



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 12:29 AM JST

PDB ID : 6AEI
EMDB ID : EMD-9615
Title : Cryo-EM structure of the receptor-activated TRPC5 ion channel
Authors : Duan, J.; Li, Z.; Li, J.; Zhang, J.
Deposited on : 2018-08-05
Resolution : 2.89 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

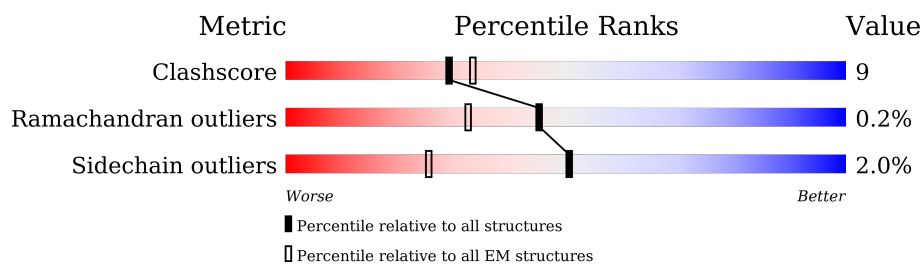
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	765	<div> <div>7%</div> <div>69%</div> <div>14%</div> <div>•</div> <div>16%</div> </div>
1	B	765	<div> <div>10%</div> <div>69%</div> <div>14%</div> <div>•</div> <div>16%</div> </div>
1	C	765	<div> <div>15%</div> <div>70%</div> <div>13%</div> <div>•</div> <div>16%</div> </div>
1	D	765	<div> <div>10%</div> <div>71%</div> <div>13%</div> <div>•</div> <div>16%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

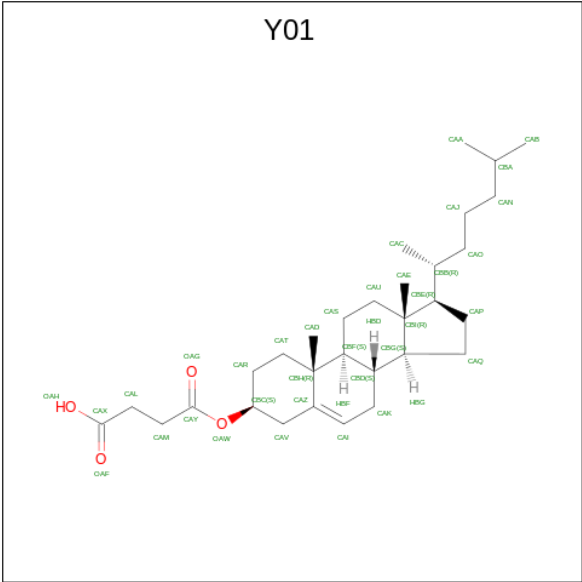
- Molecule 1 is a protein called Short transient receptor potential channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	642	Total	C	N	O	S	0	0
			5207	3404	851	926	26		
1	B	642	Total	C	N	O	S	0	0
			5204	3401	851	926	26		
1	C	642	Total	C	N	O	S	0	0
			5205	3402	851	926	26		
1	D	642	Total	C	N	O	S	0	0
			5205	3402	851	926	26		

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

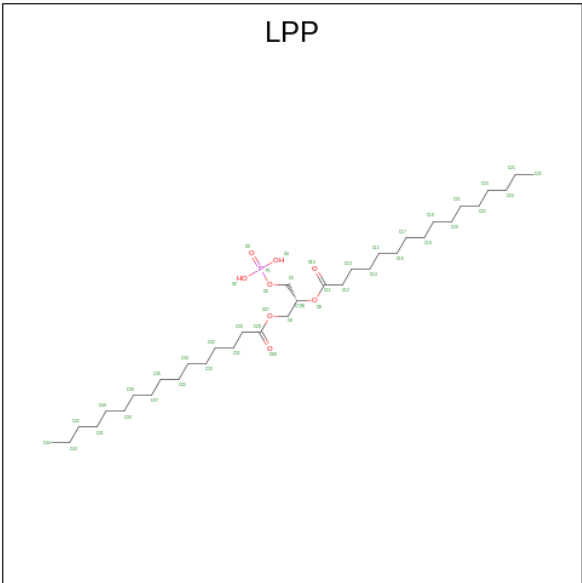
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Na	0
			2	2	
2	B	1	Total	Na	0
			1	1	
2	C	1	Total	Na	0
			1	1	
2	D	1	Total	Na	0
			1	1	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	C	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	

- Molecule 4 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P).

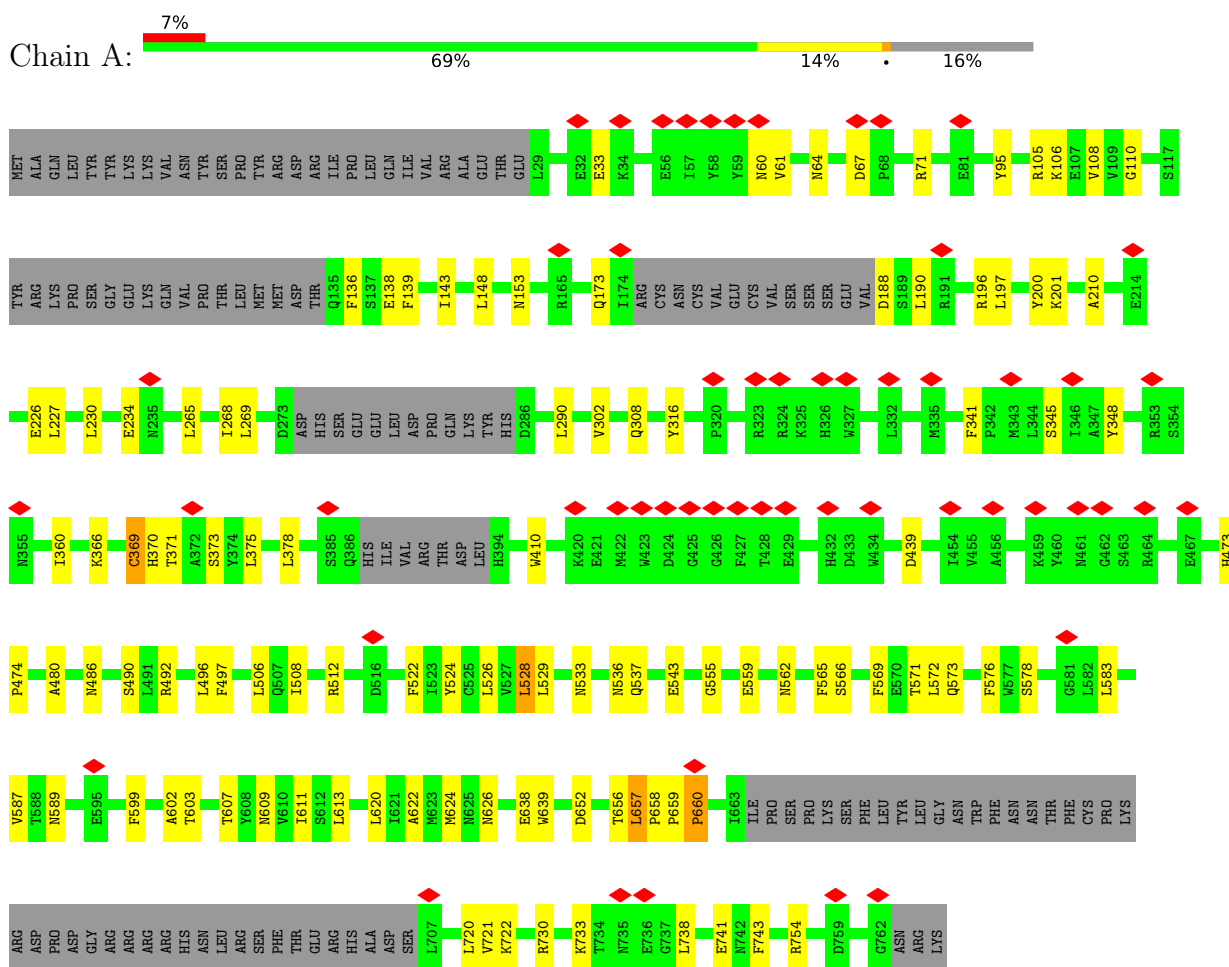


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 44	C 35	O 8	P 1	0
4	B	1	Total 44	C 35	O 8	P 1	0
4	C	1	Total 44	C 35	O 8	P 1	0
4	D	1	Total 44	C 35	O 8	P 1	0

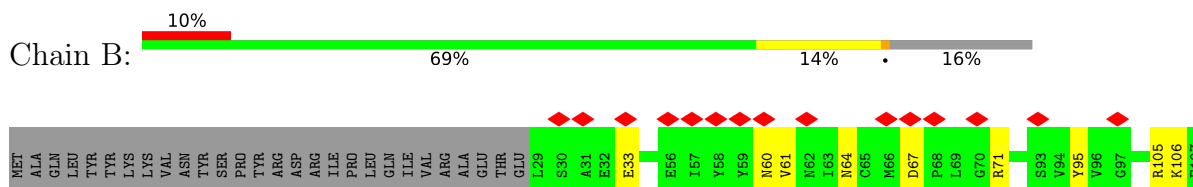
3 Residue-property plots

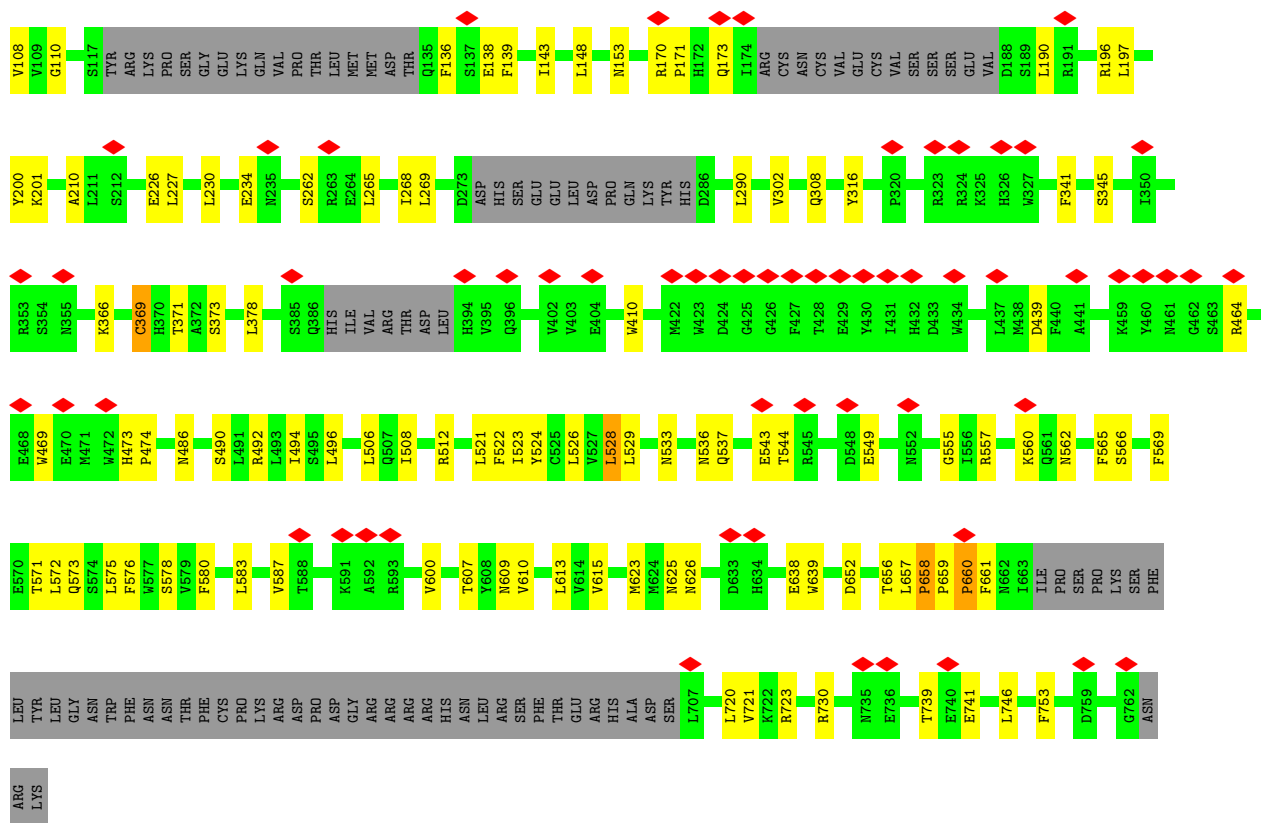
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Short transient receptor potential channel 5

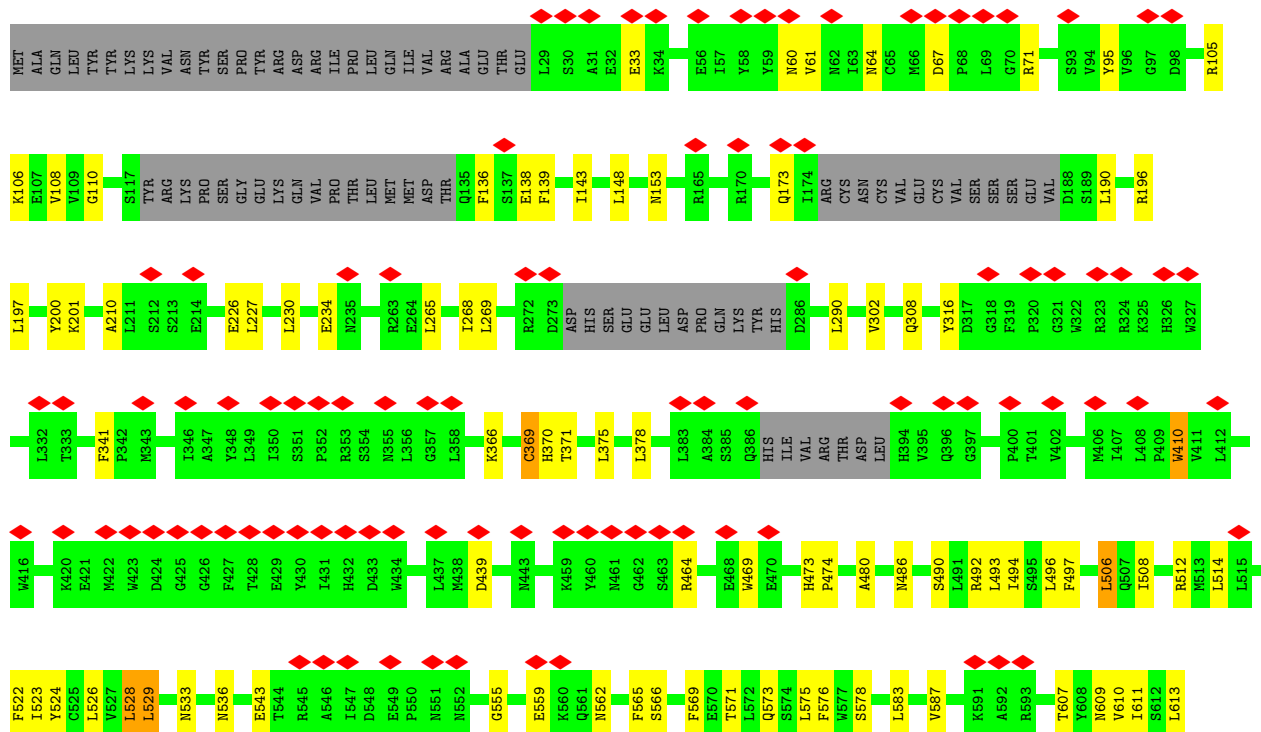


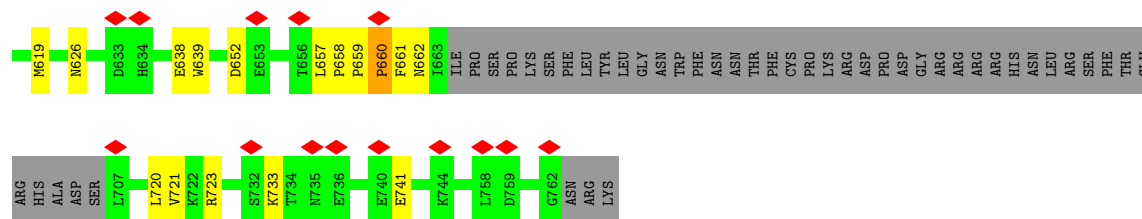
- Molecule 1: Short transient receptor potential channel 5



