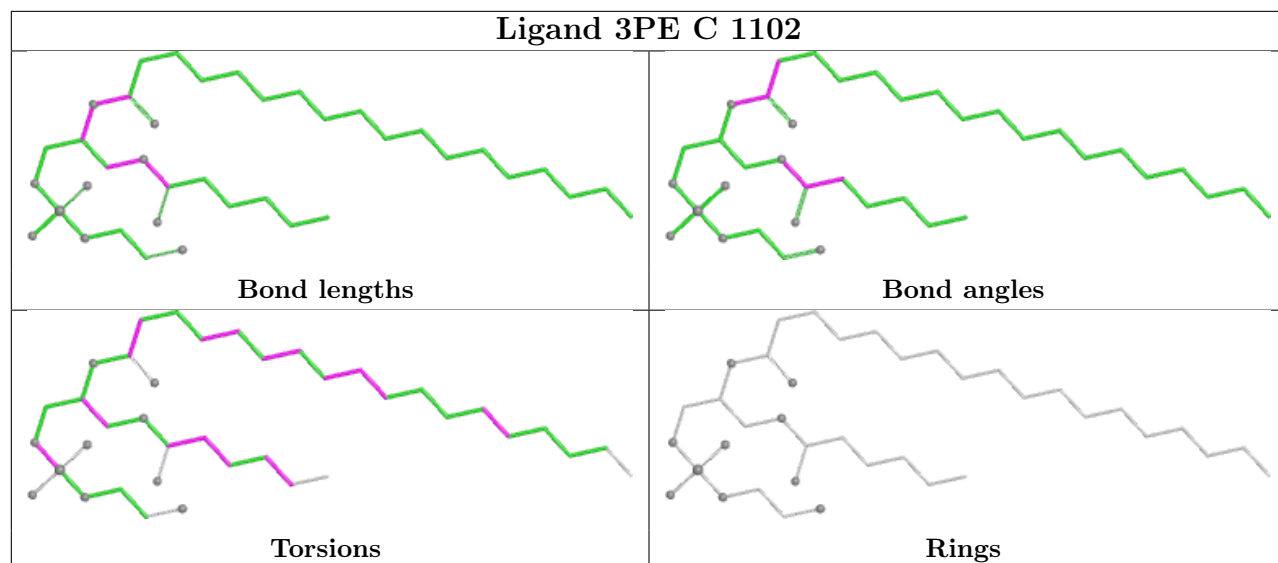
Mol	Chain	Res	Type	Atoms
2	C	1102	3PE	C27-C28-C29-C2A
2	C	1102	3PE	C25-C26-C27-C28
2	C	1103	3PE	O22-C21-O21-C2
2	C	1102	3PE	C33-C34-C35-C36
2	B	1103	3PE	O32-C31-C32-C33
2	B	1104	3PE	C2-C1-O11-P
2	B	1102	3PE	C3C-C3D-C3E-C3F
2	C	1103	3PE	C22-C21-O21-C2
2	B	1104	3PE	C32-C33-C34-C35
2	B	1104	3PE	C25-C26-C27-C28
2	C	1102	3PE	O21-C2-C3-O31
2	C	1102	3PE	C2C-C2D-C2E-C2F
2	C	1102	3PE	O31-C31-C32-C33
2	B	1102	3PE	C38-C39-C3A-C3B
2	B	1102	3PE	C2A-C2B-C2C-C2D
2	C	1102	3PE	O21-C21-C22-C23
2	B	1103	3PE	C33-C34-C35-C36
2	B	1104	3PE	C35-C36-C37-C38
2	C	1101	3PE	O21-C21-C22-C23
2	B	1104	3PE	C22-C23-C24-C25
2	C	1102	3PE	O22-C21-C22-C23
2	B	1102	3PE	C25-C26-C27-C28
2	B	1102	3PE	C23-C24-C25-C26
2	C	1103	3PE	O31-C31-C32-C33

