Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:20 PM EST

PDB ID	:	7MIL
EMDB ID	:	EMD-23855
Title	:	Mouse TRPV3 in MSP2N2 nanodiscs, sensitized state at 42 degrees Celsius
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2021-04-17
Resolution	:	3.86 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:

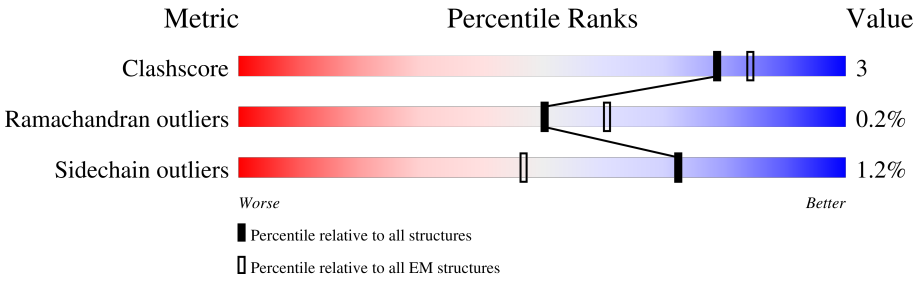
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.86 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	808	32% 74% 7% 19%
1	B	808	33% 74% 7% 19%
1	C	808	30% 73% 7% 19%
1	D	808	32% 74% 7% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21753 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	656	Total	C	N	O	S	0	0
			5347	3471	886	957	33		
1	B	656	Total	C	N	O	S	0	0
			5347	3471	886	957	33		
1	C	656	Total	C	N	O	S	0	0
			5347	3471	886	957	33		
1	D	656	Total	C	N	O	S	0	0
			5347	3471	886	957	33		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
C	801	TRP	-	expression tag	UNP Q8K424
C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424

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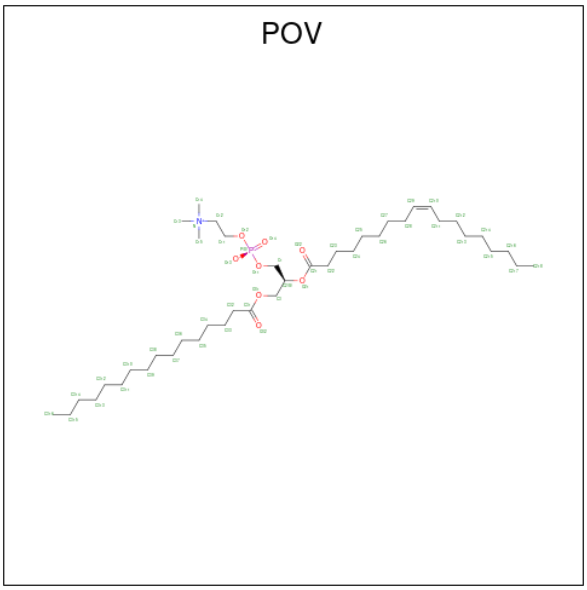
Chain	Residue	Modelled	Actual	Comment	Reference
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	A	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	B	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	B	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	C	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	C	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	D	1	Total	C	N	O	P	0
			91	71	2	16	2	
2	D	1	Total	C	N	O	P	0
			91	71	2	16	2	