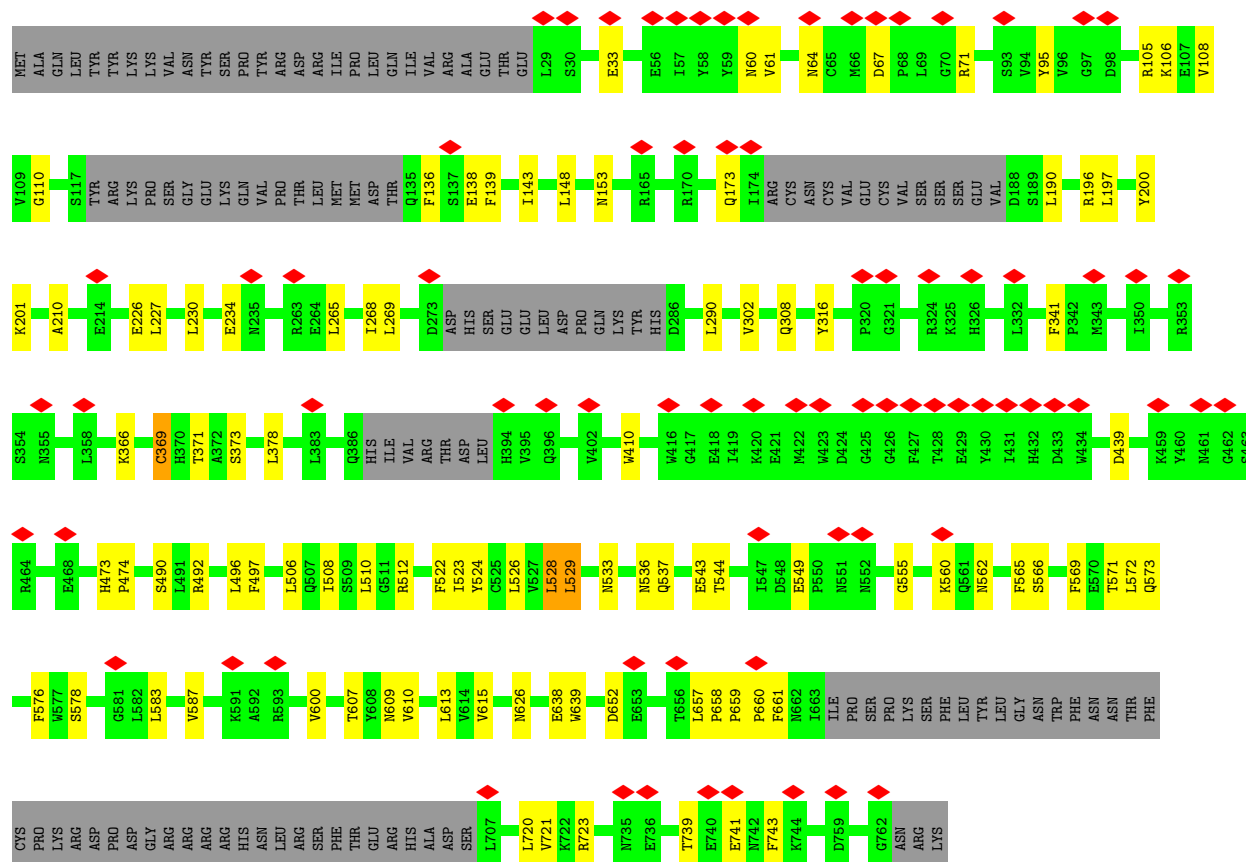


• Molecule 1: Short transient receptor potential channel 5





• Molecule 1: Short transient receptor potential channel 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	1164065	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 ($e^-/\text{\AA}^2$)	42.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.259	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.058	Depositor
Map size (\AA)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	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: Y01, NA, LPP

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	0.34	0/5331	0.57	0/7228
1	B	0.34	0/5328	0.57	0/7224
1	C	0.33	0/5328	0.57	0/7223
1	D	0.33	0/5328	0.57	0/7223
All	All	0.34	0/21315	0.57	0/28898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5207	0	5226	125	0
1	B	5204	0	5217	110	0
1	C	5205	0	5220	106	0
1	D	5205	0	5220	77	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	35	0	49	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	49	17	0
3	C	35	0	49	14	0
3	D	35	0	49	11	0
4	A	44	0	67	16	0
4	B	44	0	67	17	0
4	C	44	0	67	15	0
4	D	44	0	67	11	0
All	All	21142	0	21347	388	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 9.