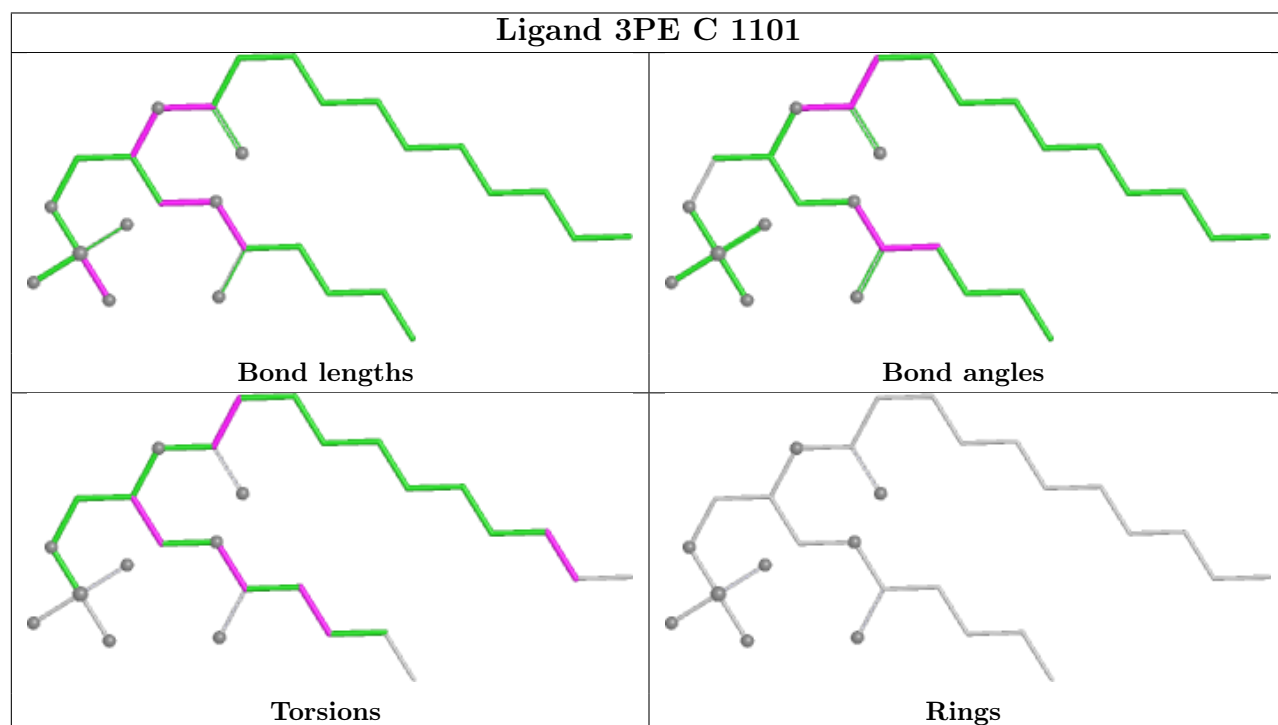
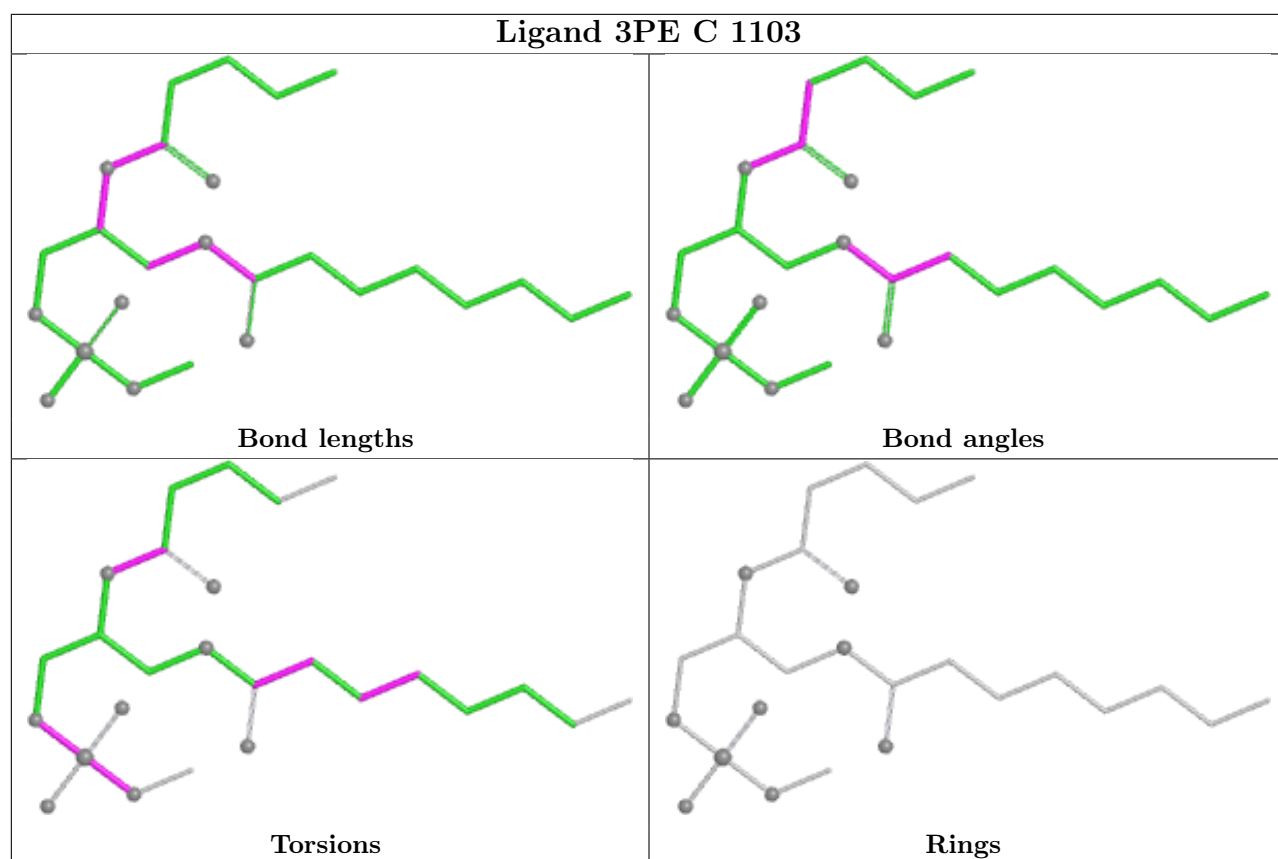
There are no ring outliers.