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

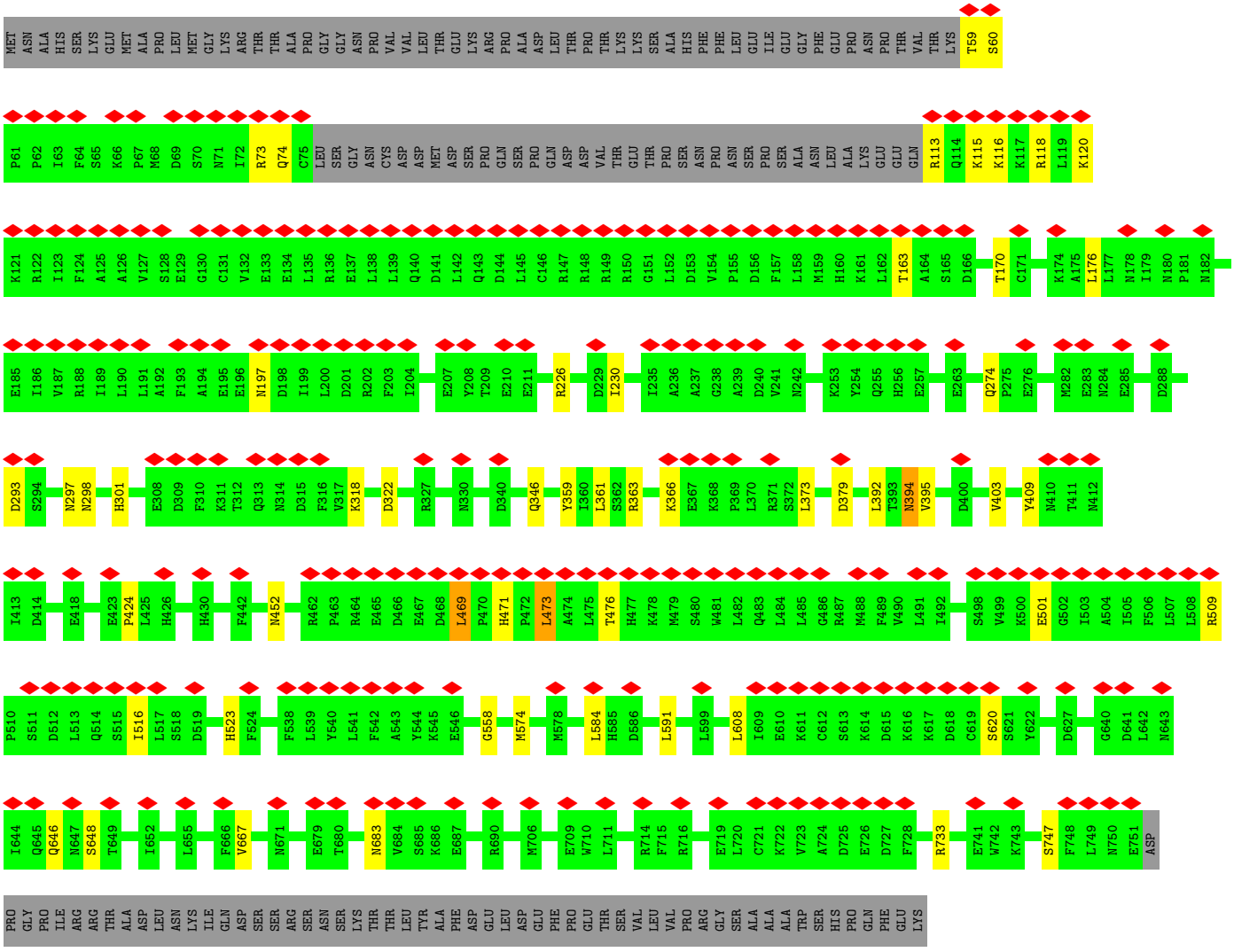
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
3	C	1	1	1	0

3 Residue-property plots (i)

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.