All (388) 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:529:LEU:CD1	3:B:802:Y01:HAA1	1.54	1.36
1:C:657:LEU:HD12	1:C:658:PRO:CD	1.64	1.28
1:C:657:LEU:CD1	1:C:658:PRO:HD3	1.68	1.24
1:C:657:LEU:CG	1:C:658:PRO:HD2	1.68	1.21
1:C:657:LEU:O	1:C:662:ASN:HB2	1.40	1.20
1:A:529:LEU:CD1	3:B:802:Y01:CAA	2.21	1.18
1:A:657:LEU:CB	1:A:659:PRO:HD3	1.75	1.17
1:A:529:LEU:HD12	3:B:802:Y01:CAA	1.75	1.17
1:D:657:LEU:HD12	1:D:658:PRO:CD	1.74	1.16
1:C:657:LEU:CD1	1:C:658:PRO:CD	2.23	1.16
1:A:607:THR:HG22	4:B:803:LPP:H311	1.12	1.11
1:B:529:LEU:HD12	3:C:802:Y01:HAA1	1.33	1.10
1:A:496:LEU:HD23	3:A:803:Y01:CAD	1.84	1.08
1:C:657:LEU:HG	1:C:658:PRO:HD2	1.08	1.08
1:C:607:THR:HG22	4:D:803:LPP:H311	1.36	1.06
1:B:526:LEU:HD21	1:C:494:ILE:HG13	1.38	1.05
1:C:496:LEU:HD23	3:C:802:Y01:CAD	1.87	1.05
1:A:657:LEU:HB3	1:A:659:PRO:HD3	1.38	1.03
1:D:657:LEU:HD12	1:D:658:PRO:HD2	1.04	1.02
1:C:657:LEU:CG	1:C:658:PRO:CD	2.36	1.02
1:D:657:LEU:CD1	1:D:658:PRO:HD2	1.90	1.01
1:B:576:PHE:CE2	4:B:803:LPP:HC82	1.95	1.01
1:D:576:PHE:CE2	4:D:803:LPP:HC82	1.97	1.00
1:A:529:LEU:HD11	3:B:802:Y01:CAA	1.91	0.98
1:B:496:LEU:HD23	3:B:802:Y01:CAD	1.98	0.93
1:A:607:THR:CG2	4:B:803:LPP:H311	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HB2	1:A:659:PRO:CD	1.99	0.92
1:B:529:LEU:HD12	3:C:802:Y01:CAA	2.01	0.90
4:A:804:LPP:H311	1:D:607:THR:HG22	1.55	0.89
1:C:657:LEU:O	1:C:662:ASN:CB	2.21	0.88
1:C:573:GLN:HG2	4:C:803:LPP:O4	1.74	0.88
1:A:657:LEU:CB	1:A:659:PRO:CD	2.52	0.87
1:B:573:GLN:HG2	4:B:803:LPP:O4	1.74	0.86
1:C:657:LEU:CD1	1:C:658:PRO:HD2	1.98	0.85
1:C:657:LEU:HG	1:C:658:PRO:CD	1.98	0.85
1:A:529:LEU:HD12	3:B:802:Y01:HAA1	0.86	0.84
1:D:496:LEU:HD23	3:D:802:Y01:CAD	2.08	0.84
1:A:370:HIS:HA	1:A:657:LEU:HD12	1.57	0.84
1:A:607:THR:HG22	4:B:803:LPP:C31	2.03	0.82
1:B:526:LEU:CD2	1:C:494:ILE:CG1	2.57	0.82
1:B:526:LEU:HD21	1:C:494:ILE:CG1	2.10	0.81
1:B:529:LEU:CD1	3:C:802:Y01:HAA1	2.09	0.79
1:B:529:LEU:HD23	1:B:572:LEU:HD21	1.64	0.79
1:B:607:THR:HG22	4:C:803:LPP:H311	1.63	0.79
1:B:610:VAL:HG11	4:C:803:LPP:H331	1.65	0.79
1:C:657:LEU:HD12	1:C:658:PRO:HD3	0.82	0.79
1:A:524:TYR:CE2	4:A:804:LPP:H221	2.18	0.79
1:B:529:LEU:CD1	3:C:802:Y01:CAA	2.61	0.78
1:B:373:SER:OG	1:B:659:PRO:HG3	1.84	0.77
1:B:136:PHE:HE1	1:C:723:ARG:HB3	1.49	0.77
1:B:576:PHE:CD2	4:B:803:LPP:HC82	2.20	0.77
1:C:576:PHE:CE2	4:C:803:LPP:HC82	2.20	0.76
1:B:526:LEU:HD11	1:C:493:LEU:HB2	1.67	0.75
1:C:524:TYR:CE2	4:C:803:LPP:H221	2.22	0.74
1:B:526:LEU:CD2	1:C:494:ILE:HG13	2.14	0.73
1:A:569:PHE:O	1:A:573:GLN:HG3	1.89	0.73
1:D:576:PHE:CD2	4:D:803:LPP:HC82	2.23	0.73
1:B:573:GLN:CG	4:B:803:LPP:O4	2.36	0.73
1:A:657:LEU:C	1:A:659:PRO:HD3	2.10	0.72
4:A:804:LPP:H331	1:D:610:VAL:HG11	1.69	0.72
1:B:528:LEU:CD2	1:B:575:LEU:HB2	2.19	0.72
1:A:657:LEU:C	1:A:659:PRO:CD	2.58	0.72
1:B:659:PRO:O	1:B:660:PRO:CB	2.37	0.71
1:B:526:LEU:CD2	1:C:494:ILE:HG12	2.19	0.71
1:B:657:LEU:CB	1:B:659:PRO:HD3	2.22	0.69
1:A:573:GLN:CD	4:A:804:LPP:O4	2.30	0.69
1:C:370:HIS:ND1	1:C:657:LEU:CD1	2.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HD23	3:A:803:Y01:HAD3	1.75	0.68
1:C:573:GLN:CG	4:C:803:LPP:O4	2.42	0.67
1:A:524:TYR:CE2	4:A:804:LPP:C22	2.78	0.67
1:A:573:GLN:CG	4:A:804:LPP:O4	2.42	0.66
1:A:108:VAL:HG12	1:A:110:GLY:H	1.61	0.66
1:D:569:PHE:O	1:D:573:GLN:HG3	1.94	0.66
1:D:543:GLU:HG2	1:D:566:SER:HB2	1.78	0.66
1:C:576:PHE:CD2	4:C:803:LPP:HC82	2.31	0.66
1:D:108:VAL:HG12	1:D:110:GLY:H	1.61	0.66
1:B:108:VAL:HG12	1:B:110:GLY:H	1.61	0.65
1:B:573:GLN:CD	4:B:803:LPP:O4	2.35	0.65
1:A:657:LEU:N	1:A:657:LEU:HD22	2.12	0.65
1:C:543:GLU:HG2	1:C:566:SER:HB2	1.78	0.64
1:A:611:ILE:HG12	4:B:803:LPP:H392	1.79	0.64
1:A:360:ILE:HD11	1:A:657:LEU:HD21	1.79	0.64
1:A:496:LEU:HD23	3:A:803:Y01:HAD1	1.75	0.64
1:C:341:PHE:HB3	1:C:369:CYS:HB2	1.79	0.64
1:C:524:TYR:CE2	4:C:803:LPP:C22	2.79	0.64
1:A:543:GLU:HG2	1:A:566:SER:HB2	1.78	0.64
1:B:543:GLU:HG2	1:B:566:SER:HB2	1.78	0.64
1:B:659:PRO:HD2	1:B:661:PHE:CD2	2.32	0.64
1:A:370:HIS:CG	1:A:657:LEU:HD13	2.33	0.64
1:B:341:PHE:HB3	1:B:369:CYS:HB2	1.79	0.64
1:B:523:ILE:O	1:B:526:LEU:HB3	1.98	0.63
1:C:108:VAL:HG12	1:C:110:GLY:H	1.61	0.63
3:A:803:Y01:HAQ2	1:D:522:PHE:CE2	2.34	0.63
1:C:496:LEU:HD23	3:C:802:Y01:HAD2	1.79	0.63
1:A:341:PHE:HB3	1:A:369:CYS:HB2	1.79	0.63
1:C:569:PHE:O	1:C:573:GLN:HG3	1.99	0.63
1:C:496:LEU:HD23	3:C:802:Y01:HAD3	1.79	0.63
1:D:341:PHE:HB3	1:D:369:CYS:HB2	1.79	0.63
3:A:803:Y01:HAQ2	1:D:522:PHE:HE2	1.64	0.63
1:B:528:LEU:HD21	1:B:575:LEU:CB	2.29	0.63
1:A:370:HIS:CD2	1:A:657:LEU:HD13	2.34	0.62
1:A:573:GLN:HG2	4:A:804:LPP:O4	1.99	0.62
1:A:722:LYS:HE2	1:D:136:PHE:CD1	2.35	0.62
1:A:265:LEU:HD22	1:D:190:LEU:HD11	1.81	0.62
1:B:659:PRO:HD2	1:B:661:PHE:HD2	1.62	0.62
1:A:529:LEU:CD1	3:B:802:Y01:HAA2	2.26	0.61
1:A:576:PHE:CE2	4:A:804:LPP:HC82	2.36	0.61
1:B:528:LEU:HD21	1:B:575:LEU:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:H	1:A:657:LEU:CD2	2.14	0.60
1:C:370:HIS:HA	1:C:657:LEU:HD11	1.82	0.60
1:D:657:LEU:HD12	1:D:658:PRO:HD3	1.77	0.60
1:B:528:LEU:CD2	1:B:575:LEU:CB	2.79	0.60
1:A:529:LEU:HD11	3:B:802:Y01:HAA2	1.79	0.59
1:C:496:LEU:HD23	3:C:802:Y01:HAD1	1.80	0.59
1:A:136:PHE:HE1	1:B:723:ARG:HB3	1.68	0.59
1:A:528:LEU:HD22	1:A:572:LEU:HD23	1.83	0.58
1:B:573:GLN:NE2	4:B:803:LPP:O4	2.37	0.58
1:C:370:HIS:CE1	1:C:657:LEU:CD1	2.87	0.58
1:A:496:LEU:HD23	3:A:803:Y01:HAD2	1.80	0.58
1:A:480:ALA:HB1	1:D:600:VAL:HG11	1.86	0.57
1:D:439:ASP:OD1	1:D:492:ARG:NH2	2.37	0.57
1:B:439:ASP:OD1	1:B:492:ARG:NH2	2.37	0.57
1:C:439:ASP:OD1	1:C:492:ARG:NH2	2.37	0.57
3:B:802:Y01:HAC1	3:B:802:Y01:HAU2	1.87	0.57
1:A:439:ASP:OD1	1:A:492:ARG:NH2	2.37	0.57
1:A:657:LEU:HD22	1:A:657:LEU:H	1.68	0.57
1:A:743:PHE:HE1	1:B:746:LEU:HG	1.70	0.56
1:A:658:PRO:N	1:A:659:PRO:HD3	2.19	0.56
3:C:802:Y01:HAC1	3:C:802:Y01:HAU2	1.87	0.56
1:C:529:LEU:HD12	3:D:802:Y01:HAA1	1.88	0.56
1:A:589:ASN:HD21	1:B:557:ARG:HB3	1.69	0.56
1:B:496:LEU:HD23	3:B:802:Y01:HAD3	1.85	0.56
1:C:196:ARG:NH1	1:C:234:GLU:OE2	2.39	0.56
1:A:196:ARG:NH1	1:A:234:GLU:OE2	2.39	0.56
1:C:316:TYR:OH	3:C:802:Y01:OAF	2.21	0.56
1:B:196:ARG:NH1	1:B:234:GLU:OE2	2.39	0.56
1:B:522:PHE:HE2	3:C:802:Y01:HAQ2	1.71	0.56
1:C:524:TYR:CD2	4:C:803:LPP:H221	2.41	0.55
3:A:803:Y01:HAC1	3:A:803:Y01:HAU2	1.87	0.55
1:B:524:TYR:CE2	4:B:803:LPP:H221	2.42	0.55
1:B:610:VAL:CG1	4:C:803:LPP:H331	2.35	0.55
1:B:522:PHE:CE2	3:C:802:Y01:HAQ2	2.41	0.55
1:D:196:ARG:NH1	1:D:234:GLU:OE2	2.39	0.55
3:D:802:Y01:HAC1	3:D:802:Y01:HAU2	1.87	0.55
1:C:528:LEU:HD21	1:C:575:LEU:HB2	1.88	0.55
1:A:524:TYR:CD2	4:A:804:LPP:H221	2.41	0.55
1:C:524:TYR:CZ	1:C:528:LEU:HD12	2.42	0.54
1:A:370:HIS:CG	1:A:657:LEU:CD1	2.91	0.54
1:A:370:HIS:HA	1:A:657:LEU:CD1	2.31	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:O	1:A:138:GLU:HG2	2.07	0.54
1:A:370:HIS:CE1	1:A:657:LEU:HD13	2.42	0.54
1:A:573:GLN:NE2	4:A:804:LPP:O4	2.40	0.54
4:A:804:LPP:H331	1:D:610:VAL:CG1	2.38	0.53
1:B:657:LEU:C	1:B:659:PRO:HD3	2.29	0.53
1:D:316:TYR:OH	3:D:802:Y01:OAF	2.27	0.53
1:A:197:LEU:O	1:A:201:LYS:HB2	2.09	0.53
1:A:67:ASP:HB2	1:A:71:ARG:HB2	1.91	0.53
1:B:67:ASP:HB2	1:B:71:ARG:HB2	1.91	0.53
1:D:67:ASP:HB2	1:D:71:ARG:HB2	1.91	0.53
1:A:657:LEU:CA	1:A:659:PRO:HD3	2.38	0.53
1:C:197:LEU:O	1:C:201:LYS:HB2	2.09	0.53
1:D:573:GLN:HG2	4:D:803:LPP:O4	2.09	0.52
1:A:658:PRO:N	1:A:659:PRO:CD	2.72	0.52
1:D:197:LEU:O	1:D:201:LYS:HB2	2.09	0.52
1:D:524:TYR:CE2	4:D:803:LPP:H221	2.44	0.52
1:C:67:ASP:HB2	1:C:71:ARG:HB2	1.91	0.52
1:A:190:LEU:HD11	1:B:265:LEU:HD22	1.92	0.52
1:B:197:LEU:O	1:B:201:LYS:HB2	2.09	0.52
1:B:529:LEU:CD2	1:B:572:LEU:HD21	2.39	0.52
1:A:657:LEU:HB2	1:A:659:PRO:HD2	1.87	0.51
1:A:657:LEU:N	1:A:657:LEU:CD2	2.73	0.51
1:A:537:GLN:HG2	1:B:486:ASN:HD22	1.75	0.51
1:C:105:ARG:HD2	1:C:139:PHE:HZ	1.76	0.51
1:C:583:LEU:HD22	1:C:587:VAL:HG21	1.93	0.51
1:B:105:ARG:HD2	1:B:139:PHE:HZ	1.76	0.51
1:D:64:ASN:HD21	1:D:95:TYR:H	1.59	0.51
1:D:105:ARG:HD2	1:D:139:PHE:HZ	1.76	0.51
1:A:64:ASN:HD21	1:A:95:TYR:H	1.59	0.51
1:A:105:ARG:HD2	1:A:139:PHE:HZ	1.76	0.50
1:A:573:GLN:HG2	4:A:804:LPP:H122	1.93	0.50
1:B:316:TYR:OH	3:B:802:Y01:OAF	2.29	0.50
1:A:576:PHE:CD2	4:A:804:LPP:HC82	2.46	0.50
1:C:138:GLU:HG2	1:C:138:GLU:O	2.12	0.50
1:A:497:PHE:CE2	1:D:523:ILE:HG12	2.46	0.50
1:A:559:GLU:OE2	1:D:560:LYS:NZ	2.45	0.50
1:B:64:ASN:HD21	1:B:95:TYR:H	1.59	0.50
1:C:659:PRO:CB	1:C:661:PHE:CE2	2.95	0.50
1:D:583:LEU:HD22	1:D:587:VAL:HG21	1.93	0.50
1:C:64:ASN:HD21	1:C:95:TYR:H	1.59	0.50
1:B:583:LEU:HD22	1:B:587:VAL:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HD11	1:A:720:LEU:HD11	1.94	0.49
1:A:373:SER:OG	1:A:659:PRO:HG3	2.12	0.49
1:A:583:LEU:HD22	1:A:587:VAL:HG21	1.93	0.49
1:C:268:ILE:HD11	1:C:720:LEU:HD11	1.95	0.49
1:D:496:LEU:HD23	3:D:802:Y01:HAD3	1.93	0.49
1:B:106:LYS:NZ	1:B:741:GLU:OE1	2.46	0.49
1:D:268:ILE:HD11	1:D:720:LEU:HD11	1.94	0.49
1:B:268:ILE:HD11	1:B:720:LEU:HD11	1.95	0.49
1:C:369:CYS:O	1:C:657:LEU:HD21	2.12	0.49
1:B:524:TYR:HE2	4:B:803:LPP:H191	1.78	0.49
1:D:106:LYS:NZ	1:D:741:GLU:OE1	2.46	0.49
1:C:370:HIS:CE1	1:C:657:LEU:HD13	2.48	0.49
1:A:106:LYS:NZ	1:A:741:GLU:OE1	2.46	0.49
1:D:578:SER:HB3	1:D:583:LEU:HD12	1.95	0.49
1:A:537:GLN:HG2	1:B:486:ASN:ND2	2.28	0.48
1:A:378:LEU:HD21	1:A:490:SER:HA	1.95	0.48
1:D:378:LEU:HD21	1:D:490:SER:HA	1.95	0.48
1:B:378:LEU:HD21	1:B:490:SER:HA	1.95	0.48
1:C:378:LEU:HD21	1:C:490:SER:HA	1.95	0.48
1:A:522:PHE:CE2	3:B:802:Y01:HAQ2	2.48	0.48
1:B:33:GLU:HG2	1:B:61:VAL:HG13	1.95	0.48
1:C:578:SER:HB3	1:C:583:LEU:HD12	1.95	0.48
1:A:33:GLU:HG2	1:A:61:VAL:HG13	1.95	0.48
1:C:190:LEU:HD11	1:D:265:LEU:HD22	1.94	0.48
1:D:657:LEU:HD23	1:D:661:PHE:CD2	2.49	0.48
1:C:106:LYS:NZ	1:C:741:GLU:OE1	2.46	0.48
1:C:526:LEU:HD23	1:C:526:LEU:O	2.13	0.48
1:C:526:LEU:HD13	1:D:497:PHE:CZ	2.49	0.48
1:D:569:PHE:CE2	1:D:573:GLN:OE1	2.67	0.48
1:B:138:GLU:O	1:B:138:GLU:HG2	2.13	0.48
1:B:537:GLN:HG2	1:C:486:ASN:ND2	2.29	0.48
1:A:105:ARG:HH22	1:B:730:ARG:HG2	1.79	0.47
1:C:524:TYR:CE2	4:C:803:LPP:H222	2.49	0.47
1:A:375:LEU:HD21	3:A:803:Y01:HAE2	1.96	0.47
1:A:578:SER:HB3	1:A:583:LEU:HD12	1.95	0.47
1:B:200:TYR:HB3	1:B:227:LEU:HD21	1.97	0.47
1:D:565:PHE:HD1	1:D:571:THR:HG23	1.80	0.47
1:A:565:PHE:HD1	1:A:571:THR:HG23	1.80	0.47
1:C:565:PHE:HD1	1:C:571:THR:HG23	1.80	0.47
1:A:316:TYR:OH	3:A:803:Y01:OAF	2.26	0.47
1:A:722:LYS:HE2	1:D:136:PHE:CG	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLU:HG2	1:C:61:VAL:HG13	1.95	0.47
1:B:578:SER:HB3	1:B:583:LEU:HD12	1.95	0.47
1:D:33:GLU:HG2	1:D:61:VAL:HG13	1.95	0.47
1:C:370:HIS:CE1	1:C:657:LEU:HD12	2.50	0.47
1:C:522:PHE:HE2	3:D:802:Y01:HAQ2	1.80	0.47
1:A:200:TYR:HB3	1:A:227:LEU:HD21	1.97	0.46
1:C:514:LEU:HD21	4:C:803:LPP:H412	1.96	0.46
1:A:369:CYS:O	1:A:657:LEU:CD1	2.63	0.46
1:B:529:LEU:HD11	3:C:802:Y01:CAA	2.44	0.46
1:C:523:ILE:O	1:C:526:LEU:HB3	2.16	0.46
1:A:496:LEU:CD2	3:A:803:Y01:CAD	2.76	0.46
1:B:190:LEU:HD11	1:C:265:LEU:HD22	1.97	0.46
1:B:565:PHE:HD1	1:B:571:THR:HG23	1.80	0.46
1:A:528:LEU:HD11	4:A:804:LPP:H152	1.96	0.46
1:A:526:LEU:CD1	3:B:802:Y01:HAP1	2.46	0.46
1:B:269:LEU:HD22	1:B:290:LEU:HG	1.98	0.46
1:C:136:PHE:CG	1:C:136:PHE:O	2.69	0.46
1:C:269:LEU:HD22	1:C:290:LEU:HG	1.98	0.46
1:C:522:PHE:CE2	3:D:802:Y01:HAQ2	2.51	0.46
1:C:610:VAL:HG11	4:D:803:LPP:H331	1.98	0.46
1:B:496:LEU:HD23	3:B:802:Y01:HAD2	1.90	0.46
1:C:200:TYR:HB3	1:C:227:LEU:HD21	1.97	0.46
1:D:200:TYR:HB3	1:D:227:LEU:HD21	1.97	0.46
1:C:607:THR:CG2	4:D:803:LPP:H311	2.25	0.45
1:A:555:GLY:N	1:A:562:ASN:OD1	2.49	0.45
1:A:733:LYS:O	1:D:739:THR:OG1	2.33	0.45
1:C:555:GLY:N	1:C:562:ASN:OD1	2.49	0.45
1:A:136:PHE:O	1:A:136:PHE:CD2	2.70	0.45
1:C:302:VAL:O	1:C:308:GLN:NE2	2.44	0.45
1:D:544:THR:OG1	1:D:549:GLU:OE2	2.28	0.45
1:A:341:PHE:O	1:A:345:SER:OG	2.35	0.45
1:D:302:VAL:O	1:D:308:GLN:NE2	2.44	0.45
1:A:188:ASP:N	1:B:262:SER:HG	2.15	0.45
1:A:371:THR:HB	1:A:496:LEU:HD21	1.99	0.45
1:A:738:LEU:HD21	1:D:743:PHE:HB2	1.98	0.45
1:C:512:ARG:HD2	1:C:638:GLU:HG2	1.99	0.45
1:D:555:GLY:N	1:D:562:ASN:OD1	2.49	0.45
1:B:560:LYS:NZ	1:C:559:GLU:OE2	2.50	0.45
1:D:512:ARG:HD2	1:D:638:GLU:HG2	1.99	0.45
1:A:370:HIS:CD2	1:A:657:LEU:CD1	3.01	0.45
1:B:341:PHE:O	1:B:345:SER:OG	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD23	1:B:529:LEU:HA	1.74	0.45
1:A:522:PHE:HE2	3:B:802:Y01:HAQ2	1.82	0.44
1:D:524:TYR:HE2	4:D:803:LPP:H191	1.82	0.44
1:B:555:GLY:N	1:B:562:ASN:OD1	2.49	0.44
1:C:366:LYS:NZ	1:C:652:ASP:O	2.51	0.44
1:D:136:PHE:CD2	1:D:136:PHE:O	2.71	0.44
1:A:136:PHE:O	1:A:136:PHE:CG	2.69	0.44
1:A:366:LYS:NZ	1:A:652:ASP:O	2.51	0.44
1:A:524:TYR:CE2	4:A:804:LPP:H222	2.51	0.44
1:B:136:PHE:CD2	1:B:136:PHE:O	2.70	0.44
1:C:370:HIS:ND1	1:C:657:LEU:HD12	2.30	0.44
1:A:269:LEU:HD22	1:A:290:LEU:HG	1.98	0.44
1:B:136:PHE:O	1:B:136:PHE:CG	2.69	0.44
1:B:210:ALA:HB1	1:B:721:VAL:HG13	2.00	0.44
1:B:371:THR:HB	1:B:496:LEU:HD21	1.99	0.44
1:A:210:ALA:HB1	1:A:721:VAL:HG13	2.00	0.44
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.88	0.44
1:D:573:GLN:CG	4:D:803:LPP:O4	2.65	0.44
1:B:366:LYS:NZ	1:B:652:ASP:O	2.51	0.44
1:B:524:TYR:CE2	4:B:803:LPP:C22	3.01	0.44
1:D:269:LEU:HD22	1:D:290:LEU:HG	1.98	0.44
1:A:754:ARG:HA	1:B:753:PHE:CE1	2.52	0.44
3:A:803:Y01:HAE2	3:A:803:Y01:HBB	1.83	0.44
1:B:512:ARG:HD2	1:B:638:GLU:HG2	1.99	0.44
1:A:512:ARG:HD2	1:A:638:GLU:HG2	1.99	0.44
1:B:496:LEU:HD23	3:B:802:Y01:HAD1	1.93	0.43
1:C:529:LEU:HD23	1:C:529:LEU:HA	1.81	0.43
1:C:611:ILE:HG12	4:D:803:LPP:H392	2.00	0.43
1:D:366:LYS:NZ	1:D:652:ASP:O	2.51	0.43
1:D:371:THR:HB	1:D:496:LEU:HD21	1.99	0.43
1:A:743:PHE:CE1	1:B:746:LEU:HG	2.51	0.43
1:C:514:LEU:HD11	4:C:803:LPP:H411	2.00	0.43
1:C:657:LEU:O	1:C:662:ASN:CA	2.66	0.43
3:D:802:Y01:HAE2	3:D:802:Y01:HBB	1.83	0.43
1:B:600:VAL:HG11	1:C:480:ALA:HB1	1.99	0.43
1:D:226:GLU:O	1:D:230:LEU:HB2	2.18	0.43
3:B:802:Y01:HAS2	3:B:802:Y01:HAE1	1.81	0.43
1:C:136:PHE:HE1	1:D:723:ARG:HB3	1.82	0.43
1:C:226:GLU:O	1:C:230:LEU:HB2	2.18	0.43
1:A:603:THR:HA	4:B:803:LPP:HC62	1.99	0.43
1:B:544:THR:OG1	1:B:549:GLU:OE2	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:THR:HB	1:C:496:LEU:HD21	1.99	0.43
3:A:803:Y01:HAS2	3:A:803:Y01:HAE1	1.81	0.43
1:B:226:GLU:O	1:B:230:LEU:HB2	2.18	0.43
1:B:615:VAL:HG11	4:C:803:LPP:H412	1.99	0.43
1:C:136:PHE:O	1:C:136:PHE:CD2	2.72	0.43
1:D:136:PHE:CG	1:D:136:PHE:O	2.69	0.43
1:C:143:ILE:HG21	1:C:148:LEU:HD12	2.01	0.43
1:A:609:ASN:O	1:A:613:LEU:HB2	2.19	0.43
1:C:210:ALA:HB1	1:C:721:VAL:HG13	2.00	0.43
1:C:619:MET:SD	1:D:510:LEU:HD22	2.58	0.43
1:A:143:ILE:HG21	1:A:148:LEU:HD12	2.01	0.43
1:B:609:ASN:O	1:B:613:LEU:HB2	2.19	0.43
1:C:659:PRO:O	1:C:660:PRO:CB	2.67	0.43
1:D:529:LEU:HD23	1:D:529:LEU:HA	1.79	0.43
1:B:143:ILE:HG21	1:B:148:LEU:HD12	2.01	0.42
1:B:657:LEU:C	1:B:659:PRO:CD	2.88	0.42
1:A:613:LEU:HD23	1:A:613:LEU:HA	1.90	0.42
1:D:143:ILE:HG21	1:D:148:LEU:HD12	2.01	0.42
1:D:210:ALA:HB1	1:D:721:VAL:HG13	2.00	0.42
1:A:473:HIS:HD2	1:A:474:PRO:HD2	1.85	0.42
1:A:486:ASN:ND2	1:D:537:GLN:HG2	2.35	0.42
1:C:609:ASN:O	1:C:613:LEU:HB2	2.19	0.42
1:D:373:SER:OG	1:D:659:PRO:CB	2.67	0.42
1:A:302:VAL:O	1:A:308:GLN:NE2	2.44	0.42
3:A:803:Y01:HAS1	3:A:803:Y01:HAT1	1.92	0.42
3:D:802:Y01:HAS2	3:D:802:Y01:HAE1	1.81	0.42
1:A:226:GLU:O	1:A:230:LEU:HB2	2.18	0.42
1:A:508:ILE:HD12	1:A:639:TRP:HD1	1.85	0.42
3:A:803:Y01:HAD3	3:A:803:Y01:HBD	1.79	0.42
1:B:170:ARG:HA	1:B:171:PRO:HD3	1.86	0.42
1:B:508:ILE:HD12	1:B:639:TRP:HD1	1.85	0.42
4:C:803:LPP:H411	4:C:803:LPP:H442	1.88	0.42
1:D:138:GLU:O	1:D:138:GLU:HG2	2.20	0.42
1:D:609:ASN:O	1:D:613:LEU:HB2	2.19	0.42
1:B:658:PRO:N	1:B:659:PRO:HD3	2.35	0.42
1:C:508:ILE:HD12	1:C:639:TRP:HD1	1.85	0.42
1:C:526:LEU:CD1	1:D:497:PHE:CZ	3.03	0.42
1:A:348:TYR:HD2	1:A:656:THR:HG23	1.85	0.41
1:A:659:PRO:O	1:A:660:PRO:CB	2.68	0.41
1:A:730:ARG:HG2	1:D:105:ARG:HH22	1.83	0.41
1:B:521:LEU:HD22	4:B:803:LPP:H202	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ILE:HD12	1:D:639:TRP:HD1	1.85	0.41
1:A:609:ASN:HB3	1:B:580:PHE:CZ	2.55	0.41
1:A:620:LEU:HG	1:A:624:MET:HE2	2.01	0.41
1:B:739:THR:OG1	1:C:733:LYS:O	2.38	0.41
1:D:496:LEU:HD23	3:D:802:Y01:HAD1	1.98	0.41
3:D:802:Y01:HAD3	3:D:802:Y01:HBD	1.80	0.41
3:A:803:Y01:HAD2	3:A:803:Y01:HAS2	1.87	0.41
1:B:473:HIS:HD2	1:B:474:PRO:HD2	1.85	0.41
1:A:589:ASN:ND2	1:B:557:ARG:O	2.54	0.41
1:C:473:HIS:HD2	1:C:474:PRO:HD2	1.85	0.41
1:D:473:HIS:HD2	1:D:474:PRO:HD2	1.85	0.41
1:B:523:ILE:HG12	1:C:497:PHE:CE2	2.56	0.41
1:A:370:HIS:ND1	1:A:657:LEU:HD13	2.36	0.41
1:A:599:PHE:CZ	1:B:569:PHE:HZ	2.38	0.41
1:B:473:HIS:CD2	1:B:474:PRO:HD2	2.56	0.41
1:C:410:TRP:NE1	1:C:659:PRO:HA	2.36	0.41
4:A:804:LPP:H412	1:D:615:VAL:HG11	2.03	0.41
1:B:623:MET:HE1	1:C:506:LEU:HD11	2.02	0.41
1:C:370:HIS:CG	1:C:657:LEU:CD1	3.03	0.41
1:D:524:TYR:CE2	4:D:803:LPP:C22	3.03	0.41
1:A:602:ALA:HB1	4:B:803:LPP:O2	2.21	0.41
1:A:622:ALA:HA	1:B:625:ASN:ND2	2.36	0.41
1:B:138:GLU:O	1:B:138:GLU:CG	2.69	0.41
3:A:803:Y01:CAP	1:D:526:LEU:HD12	2.51	0.40
3:A:803:Y01:HAA1	1:D:529:LEU:HD12	2.02	0.40
1:C:106:LYS:HB3	1:C:106:LYS:HE3	1.88	0.40
1:A:526:LEU:CD2	1:B:494:ILE:HG13	2.51	0.40
1:B:464:ARG:HH12	1:B:469:TRP:HA	1.87	0.40
1:C:464:ARG:HH12	1:C:469:TRP:HA	1.87	0.40
1:C:375:LEU:HD21	3:C:802:Y01:HAE2	2.03	0.40
1:A:607:THR:HG22	4:B:803:LPP:H332	2.04	0.40
1:B:302:VAL:O	1:B:308:GLN:NE2	2.44	0.40
1:C:524:TYR:OH	1:C:528:LEU:HD12	2.20	0.40
1:D:528:LEU:HD23	1:D:572:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	630/765 (82%)	615 (98%)	14 (2%)	1 (0%)	44	73
1	B	630/765 (82%)	613 (97%)	16 (2%)	1 (0%)	44	73
1	C	630/765 (82%)	614 (98%)	15 (2%)	1 (0%)	44	73
1	D	630/765 (82%)	617 (98%)	12 (2%)	1 (0%)	44	73
All	All	2520/3060 (82%)	2459 (98%)	57 (2%)	4 (0%)	45	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	660	PRO
1	B	660	PRO
1	C	660	PRO
1	D	660	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	564/687 (82%)	553 (98%)	11 (2%)	50	79
1	B	563/687 (82%)	551 (98%)	12 (2%)	48	78
1	C	563/687 (82%)	552 (98%)	11 (2%)	50	79
1	D	563/687 (82%)	552 (98%)	11 (2%)	50	79
All	All	2253/2748 (82%)	2208 (98%)	45 (2%)	50	79