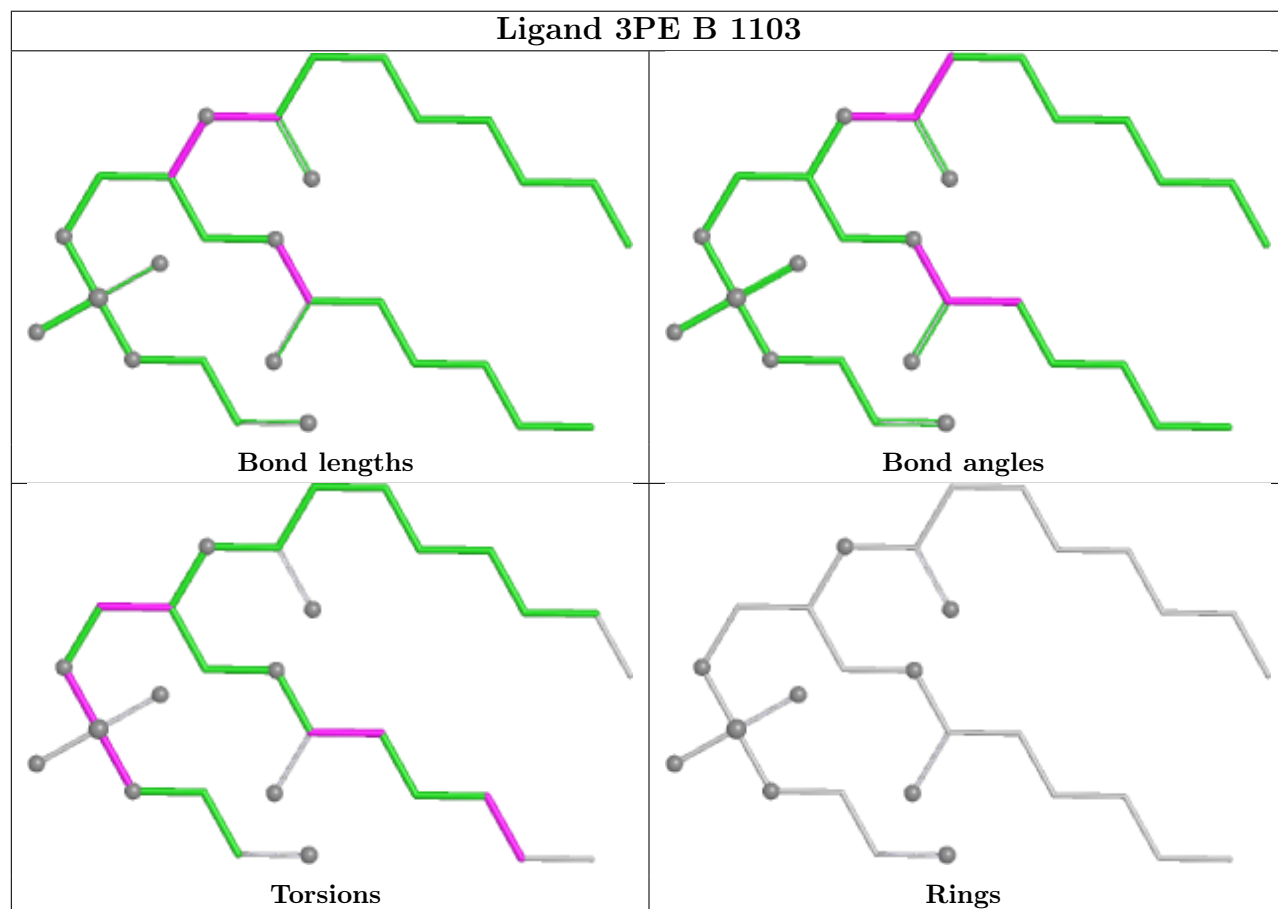
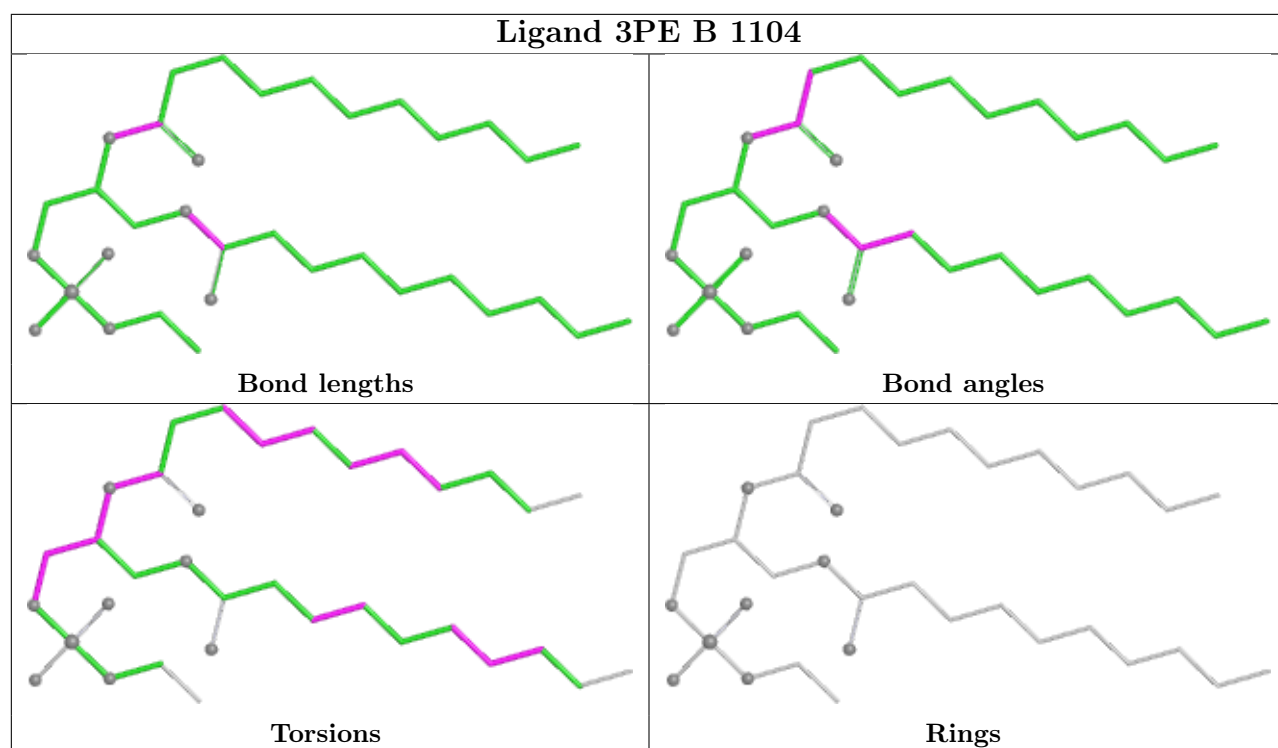
No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