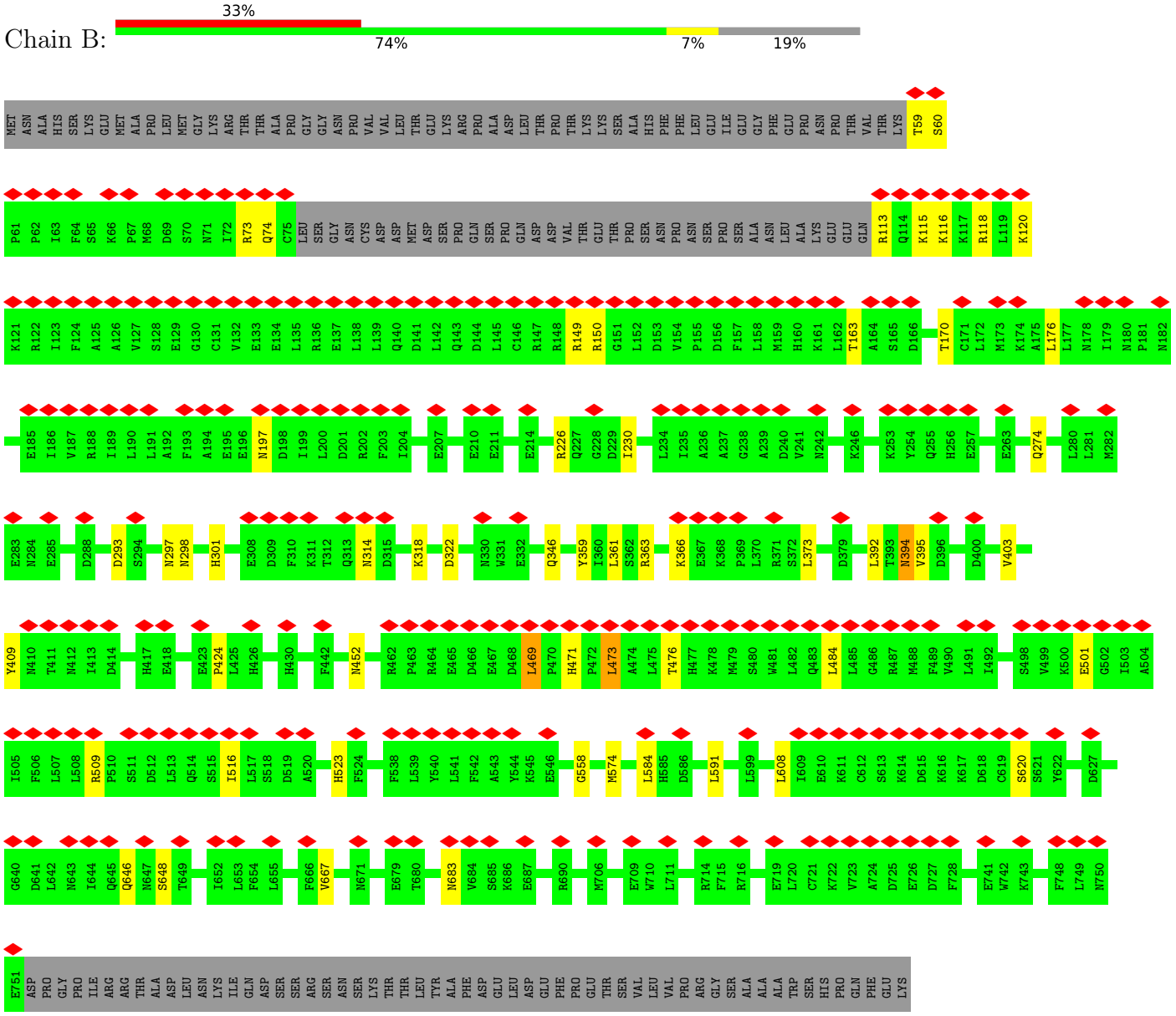
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain A:



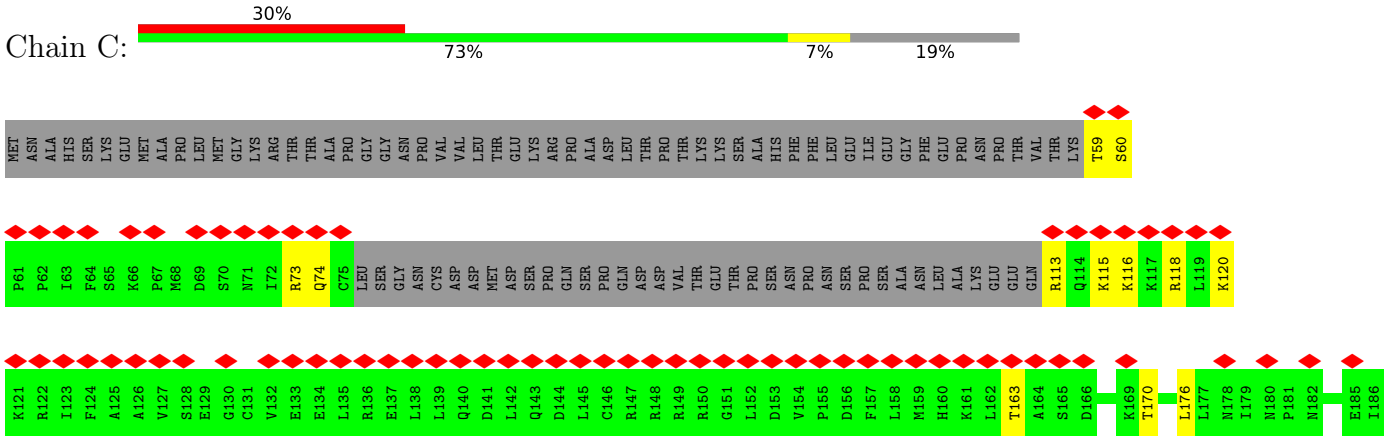
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