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

Mol	Chain	Res	Type
1	A	60	ASN
1	A	153	ASN
1	A	173	GLN
1	A	369	CYS
1	A	410	TRP
1	A	506	LEU
1	A	528	LEU
1	A	533	ASN
1	A	536	ASN
1	A	626	ASN
1	A	657	LEU
1	B	60	ASN
1	B	153	ASN
1	B	173	GLN
1	B	369	CYS
1	B	410	TRP
1	B	506	LEU
1	B	528	LEU
1	B	533	ASN
1	B	536	ASN
1	B	626	ASN
1	B	656	THR
1	B	658	PRO
1	C	60	ASN
1	C	153	ASN
1	C	173	GLN
1	C	369	CYS
1	C	410	TRP
1	C	506	LEU
1	C	528	LEU
1	C	529	LEU
1	C	533	ASN
1	C	536	ASN
1	C	626	ASN
1	D	60	ASN
1	D	153	ASN
1	D	173	GLN
1	D	369	CYS
1	D	410	TRP
1	D	506	LEU
1	D	528	LEU
1	D	529	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	533	ASN
1	D	536	ASN
1	D	626	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	64	ASN
1	A	258	GLN
1	A	297	HIS
1	A	298	GLN
1	A	306	ASN
1	A	533	ASN
1	A	536	ASN
1	A	563	ASN
1	A	573	GLN
1	A	626	ASN
1	B	60	ASN
1	B	64	ASN
1	B	258	GLN
1	B	297	HIS
1	B	298	GLN
1	B	306	ASN
1	B	533	ASN
1	B	536	ASN
1	B	563	ASN
1	B	573	GLN
1	B	626	ASN
1	C	60	ASN
1	C	64	ASN
1	C	258	GLN
1	C	297	HIS
1	C	298	GLN
1	C	306	ASN
1	C	533	ASN
1	C	536	ASN
1	C	537	GLN
1	C	563	ASN
1	C	573	GLN
1	C	626	ASN
1	D	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	64	ASN
1	D	258	GLN
1	D	297	HIS
1	D	298	GLN
1	D	306	ASN
1	D	533	ASN
1	D	536	ASN
1	D	563	ASN
1	D	573	GLN
1	D	626	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](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	Y01	C	802	-	38,38,38	1.79	7 (18%)	57,57,57	1.98	16 (28%)
3	Y01	A	803	-	38,38,38	1.79	7 (18%)	57,57,57	1.99	16 (28%)
4	LPP	D	803	-	43,43,43	0.98	2 (4%)	47,48,48	1.36	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LPP	B	803	-	43,43,43	0.97	2 (4%)	47,48,48	1.36	4 (8%)
3	Y01	D	802	-	38,38,38	1.79	7 (18%)	57,57,57	1.99	16 (28%)
4	LPP	C	803	-	43,43,43	0.98	2 (4%)	47,48,48	1.36	4 (8%)
4	LPP	A	804	-	43,43,43	0.99	2 (4%)	47,48,48	1.36	4 (8%)
3	Y01	B	802	-	38,38,38	1.79	7 (18%)	57,57,57	1.98	16 (28%)

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	Y01	C	802	-	-	8/19/77/77	0/4/4/4
3	Y01	A	803	-	-	8/19/77/77	0/4/4/4
4	LPP	D	803	-	-	31/45/45/45	-
4	LPP	B	803	-	-	31/45/45/45	-
3	Y01	D	802	-	-	6/19/77/77	0/4/4/4
4	LPP	C	803	-	-	31/45/45/45	-
4	LPP	A	804	-	-	31/45/45/45	-
3	Y01	B	802	-	-	6/19/77/77	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	Y01	CAV-CAZ	-5.68	1.39	1.51
3	C	802	Y01	CAV-CAZ	-5.65	1.39	1.51
3	A	803	Y01	CAV-CAZ	-5.64	1.39	1.51
3	D	802	Y01	CAV-CAZ	-5.62	1.39	1.51
3	A	803	Y01	CBH-CAZ	-4.69	1.43	1.52
3	D	802	Y01	CBH-CAZ	-4.65	1.43	1.52
3	C	802	Y01	CBH-CAZ	-4.64	1.43	1.52
3	B	802	Y01	CBH-CAZ	-4.64	1.43	1.52
4	A	804	LPP	O9-C11	4.28	1.46	1.34
4	C	803	LPP	O9-C11	4.23	1.46	1.34
4	D	803	LPP	O9-C11	4.23	1.46	1.34
4	B	803	LPP	O9-C11	4.20	1.46	1.34
3	D	802	Y01	CAK-CAI	-4.15	1.41	1.50
3	B	802	Y01	CAK-CAI	-4.12	1.41	1.50
3	C	802	Y01	CAK-CAI	-4.11	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	Y01	CAK-CAI	-4.10	1.41	1.50
4	A	804	LPP	O27-C29	3.90	1.44	1.33
4	D	803	LPP	O27-C29	3.88	1.44	1.33
4	C	803	LPP	O27-C29	3.86	1.44	1.33
4	B	803	LPP	O27-C29	3.84	1.44	1.33
3	A	803	Y01	CAI-CAZ	3.32	1.40	1.33
3	D	802	Y01	CAI-CAZ	3.29	1.40	1.33
3	B	802	Y01	CAI-CAZ	3.28	1.40	1.33
3	C	802	Y01	CAI-CAZ	3.27	1.40	1.33
3	B	802	Y01	CBI-CBG	-2.78	1.49	1.55
3	C	802	Y01	CBI-CBG	-2.77	1.49	1.55
3	D	802	Y01	CBI-CBG	-2.77	1.49	1.55
3	A	803	Y01	CBI-CBG	-2.74	1.49	1.55
3	C	802	Y01	CAR-CBC	2.68	1.58	1.51
3	B	802	Y01	CAR-CBC	2.66	1.58	1.51
3	D	802	Y01	CAR-CBC	2.64	1.58	1.51
3	A	803	Y01	CAR-CBC	2.61	1.58	1.51
3	A	803	Y01	CBI-CBE	-2.53	1.50	1.55
3	C	802	Y01	CBI-CBE	-2.52	1.50	1.55
3	B	802	Y01	CBI-CBE	-2.50	1.50	1.55
3	D	802	Y01	CBI-CBE	-2.47	1.50	1.55