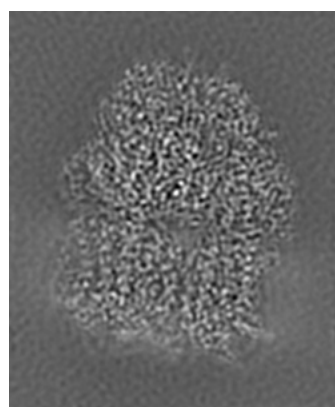
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23664. These allow visual inspection of the internal detail of the map and identification of artifacts.

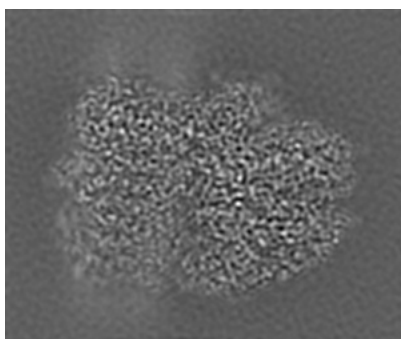
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

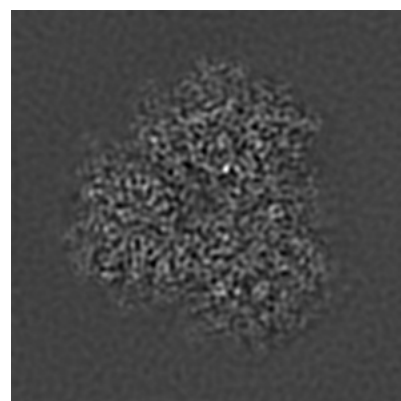
6.1.1 Primary map



X



Y

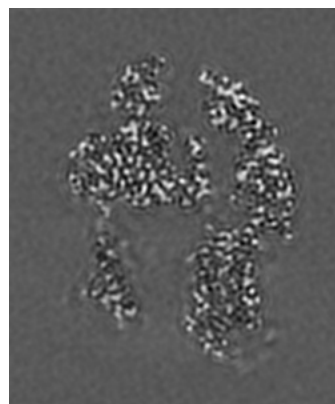


Z

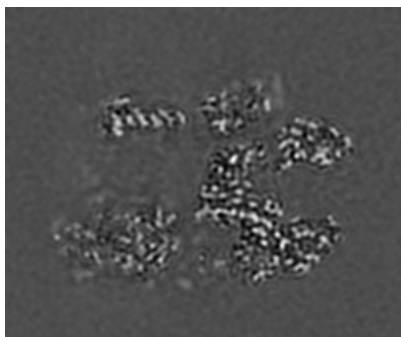
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

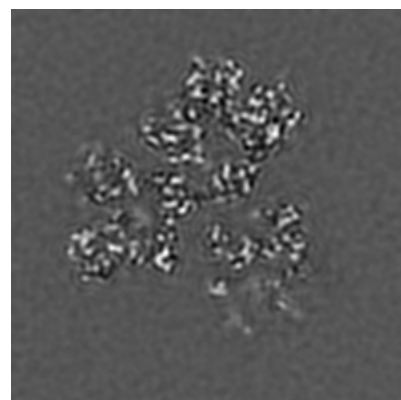
6.2.1 Primary map



X Index: 66



Y Index: 65

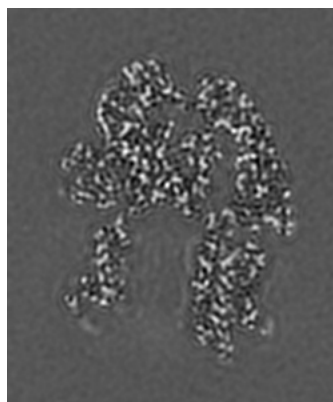


Z Index: 80

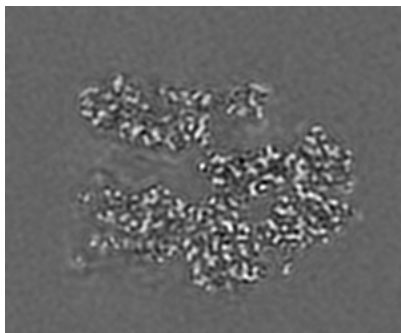
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