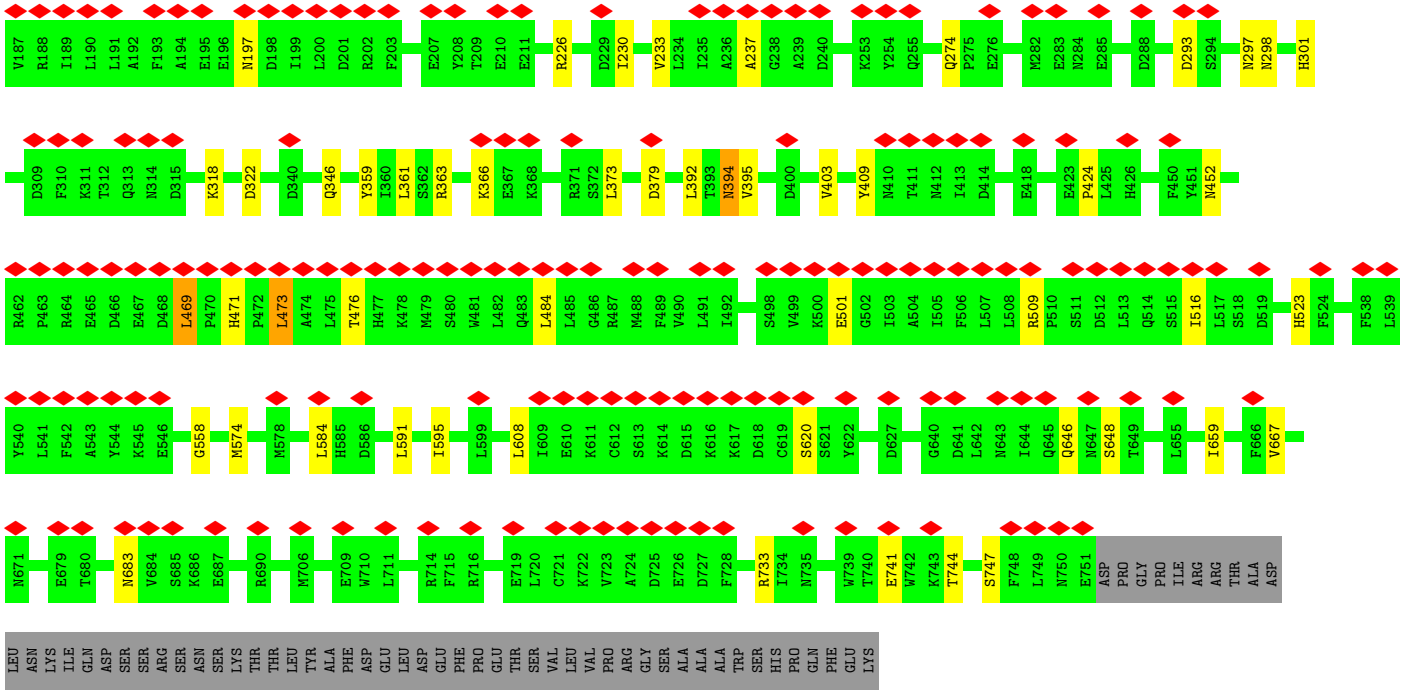
Chain B:



• Molecule 1: Transient receptor potential cation channel subfamily V member 3

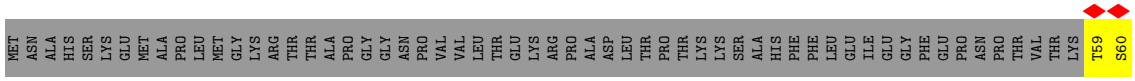
Chain C:

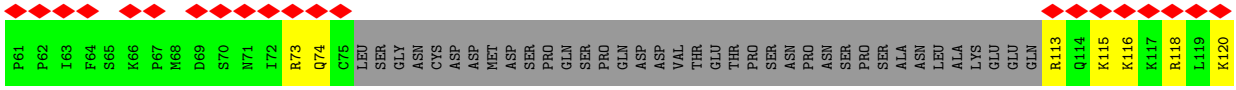


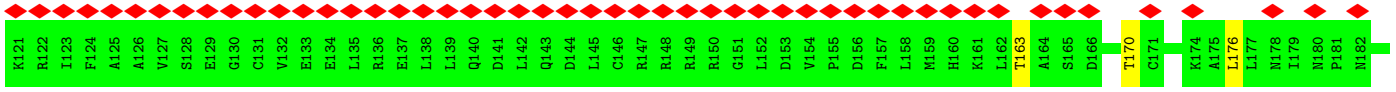


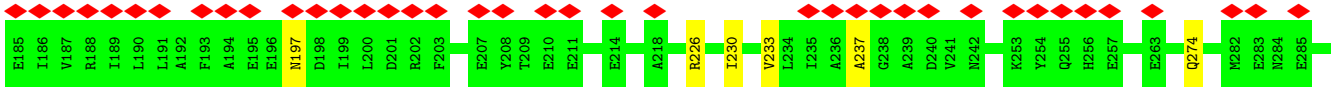
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

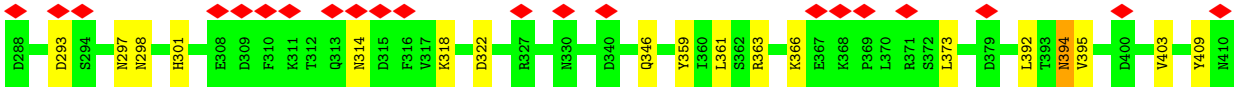
Chain D:

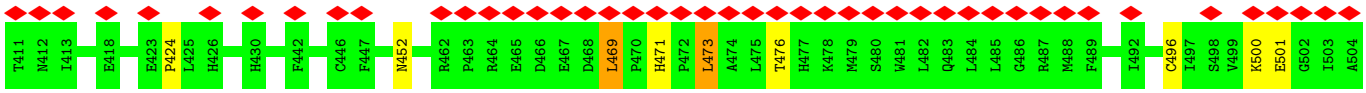


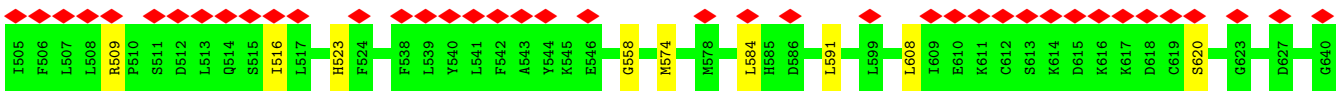


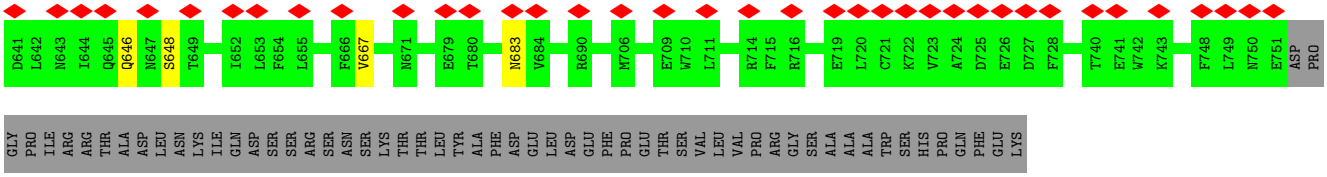











D641 L642 N643 I644 Q645 Q646 N647 S648 T649 I652 L653 F654 L655 F666 V667 N671 E679 T680 N683 V684 R690 M706 E709 W710 L711 R714 F715 R716 E719 L720 C721 K722 V723 A724 D725 E726 D727 F728 T740 E741 W742 K743 F748 L749 N750 E751 ASP PRO
GLY PRO ILE ARG ARG THR ALA ASP LEU ASN LYS ILE GLN ASP SER SER ARG SER ASN SER LYS THR THR LEU TYR ALA PHE ASP GLU LEU ASP GLU PHE PRO GLU THR SER VAL LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22925	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58.5	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0225	Depositor
Map size (Å)	219.648, 219.648, 219.648	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, NA

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	0.31	0/5462	0.56	4/7387 (0.1%)
1	B	0.31	0/5462	0.56	4/7387 (0.1%)
1	C	0.31	0/5462	0.56	4/7387 (0.1%)
1	D	0.31	0/5462	0.56	4/7387 (0.1%)
All	All	0.31	0/21848	0.56	16/29548 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	469	LEU	CA-CB-CG	8.90	135.77	115.30
1	A	469	LEU	CA-CB-CG	8.89	135.76	115.30
1	B	469	LEU	CA-CB-CG	8.89	135.74	115.30
1	D	469	LEU	CA-CB-CG	8.87	135.69	115.30
1	A	392	LEU	CA-CB-CG	7.20	131.85	115.30
1	D	392	LEU	CA-CB-CG	7.20	131.85	115.30
1	C	392	LEU	CA-CB-CG	7.19	131.85	115.30
1	B	392	LEU	CA-CB-CG	7.19	131.84	115.30
1	C	473	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	473	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	473	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	473	LEU	CA-CB-CG	5.35	127.61	115.30
1	D	469	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	469	LEU	CB-CG-CD1	5.21	119.86	111.00
1	B	469	LEU	CB-CG-CD1	5.21	119.85	111.00
1	C	469	LEU	CB-CG-CD1	5.19	119.83	111.00