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	Y01	CBC-CAV-CAZ	-5.03	103.70	111.52
3	D	802	Y01	CBC-CAV-CAZ	-5.01	103.73	111.52
3	B	802	Y01	CBI-CBE-CBB	-4.98	111.69	119.49
3	C	802	Y01	CBC-CAV-CAZ	-4.97	103.79	111.52
3	C	802	Y01	CBI-CBE-CBB	-4.97	111.70	119.49
3	D	802	Y01	CBI-CBE-CBB	-4.96	111.71	119.49
3	B	802	Y01	CBC-CAV-CAZ	-4.96	103.81	111.52
3	A	803	Y01	CBI-CBE-CBB	-4.95	111.73	119.49
3	B	802	Y01	CBH-CBF-CBD	-4.52	105.95	112.73
3	D	802	Y01	CBH-CBF-CBD	-4.51	105.97	112.73
3	C	802	Y01	CBH-CBF-CBD	-4.49	105.99	112.73
3	A	803	Y01	CBH-CBF-CBD	-4.49	106.00	112.73
4	A	804	LPP	O27-C29-C30	4.44	125.84	111.91
4	B	803	LPP	O27-C29-C30	4.44	125.83	111.91
4	C	803	LPP	O27-C29-C30	4.42	125.78	111.91
4	D	803	LPP	O27-C29-C30	4.42	125.76	111.91
3	A	803	Y01	CAD-CBH-CBF	-4.36	106.48	111.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	Y01	CAD-CBH-CBF	-4.32	106.53	111.68
3	C	802	Y01	CAD-CBH-CBF	-4.31	106.54	111.68
3	B	802	Y01	CAD-CBH-CBF	-4.30	106.56	111.68
3	A	803	Y01	CAQ-CBG-CBD	-4.20	112.16	119.08
3	D	802	Y01	CAQ-CBG-CBD	-4.18	112.20	119.08
3	C	802	Y01	CAQ-CBG-CBD	-4.16	112.23	119.08
3	B	802	Y01	CAQ-CBG-CBD	-4.15	112.25	119.08
4	D	803	LPP	O9-C11-C12	3.90	119.91	111.50
4	B	803	LPP	O9-C11-C12	3.90	119.91	111.50
4	C	803	LPP	O9-C11-C12	3.89	119.89	111.50
4	A	804	LPP	O9-C11-C12	3.89	119.89	111.50
3	A	803	Y01	CBI-CBG-CBD	-3.68	108.93	114.38
3	D	802	Y01	CBI-CBG-CBD	-3.65	108.97	114.38
3	B	802	Y01	CBI-CBG-CBD	-3.64	109.00	114.38
3	C	802	Y01	CBI-CBG-CBD	-3.63	109.00	114.38
4	C	803	LPP	C8-C7-C6	-3.49	103.53	111.79
4	D	803	LPP	C8-C7-C6	-3.49	103.54	111.79
4	B	803	LPP	C8-C7-C6	-3.48	103.55	111.79
4	A	804	LPP	C8-C7-C6	-3.45	103.62	111.79
4	A	804	LPP	O27-C29-O28	-3.13	115.68	123.59
4	D	803	LPP	O27-C29-O28	-3.09	115.80	123.59
3	C	802	Y01	CAS-CAU-CBI	-3.08	107.50	112.78
4	B	803	LPP	O27-C29-O28	-3.08	115.82	123.59
4	C	803	LPP	O27-C29-O28	-3.08	115.83	123.59
3	D	802	Y01	CAS-CAU-CBI	-3.05	107.55	112.78
3	B	802	Y01	CAS-CAU-CBI	-3.05	107.56	112.78
3	A	803	Y01	CAS-CAU-CBI	-3.05	107.56	112.78
3	A	803	Y01	CAT-CBH-CAZ	2.85	113.98	108.75
3	C	802	Y01	CAT-CBH-CAZ	2.85	113.96	108.75
3	D	802	Y01	CAT-CBH-CAZ	2.84	113.95	108.75
3	B	802	Y01	CAT-CBH-CAZ	2.81	113.90	108.75
3	B	802	Y01	CAC-CBB-CBE	-2.60	108.94	112.92
3	A	803	Y01	CAC-CBB-CBE	-2.60	108.94	112.92
3	D	802	Y01	CAC-CBB-CBE	-2.59	108.96	112.92
3	C	802	Y01	CAC-CBB-CBE	-2.57	108.98	112.92
3	A	803	Y01	CAR-CBC-CAV	2.43	114.61	110.99
3	B	802	Y01	CAR-CBC-CAV	2.42	114.59	110.99
3	D	802	Y01	CAR-CBC-CAV	2.41	114.58	110.99
3	C	802	Y01	CAD-CBH-CAT	-2.41	105.63	109.43
3	D	802	Y01	CAD-CBH-CAT	-2.41	105.63	109.43
3	B	802	Y01	CAD-CBH-CAT	-2.39	105.65	109.43
3	C	802	Y01	CAR-CBC-CAV	2.38	114.54	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	Y01	CAD-CBH-CAT	-2.35	105.71	109.43
3	D	802	Y01	CBD-CAK-CAI	2.25	115.97	112.73
3	C	802	Y01	CBD-CAK-CAI	2.25	115.96	112.73
3	A	803	Y01	CAV-CAZ-CBH	2.21	119.36	116.42
3	B	802	Y01	CBD-CAK-CAI	2.20	115.90	112.73
3	B	802	Y01	CAV-CAZ-CBH	2.20	119.34	116.42
3	D	802	Y01	CAP-CBE-CBI	-2.19	101.21	103.84
3	A	803	Y01	CBD-CAK-CAI	2.18	115.86	112.73
3	A	803	Y01	CAJ-CAO-CBB	-2.18	108.77	115.03
3	C	802	Y01	CAV-CAZ-CBH	2.18	119.31	116.42
3	D	802	Y01	CAV-CAZ-CBH	2.17	119.31	116.42
3	A	803	Y01	CAP-CBE-CBI	-2.16	101.24	103.84
3	D	802	Y01	CAJ-CAO-CBB	-2.16	108.82	115.03
3	B	802	Y01	CAJ-CAO-CBB	-2.16	108.84	115.03
3	C	802	Y01	CAJ-CAO-CBB	-2.16	108.84	115.03
3	A	803	Y01	CBG-CBI-CBE	-2.15	97.52	100.07
3	B	802	Y01	CAP-CBE-CBI	-2.15	101.25	103.84
3	B	802	Y01	CBG-CBI-CBE	-2.13	97.55	100.07
3	C	802	Y01	CBG-CBI-CBE	-2.13	97.55	100.07
3	C	802	Y01	CAP-CBE-CBI	-2.13	101.28	103.84
3	D	802	Y01	CBG-CBI-CBE	-2.12	97.56	100.07

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	LPP	C6-O5-P1-O2
4	A	804	LPP	C6-O5-P1-O3
4	A	804	LPP	C6-O5-P1-O4
4	A	804	LPP	O5-C6-C7-O9
4	B	803	LPP	C6-O5-P1-O2
4	B	803	LPP	C6-O5-P1-O3
4	B	803	LPP	C6-O5-P1-O4
4	B	803	LPP	O5-C6-C7-O9
4	C	803	LPP	C6-O5-P1-O2
4	C	803	LPP	C6-O5-P1-O3
4	C	803	LPP	C6-O5-P1-O4
4	C	803	LPP	O5-C6-C7-O9
4	D	803	LPP	C6-O5-P1-O2
4	D	803	LPP	C6-O5-P1-O3
4	D	803	LPP	C6-O5-P1-O4
4	D	803	LPP	O5-C6-C7-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	804	LPP	C7-C6-O5-P1
4	C	803	LPP	C7-C6-O5-P1
4	D	803	LPP	C7-C6-O5-P1
4	A	804	LPP	C29-C30-C31-C32
4	C	803	LPP	C29-C30-C31-C32
4	D	803	LPP	C29-C30-C31-C32
4	B	803	LPP	C29-C30-C31-C32
4	A	804	LPP	C30-C29-O27-C8
4	B	803	LPP	C30-C29-O27-C8
4	C	803	LPP	C30-C29-O27-C8
4	D	803	LPP	C30-C29-O27-C8
4	A	804	LPP	C21-C22-C23-C24
4	A	804	LPP	C33-C34-C35-C36
4	B	803	LPP	C21-C22-C23-C24
4	B	803	LPP	C33-C34-C35-C36
4	C	803	LPP	C21-C22-C23-C24
4	C	803	LPP	C33-C34-C35-C36
4	D	803	LPP	C21-C22-C23-C24
4	D	803	LPP	C33-C34-C35-C36
4	B	803	LPP	C37-C38-C39-C40
4	C	803	LPP	C37-C38-C39-C40
4	D	803	LPP	C37-C38-C39-C40
4	A	804	LPP	C37-C38-C39-C40
4	A	804	LPP	C39-C40-C41-C42
4	B	803	LPP	C39-C40-C41-C42
4	C	803	LPP	C39-C40-C41-C42
4	D	803	LPP	C39-C40-C41-C42
4	C	803	LPP	C13-C14-C15-C16
4	A	804	LPP	C13-C14-C15-C16
4	B	803	LPP	C13-C14-C15-C16
4	D	803	LPP	C13-C14-C15-C16
4	A	804	LPP	C22-C23-C24-C25
4	B	803	LPP	C22-C23-C24-C25
4	C	803	LPP	C22-C23-C24-C25
4	D	803	LPP	C22-C23-C24-C25
3	A	803	Y01	CAN-CAJ-CAO-CBB
3	B	802	Y01	CAN-CAJ-CAO-CBB
3	C	802	Y01	CAN-CAJ-CAO-CBB
3	D	802	Y01	CAN-CAJ-CAO-CBB
4	A	804	LPP	C16-C17-C18-C19
4	B	803	LPP	C16-C17-C18-C19
4	C	803	LPP	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	803	LPP	C16-C17-C18-C19
4	B	803	LPP	C38-C39-C40-C41
4	C	803	LPP	C38-C39-C40-C41
4	A	804	LPP	C38-C39-C40-C41
4	D	803	LPP	C38-C39-C40-C41
4	A	804	LPP	O28-C29-O27-C8
4	C	803	LPP	O28-C29-O27-C8
4	A	804	LPP	C31-C32-C33-C34
4	B	803	LPP	C31-C32-C33-C34
4	C	803	LPP	C31-C32-C33-C34
4	D	803	LPP	C31-C32-C33-C34
4	B	803	LPP	O28-C29-O27-C8
4	D	803	LPP	O28-C29-O27-C8
4	A	804	LPP	C40-C41-C42-C43
4	B	803	LPP	C40-C41-C42-C43
4	C	803	LPP	C40-C41-C42-C43
4	D	803	LPP	C40-C41-C42-C43
3	A	803	Y01	CAC-CBB-CBE-CBI
3	B	802	Y01	CAC-CBB-CBE-CBI
3	C	802	Y01	CAC-CBB-CBE-CBI
3	D	802	Y01	CAC-CBB-CBE-CBI
4	A	804	LPP	C41-C42-C43-C44
4	B	803	LPP	C41-C42-C43-C44
4	C	803	LPP	C41-C42-C43-C44
4	D	803	LPP	C30-C31-C32-C33
4	D	803	LPP	C41-C42-C43-C44
4	A	804	LPP	C30-C31-C32-C33
4	B	803	LPP	C30-C31-C32-C33
4	C	803	LPP	C30-C31-C32-C33
4	C	803	LPP	C36-C37-C38-C39
4	D	803	LPP	C36-C37-C38-C39
4	A	804	LPP	C36-C37-C38-C39
4	B	803	LPP	C36-C37-C38-C39
4	B	803	LPP	C7-C6-O5-P1
3	A	803	Y01	CAO-CAJ-CAN-CBA
3	C	802	Y01	CAO-CAJ-CAN-CBA
3	D	802	Y01	CAO-CAJ-CAN-CBA
3	B	802	Y01	CAO-CAJ-CAN-CBA
3	A	803	Y01	CAO-CBB-CBE-CBI
3	B	802	Y01	CAO-CBB-CBE-CBI
3	C	802	Y01	CAO-CBB-CBE-CBI
3	D	802	Y01	CAO-CBB-CBE-CBI

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	804	LPP	O5-C6-C7-C8
4	B	803	LPP	O5-C6-C7-C8
4	C	803	LPP	O5-C6-C7-C8
4	D	803	LPP	O5-C6-C7-C8
4	B	803	LPP	C32-C33-C34-C35
4	D	803	LPP	C32-C33-C34-C35
4	A	804	LPP	C32-C33-C34-C35
4	C	803	LPP	C32-C33-C34-C35
4	B	803	LPP	O9-C7-C8-O27
4	A	804	LPP	C6-C7-C8-O27
4	B	803	LPP	C6-C7-C8-O27
4	C	803	LPP	C6-C7-C8-O27
4	D	803	LPP	C6-C7-C8-O27
4	B	803	LPP	C34-C35-C36-C37
4	D	803	LPP	C34-C35-C36-C37
4	C	803	LPP	C34-C35-C36-C37
4	A	804	LPP	C34-C35-C36-C37
4	A	804	LPP	O9-C7-C8-O27
4	C	803	LPP	O9-C7-C8-O27
4	D	803	LPP	O9-C7-C8-O27
4	A	804	LPP	O9-C11-C12-C13
4	B	803	LPP	O9-C11-C12-C13
4	C	803	LPP	O9-C11-C12-C13
4	D	803	LPP	O9-C11-C12-C13
4	A	804	LPP	C18-C19-C20-C21
4	B	803	LPP	C18-C19-C20-C21
4	C	803	LPP	C18-C19-C20-C21
4	D	803	LPP	C18-C19-C20-C21
3	A	803	Y01	CAL-CAM-CAY-OAW
3	B	802	Y01	CAL-CAM-CAY-OAW
3	C	802	Y01	CAL-CAM-CAY-OAW
3	D	802	Y01	CAL-CAM-CAY-OAW
4	C	803	LPP	C35-C36-C37-C38
4	A	804	LPP	C35-C36-C37-C38
4	B	803	LPP	C35-C36-C37-C38
4	D	803	LPP	C35-C36-C37-C38
4	C	803	LPP	O10-C11-C12-C13
4	D	803	LPP	O10-C11-C12-C13
4	B	803	LPP	O10-C11-C12-C13
3	C	802	Y01	CAM-CAL-CAX-OAH
4	A	804	LPP	O10-C11-C12-C13
3	A	803	Y01	CAM-CAL-CAX-OAH

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	803	LPP	C11-C12-C13-C14
4	D	803	LPP	C11-C12-C13-C14
4	A	804	LPP	C11-C12-C13-C14
4	B	803	LPP	C11-C12-C13-C14
3	A	803	Y01	CAC-CBB-CBE-CAP
3	C	802	Y01	CAC-CBB-CBE-CAP
3	B	802	Y01	CAC-CBB-CBE-CAP
3	D	802	Y01	CAC-CBB-CBE-CAP
3	A	803	Y01	CAM-CAL-CAX-OAF
3	C	802	Y01	CAM-CAL-CAX-OAF

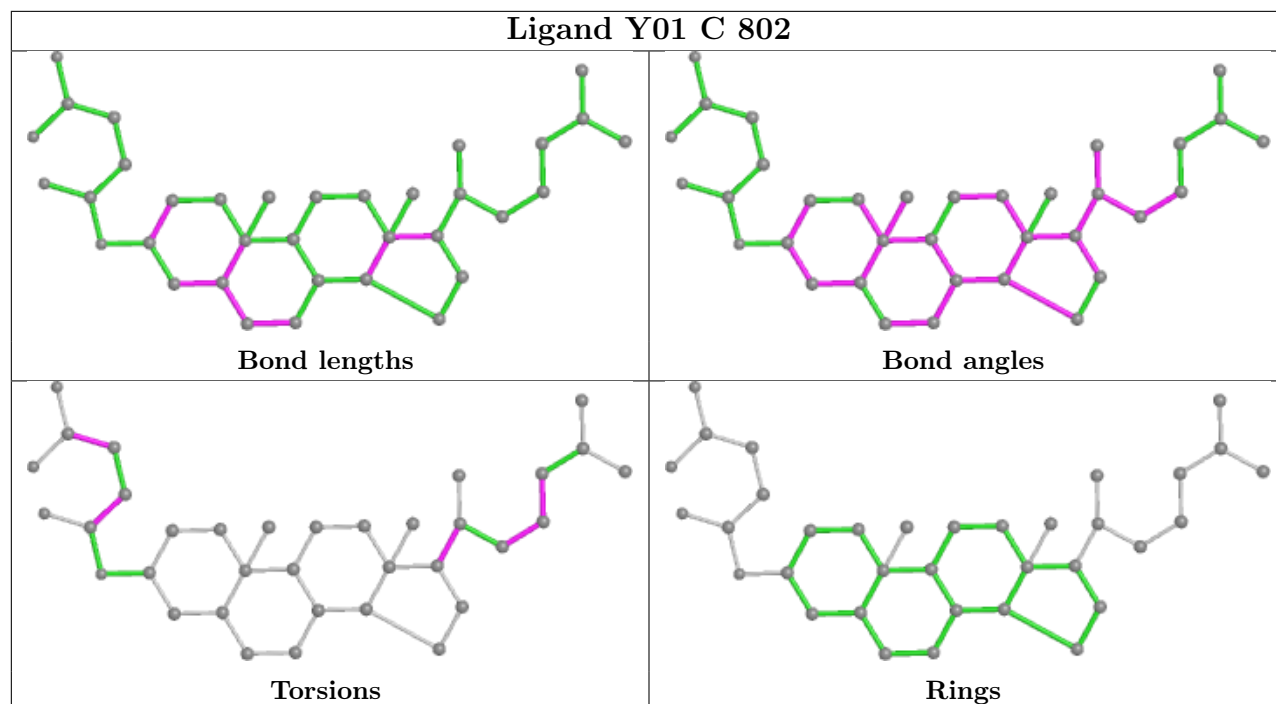
There are no ring outliers.