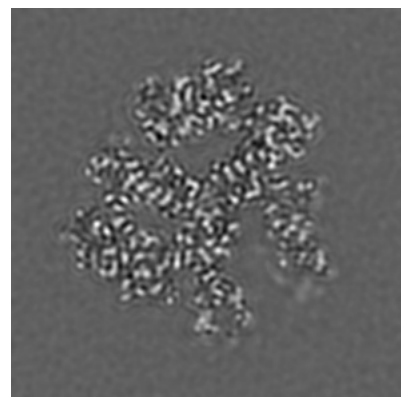
6.3.1 Primary map



X Index: 70



Y Index: 52

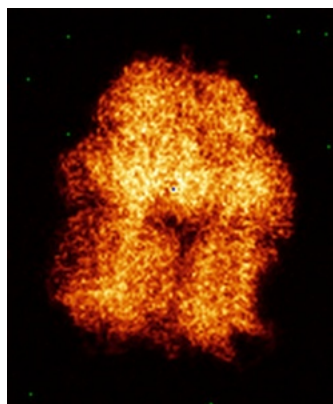


Z Index: 93

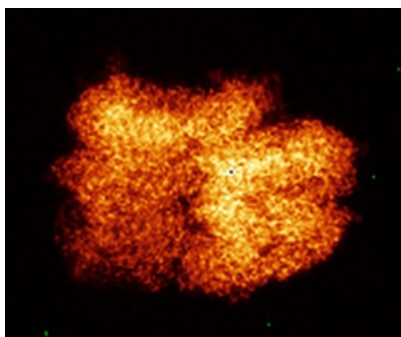
The images above show the largest variance slices of the map in three orthogonal directions.

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

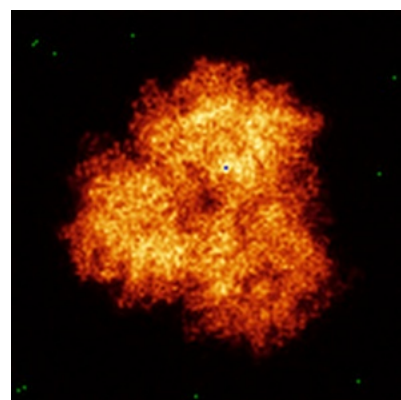
6.4.1 Primary map



X



Y

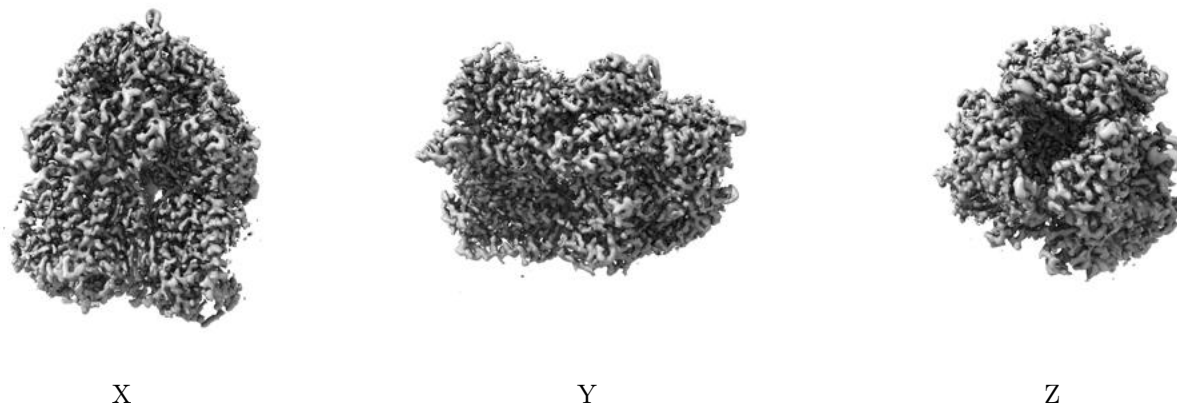


Z

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 0.192. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

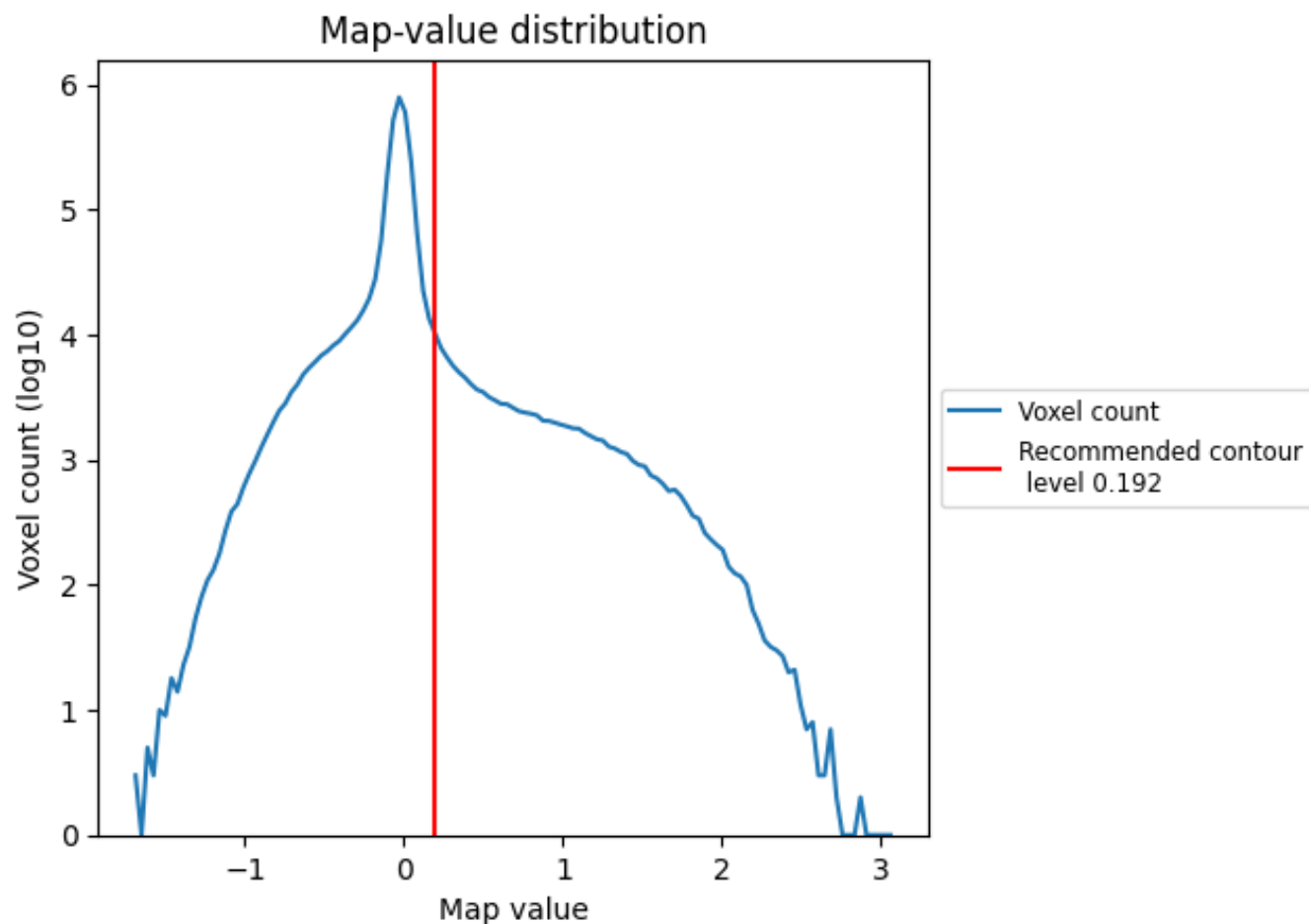
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

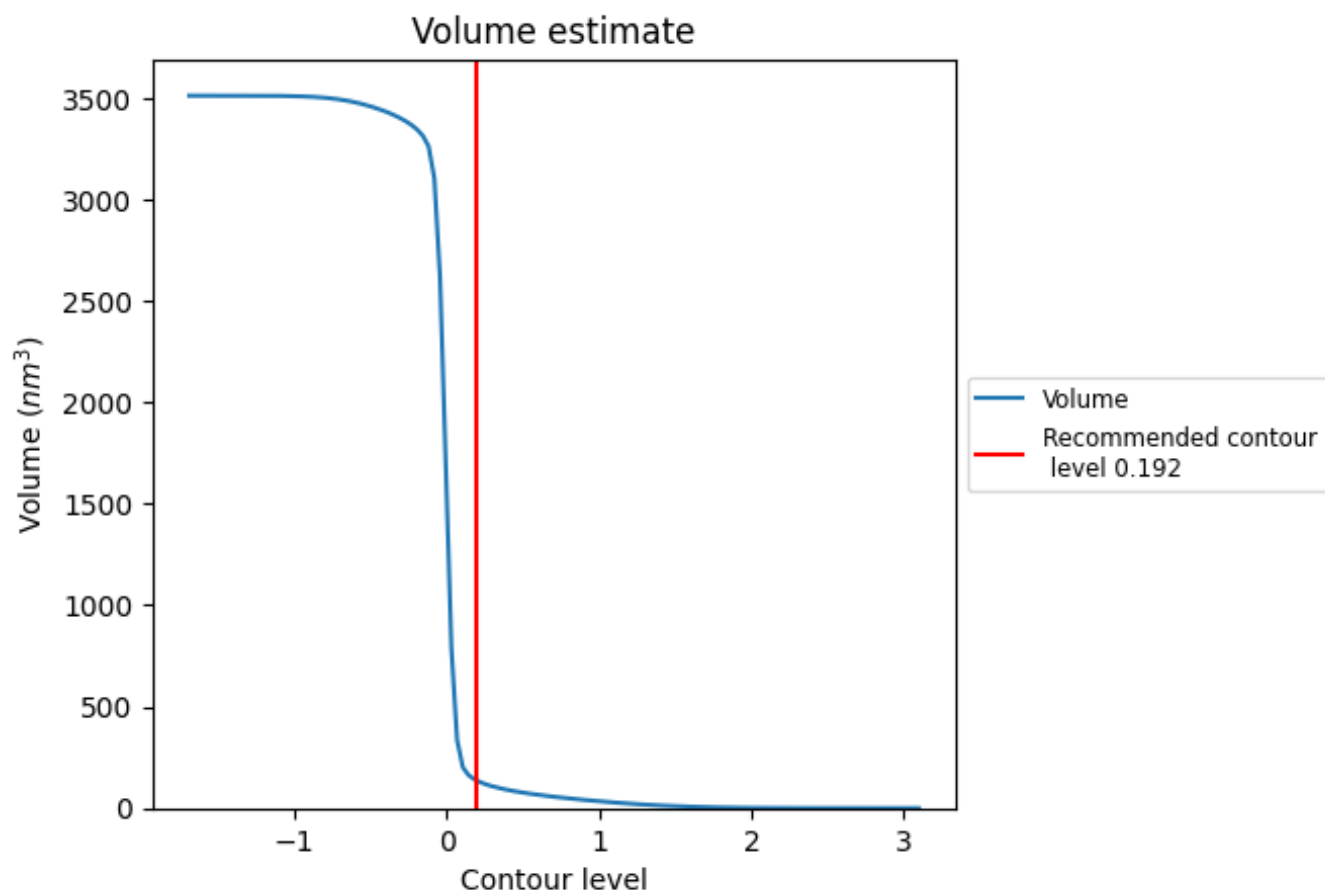
This section contains the results of statistical analysis of the map.