8 monomers are involved in 118 short contacts:

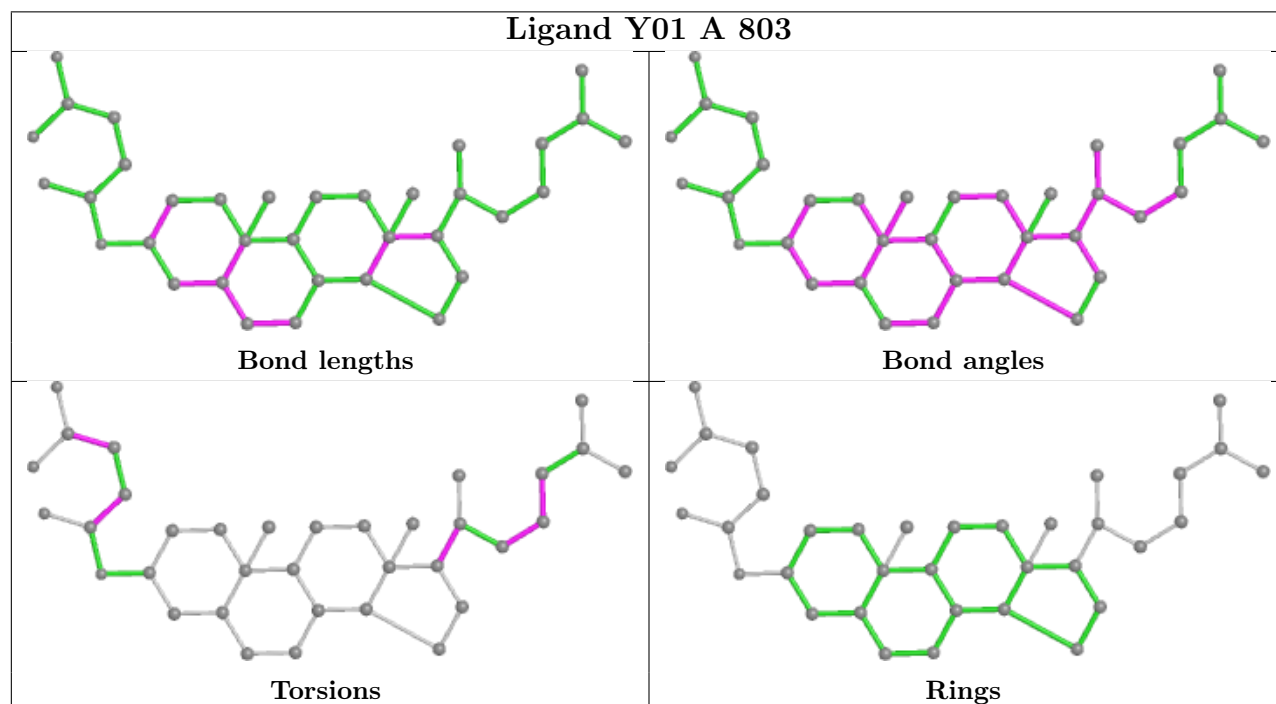
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	Y01	14	0
3	A	803	Y01	17	0
4	D	803	LPP	11	0
4	B	803	LPP	17	0
3	D	802	Y01	11	0
4	C	803	LPP	15	0
4	A	804	LPP	16	0
3	B	802	Y01	17	0

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.

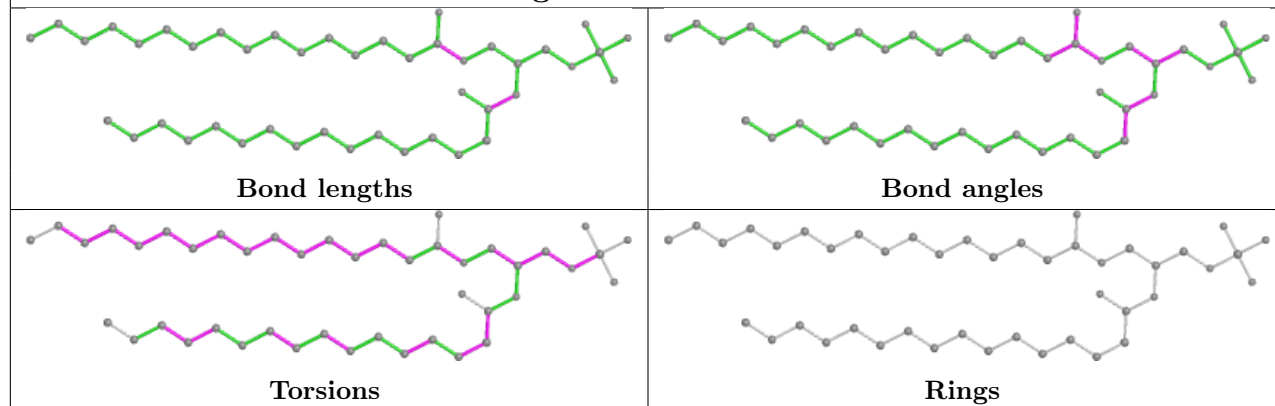
Ligand Y01 C 802



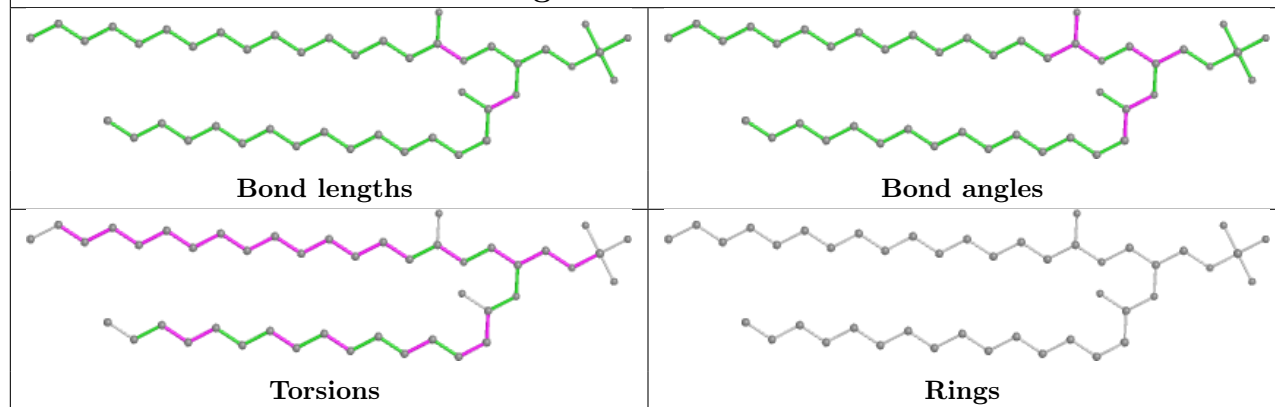
Ligand Y01 A 803



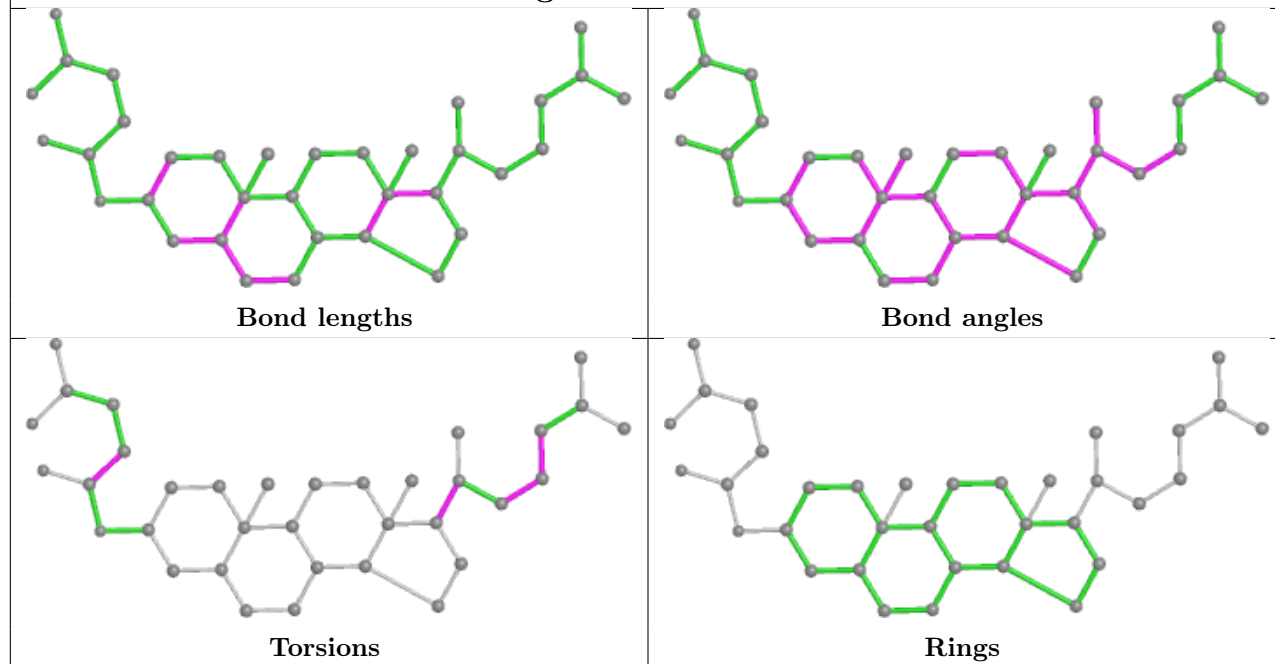
Ligand LPP D 803



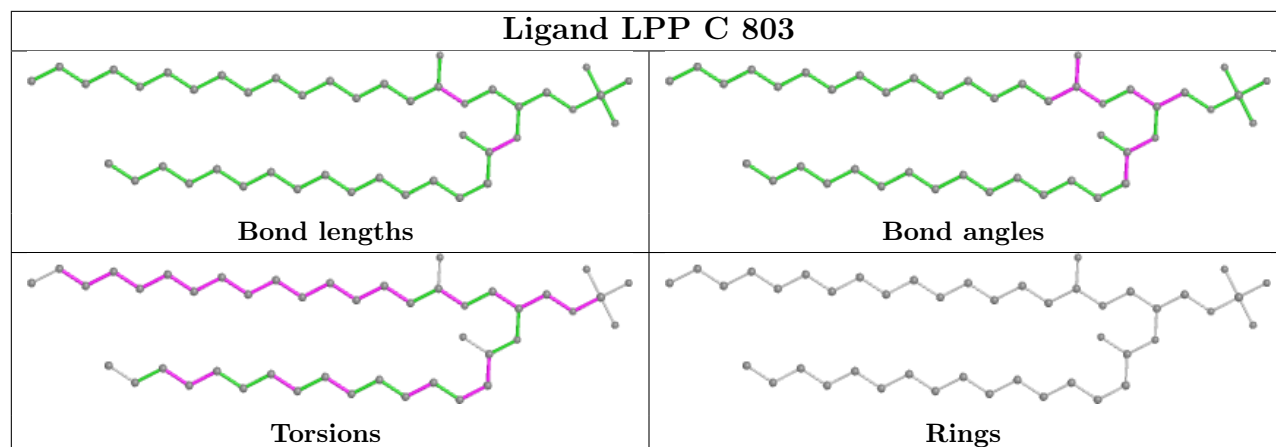
Ligand LPP B 803



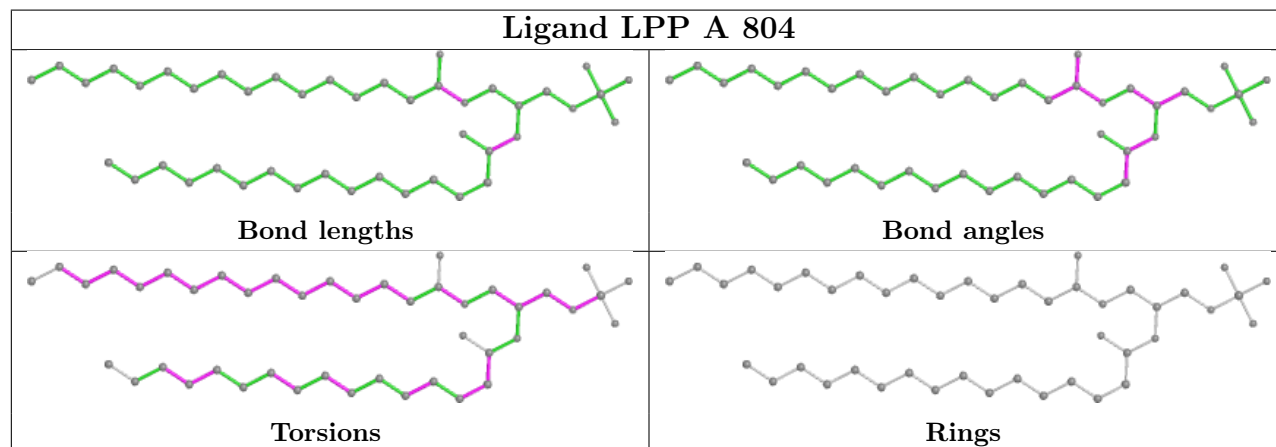
Ligand Y01 D 802



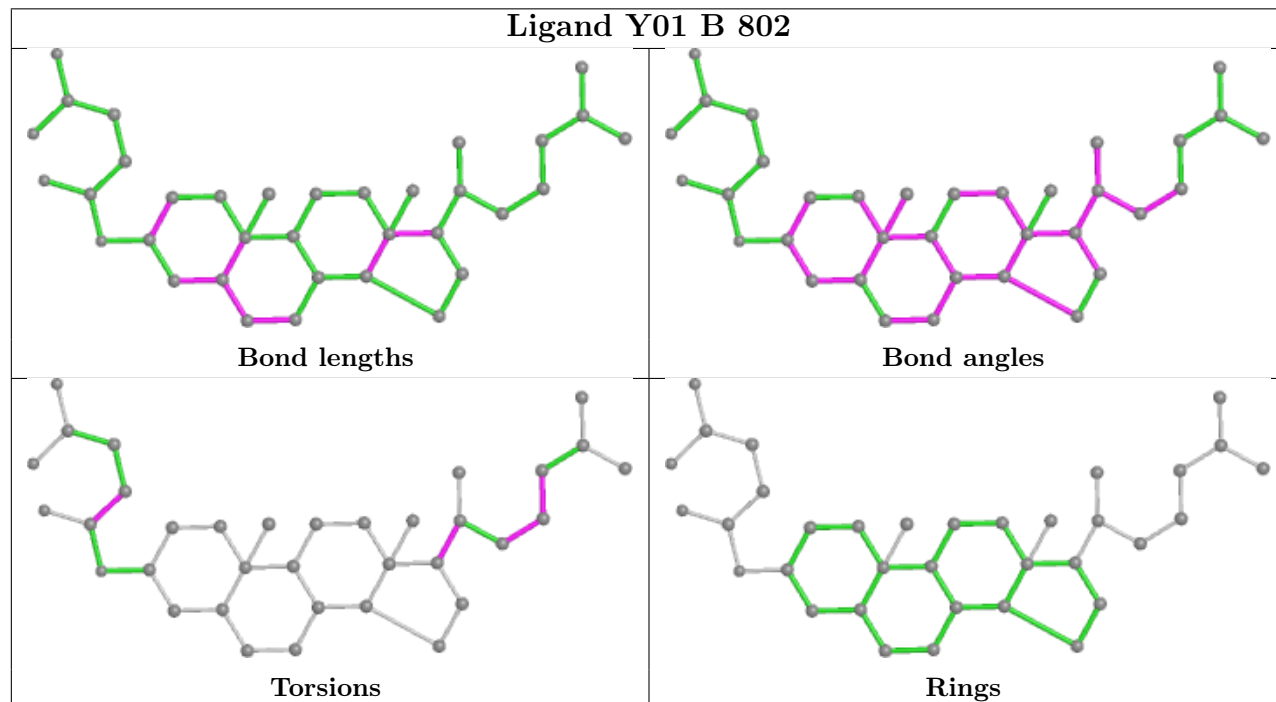
Ligand LPP C 803



Ligand LPP A 804



Ligand Y01 B 802



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.