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 139 nm³; this corresponds to an approximate mass of 125 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

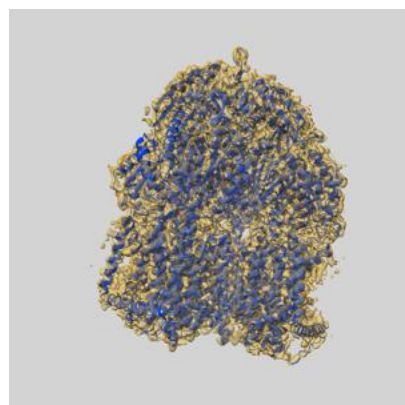
8 Fourier-Shell correlation

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

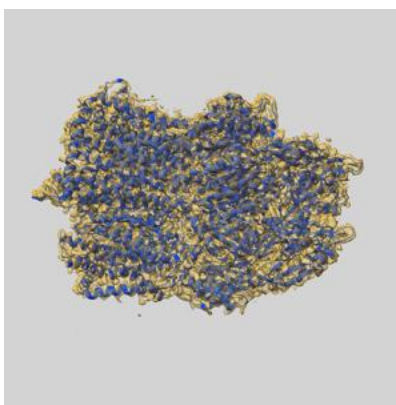
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23664 and PDB model 7M4Q. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

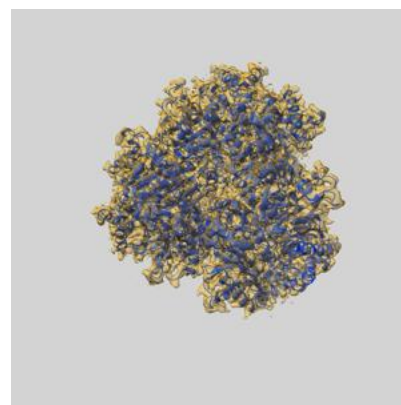
9.1 Map-model overlay [i](#)