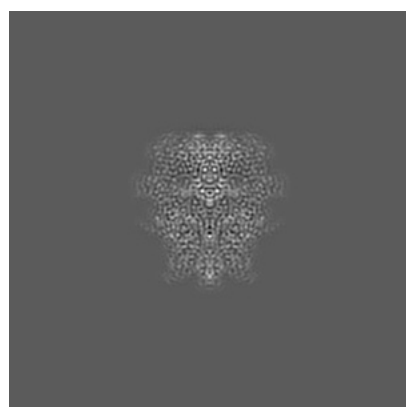
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9615. These allow visual inspection of the internal detail of the map and identification of artifacts.

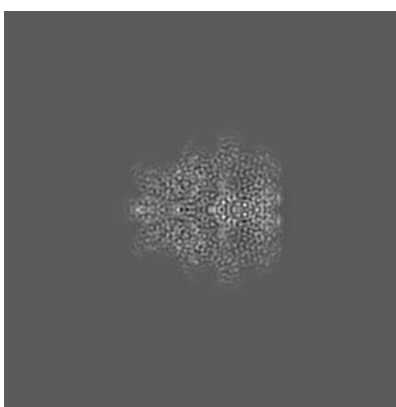
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

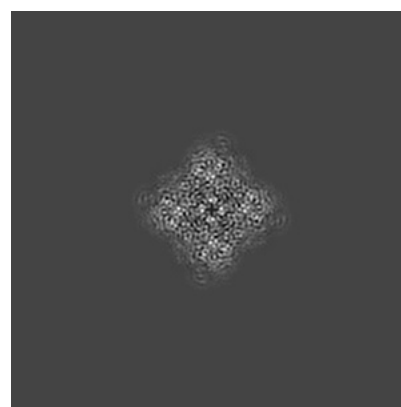
6.1.1 Primary map



X



Y

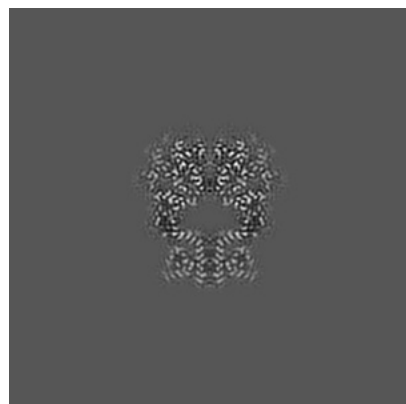


Z

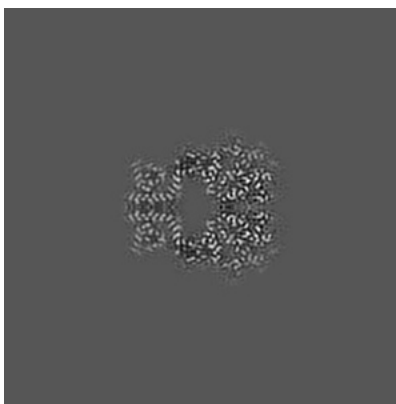
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

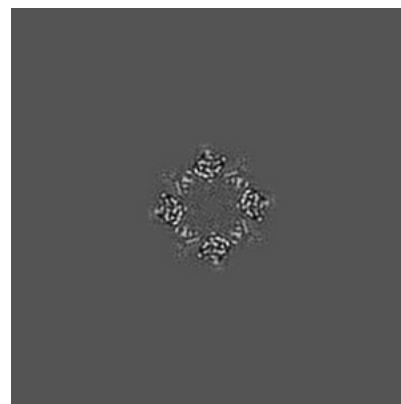
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices [i](#)

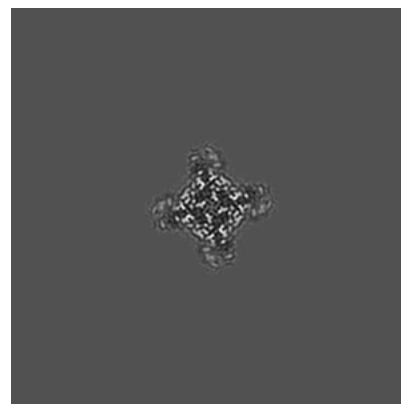
6.3.1 Primary map



X Index: 127



Y Index: 129

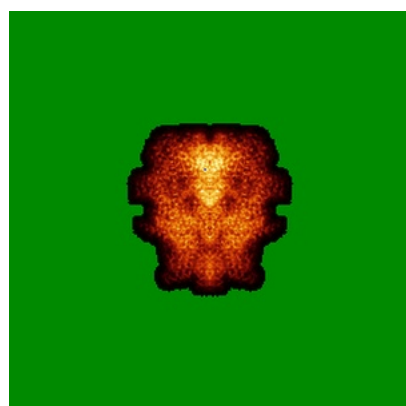


Z Index: 161

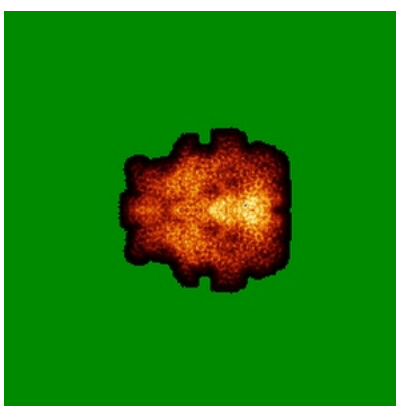
The images above show the largest variance slices of the map in three orthogonal directions.

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

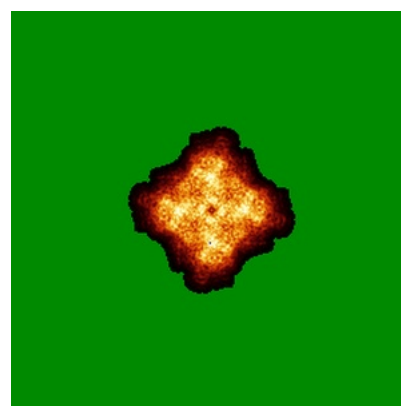
6.4.1 Primary map



X



Y

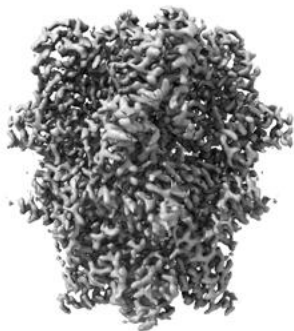


Z

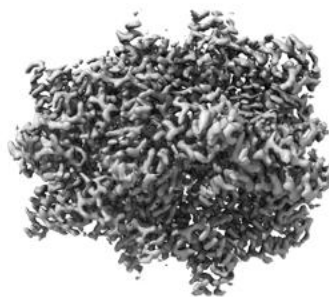
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.058. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

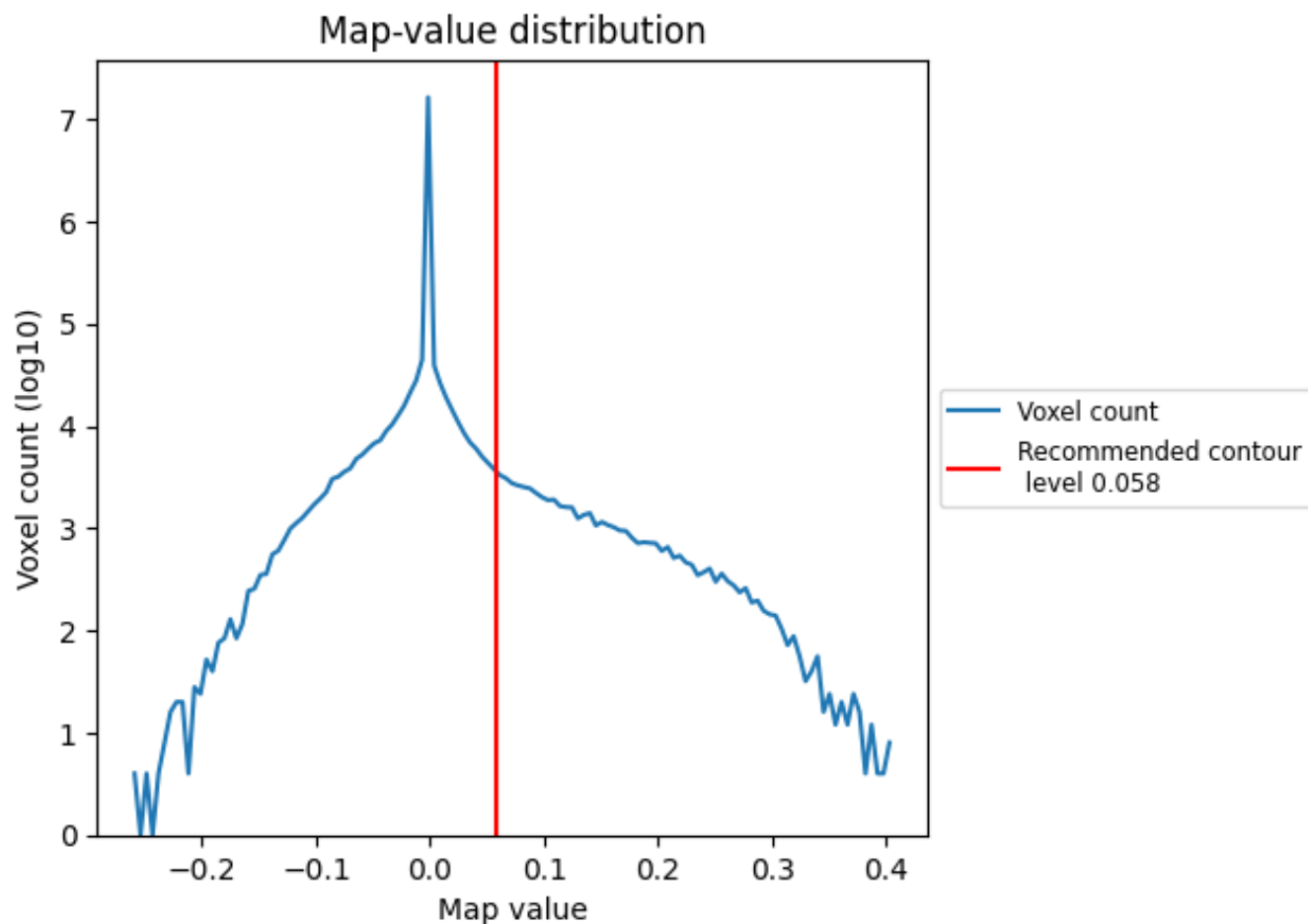
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

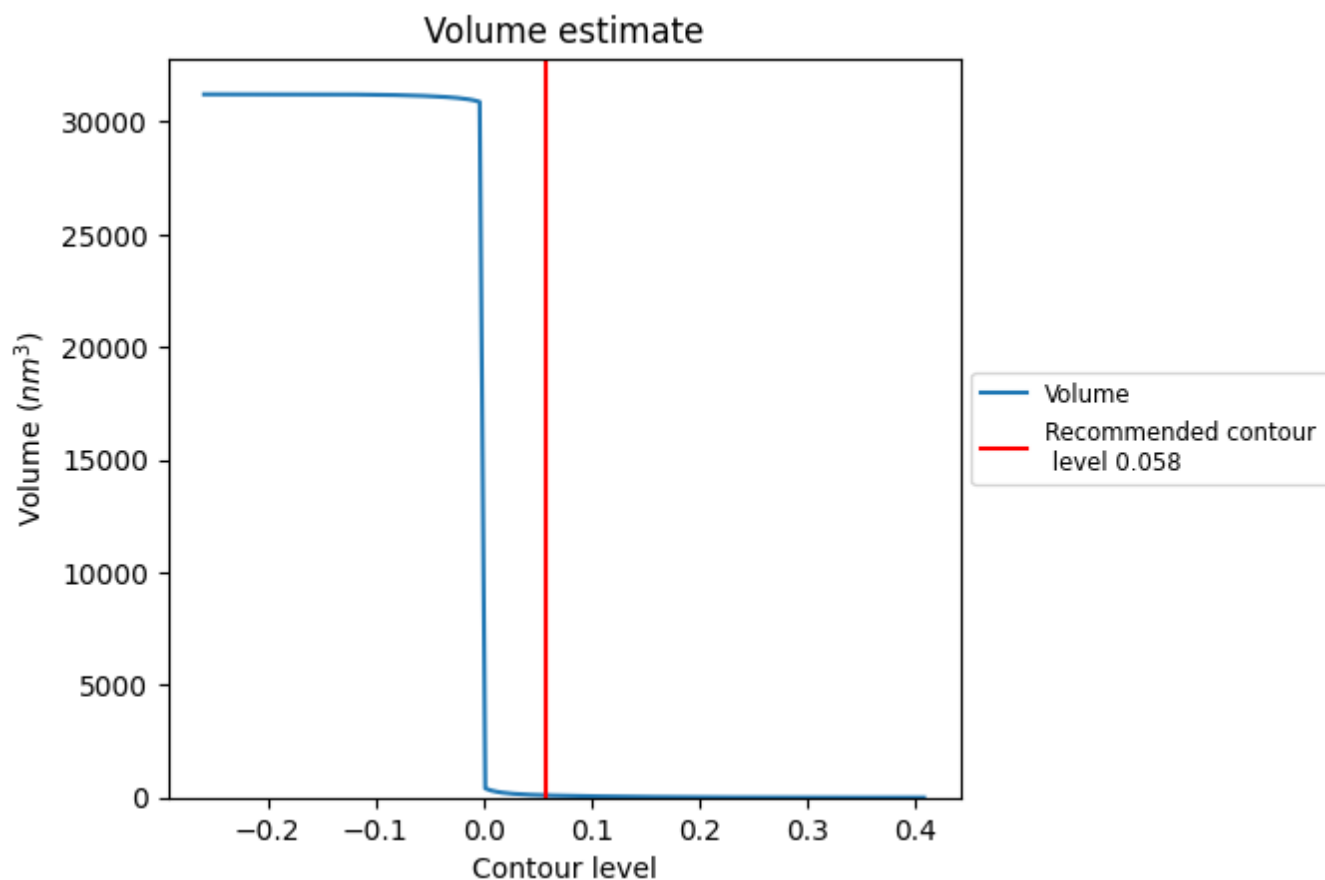
This section contains the results of statistical analysis of the map.

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.

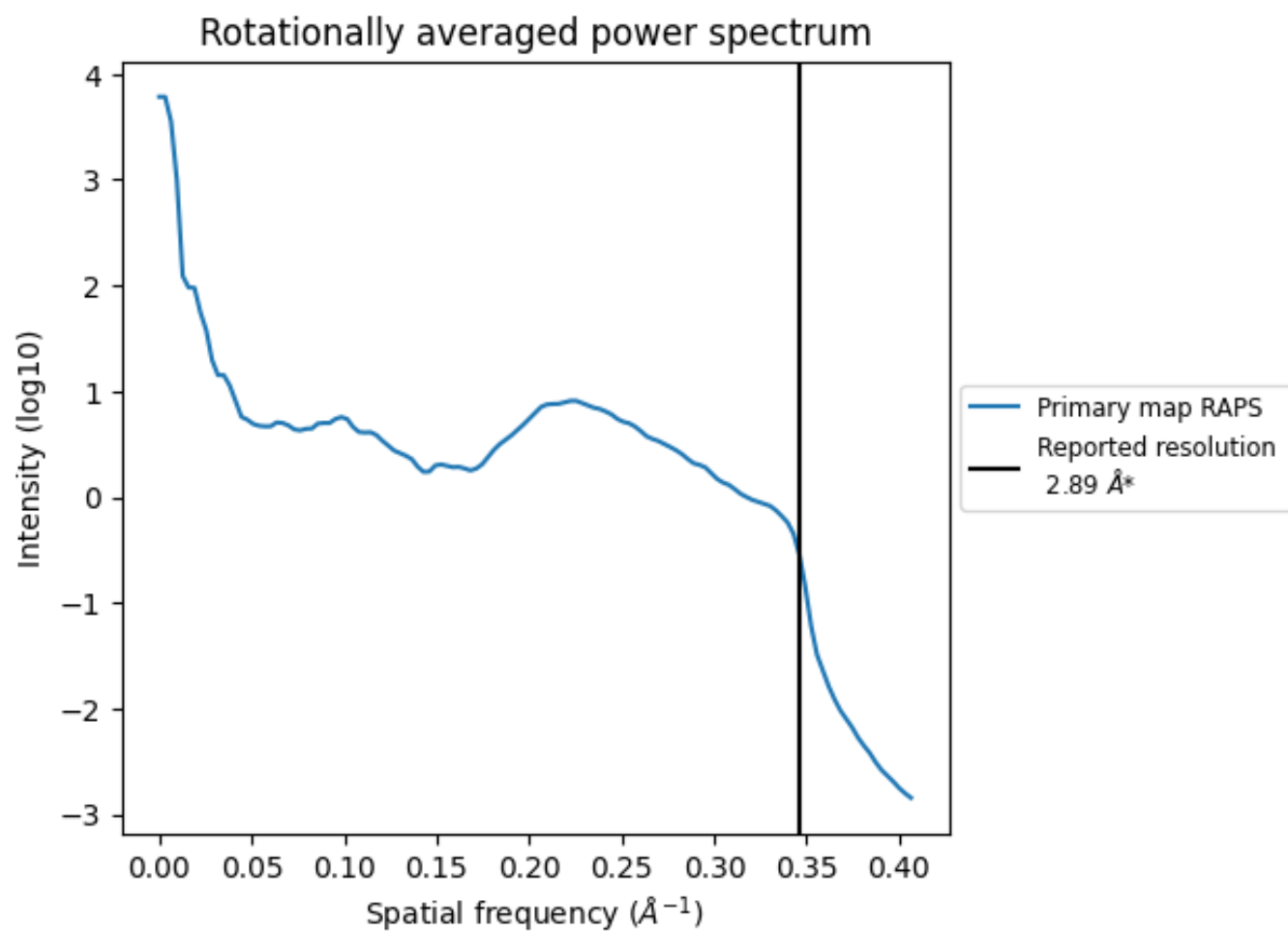
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 90 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 ⓘ

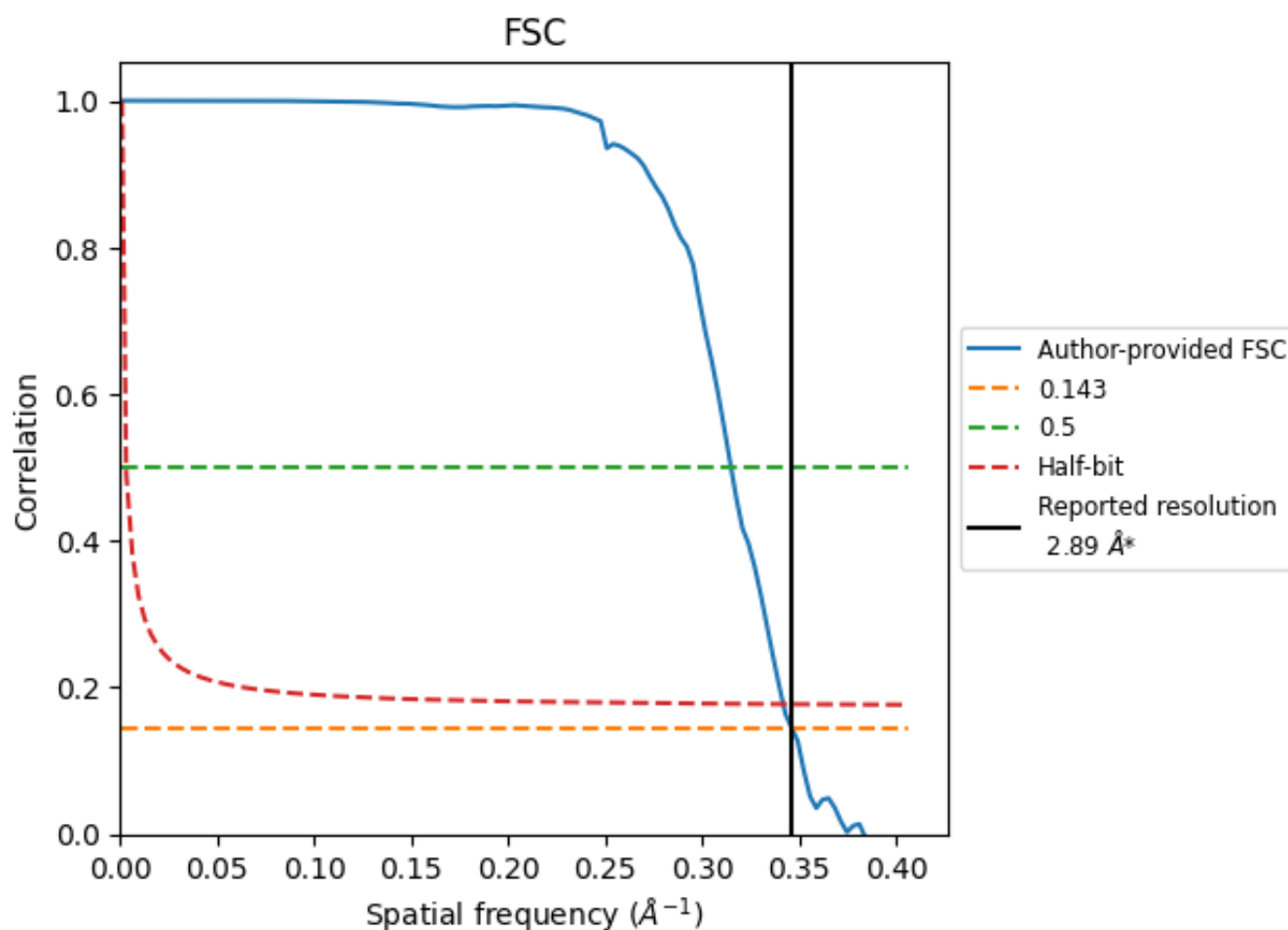


*Reported resolution corresponds to spatial frequency of 0.346 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

8.2 Resolution estimates [i](#)

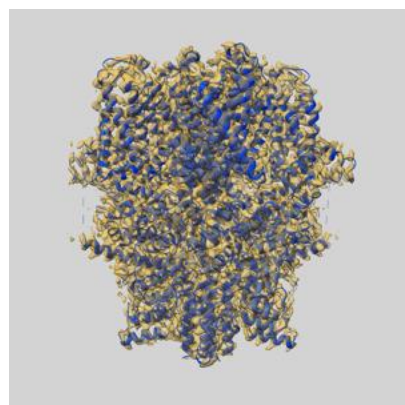
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.18	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

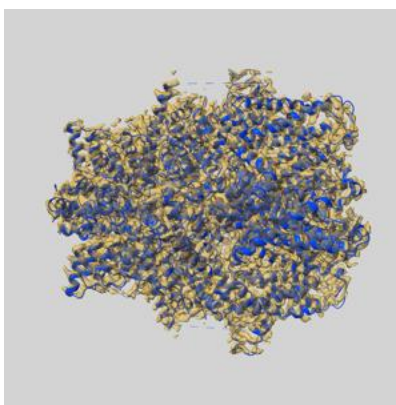
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9615 and PDB model 6AEI. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

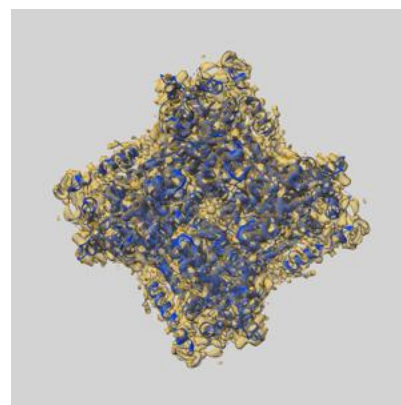
9.1 Map-model overlay [i](#)



X



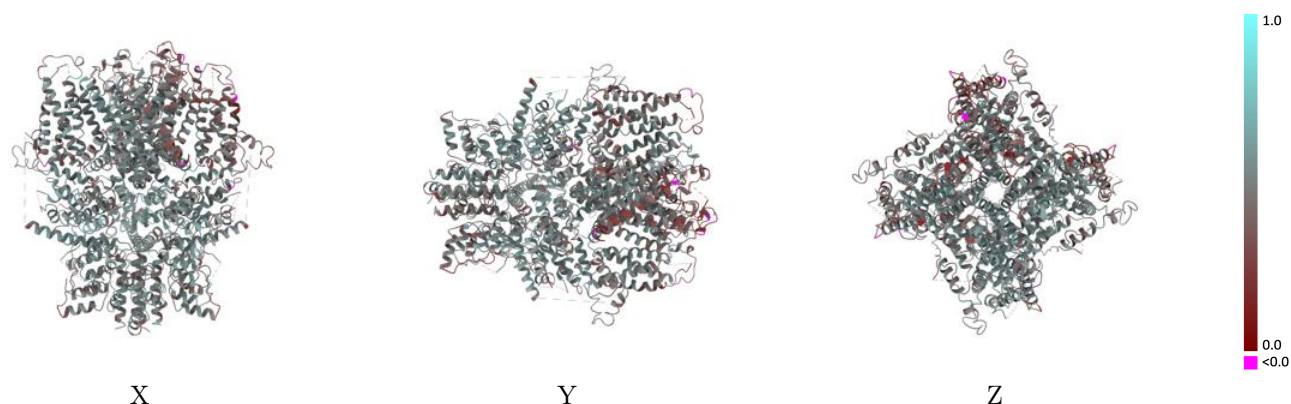
Y



Z

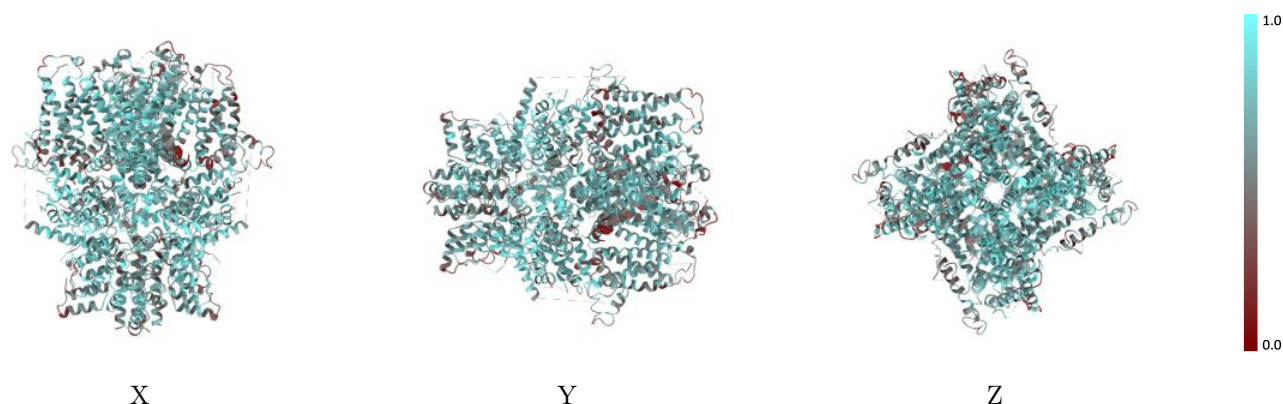
The images above show the 3D surface view of the map at the recommended contour level 0.058 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



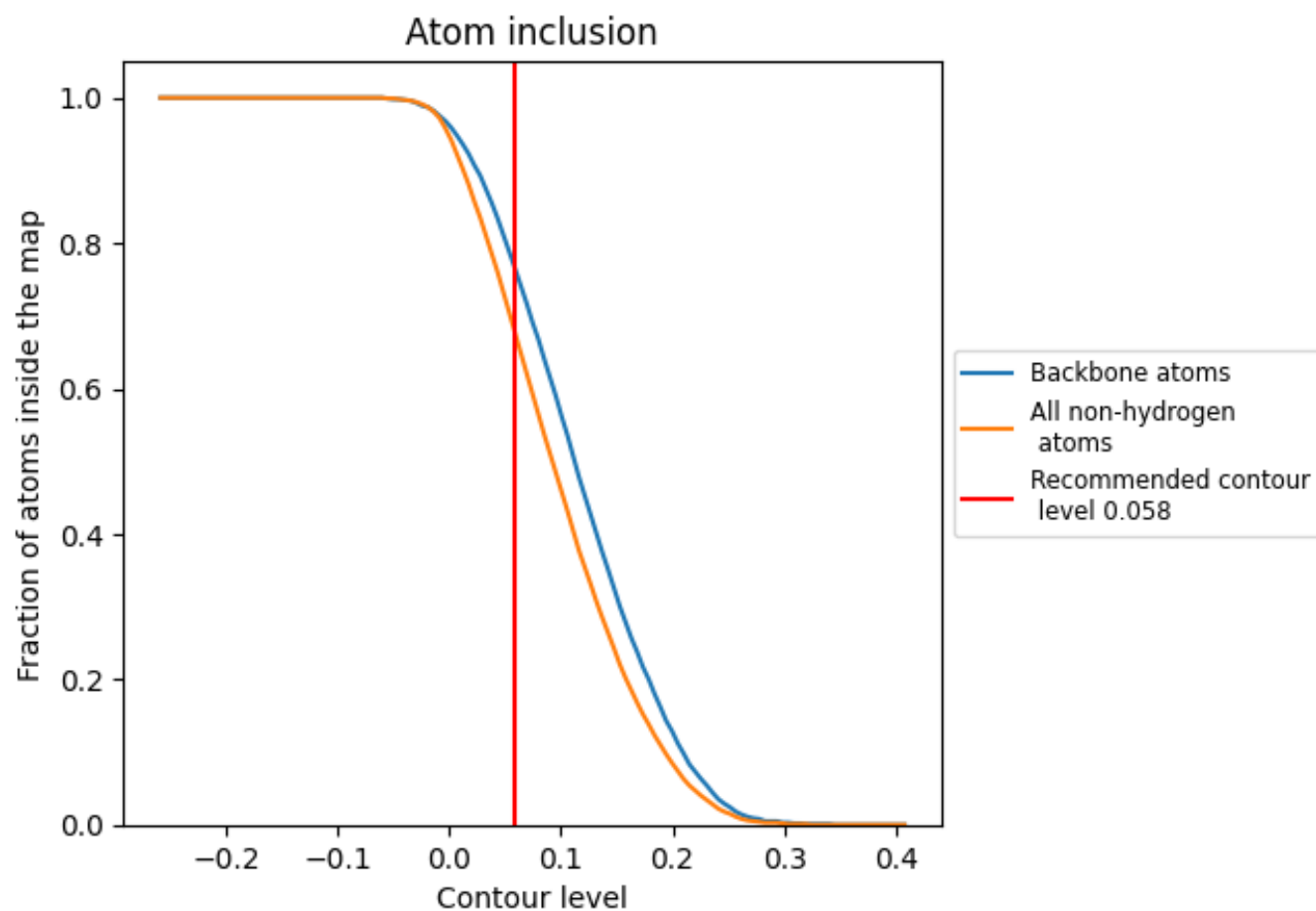
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.058).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 68% 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 (0.058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6800	<div></div> 0.4840
A	<div></div> 0.7060	<div></div> 0.5170
B	<div></div> 0.6760	<div></div> 0.4720
C	<div></div> 0.6550	<div></div> 0.4490
D	<div></div> 0.6850	<div></div> 0.4990