X



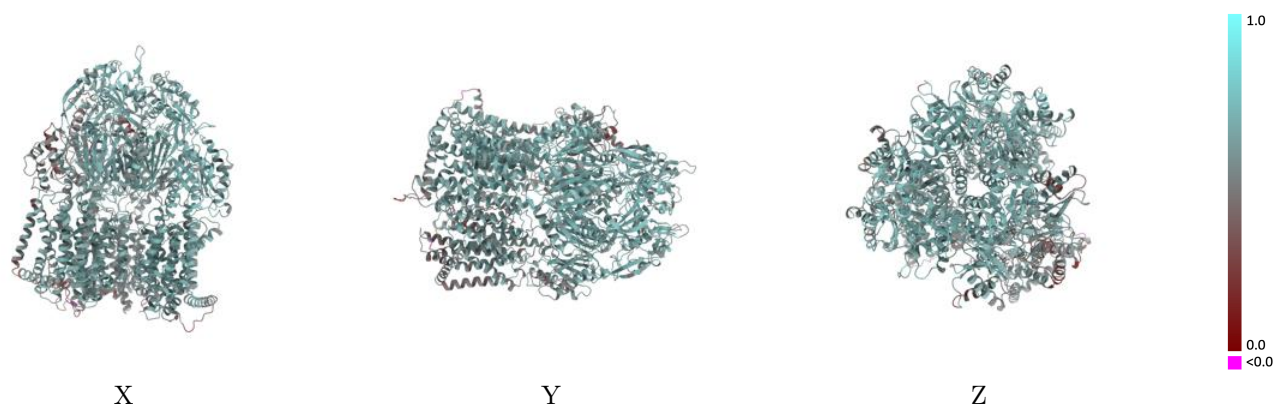
Y



Z

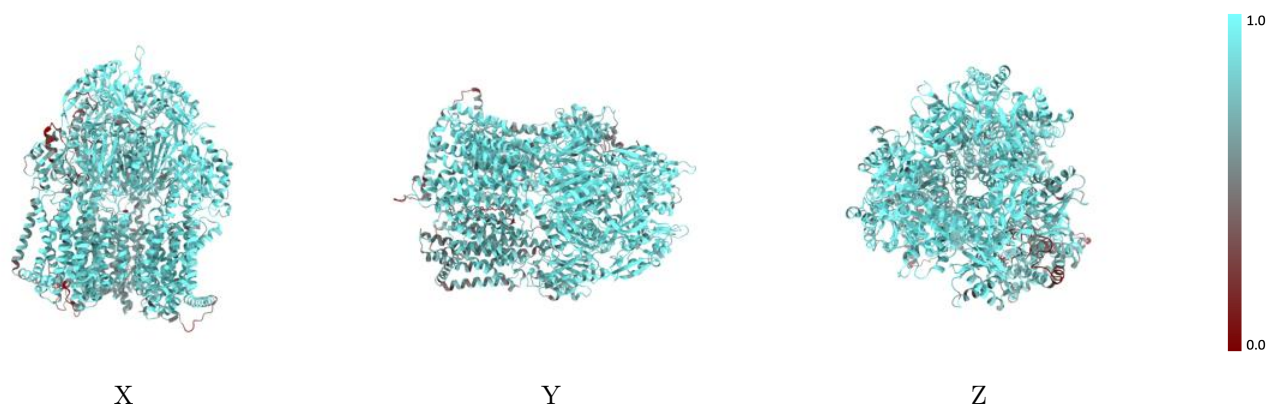
The images above show the 3D surface view of the map at the recommended contour level 0.192 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



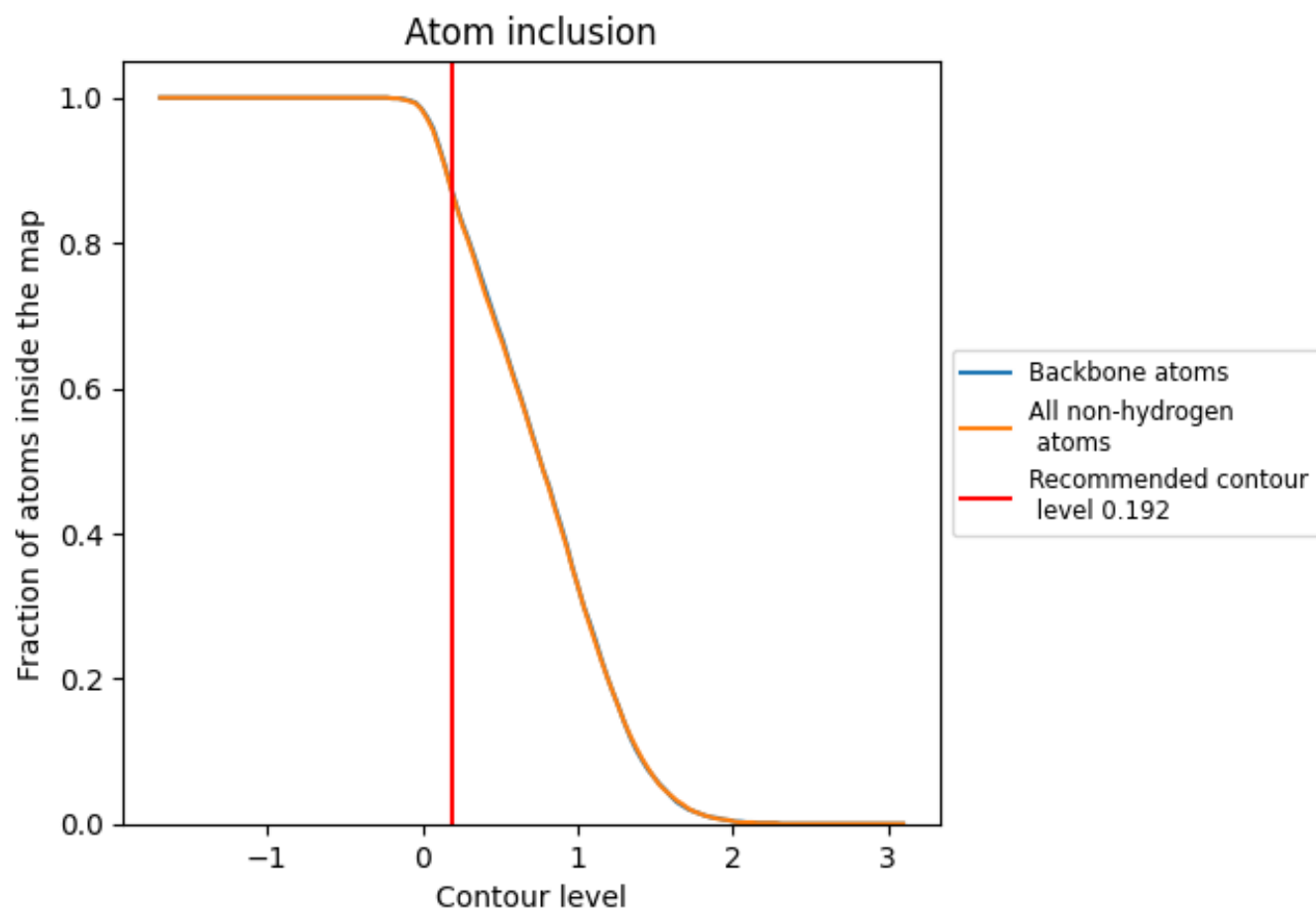
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.192).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.6010
A	0.8590	0.5950
B	0.8390	0.5820
C	0.9160	0.6270