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	5347	0	5424	26	0
1	B	5347	0	5424	27	0
1	C	5347	0	5424	31	0
1	D	5347	0	5424	28	0
2	A	91	0	137	3	0
2	B	91	0	137	3	0
2	C	91	0	137	5	0
2	D	91	0	137	8	0
3	C	1	0	0	0	0
All	All	21753	0	22244	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HG2	1:A:120:LYS:HE3	1.76	0.67
1:B:116:LYS:HG2	1:B:120:LYS:HE3	1.76	0.67
1:B:667:VAL:HG21	2:C:901:POV:H21G	1.78	0.66
1:D:116:LYS:HG2	1:D:120:LYS:HE3	1.76	0.66
1:A:747:SER:HB2	1:D:314:ASN:HD22	1.60	0.65
1:C:116:LYS:HG2	1:C:120:LYS:HE3	1.76	0.65
1:A:667:VAL:HG21	2:B:901:POV:H21G	1.79	0.64
2:A:901:POV:H21G	1:D:667:VAL:HG21	1.79	0.64
1:B:620:SER:OG	1:B:646:GLN:NE2	2.32	0.63
1:A:620:SER:OG	1:A:646:GLN:NE2	2.32	0.62
1:D:620:SER:OG	1:D:646:GLN:NE2	2.32	0.62
1:C:620:SER:OG	1:C:646:GLN:NE2	2.32	0.62
1:C:667:VAL:HG21	2:D:901:POV:H21G	1.82	0.61
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.36	0.58
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.36	0.58
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.36	0.57
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.36	0.56
1:B:516:ILE:HD11	1:B:584:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:ILE:HD11	1:D:584:LEU:HD22	1.87	0.56
1:C:516:ILE:HD11	1:C:584:LEU:HD22	1.88	0.55
1:A:452:ASN:ND2	1:A:558:GLY:O	2.40	0.55
1:A:516:ILE:HD11	1:A:584:LEU:HD22	1.87	0.55
1:D:452:ASN:ND2	1:D:558:GLY:O	2.40	0.55
1:B:452:ASN:ND2	1:B:558:GLY:O	2.40	0.54
1:C:452:ASN:ND2	1:C:558:GLY:O	2.40	0.54
1:B:314:ASN:HD22	1:C:747:SER:HB2	1.73	0.52
1:C:176:LEU:HD11	1:C:230:ILE:HG21	1.92	0.52
1:D:176:LEU:HD11	1:D:230:ILE:HG21	1.92	0.51
1:A:409:TYR:O	1:A:509:ARG:NH1	2.44	0.51
1:B:395:VAL:HA	1:B:403:VAL:HG22	1.93	0.51
1:B:409:TYR:O	1:B:509:ARG:NH1	2.44	0.51
1:B:176:LEU:HD11	1:B:230:ILE:HG21	1.92	0.51
1:D:395:VAL:HA	1:D:403:VAL:HG22	1.93	0.51
1:A:395:VAL:HA	1:A:403:VAL:HG22	1.93	0.50
1:C:395:VAL:HA	1:C:403:VAL:HG22	1.93	0.50
1:C:409:TYR:O	1:C:509:ARG:NH1	2.44	0.50
1:D:409:TYR:O	1:D:509:ARG:NH1	2.44	0.50
1:A:176:LEU:HD11	1:A:230:ILE:HG21	1.92	0.50
1:C:322:ASP:OD1	1:C:359:TYR:OH	2.30	0.49
1:D:322:ASP:OD1	1:D:359:TYR:OH	2.30	0.49
1:A:322:ASP:OD1	1:A:359:TYR:OH	2.30	0.48
1:B:293:ASP:OD1	1:B:297:ASN:N	2.46	0.48
1:B:322:ASP:OD1	1:B:359:TYR:OH	2.31	0.48
1:C:163:THR:HG22	1:C:170:THR:HG22	1.95	0.48
1:A:293:ASP:OD1	1:A:297:ASN:N	2.47	0.48
1:B:163:THR:HG22	1:B:170:THR:HG22	1.95	0.48
1:C:293:ASP:OD1	1:C:297:ASN:N	2.46	0.48
1:D:163:THR:HG22	1:D:170:THR:HG22	1.95	0.47
1:D:293:ASP:OD1	1:D:297:ASN:N	2.46	0.47
1:A:163:THR:HG22	1:A:170:THR:HG22	1.95	0.47
1:A:226:ARG:HD2	1:A:274:GLN:HE21	1.78	0.47
2:A:901:POV:H37	2:A:901:POV:H34A	1.65	0.47
1:B:226:ARG:HD2	1:B:274:GLN:HE21	1.78	0.47
1:C:226:ARG:HD2	1:C:274:GLN:HE21	1.78	0.47
1:A:361:LEU:HD12	1:A:424:PRO:HG2	1.97	0.47
1:D:361:LEU:HD12	1:D:424:PRO:HG2	1.97	0.47
1:D:496:CYS:HB3	2:D:902:POV:H22A	1.97	0.47
1:D:226:ARG:HD2	1:D:274:GLN:HE21	1.78	0.46
2:D:901:POV:H34A	2:D:901:POV:H37	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LEU:HD12	1:B:424:PRO:HG2	1.97	0.46
1:C:318:LYS:HE2	1:C:359:TYR:HB2	1.97	0.46
1:B:484:LEU:HD13	1:B:484:LEU:HA	1.77	0.46
1:A:501:GLU:OE1	1:A:523:HIS:ND1	2.35	0.46
2:D:901:POV:H210	2:D:901:POV:H21C	1.62	0.46
1:C:361:LEU:HD12	1:C:424:PRO:HG2	1.97	0.46
1:C:484:LEU:HD13	1:C:484:LEU:HA	1.77	0.45
1:C:608:LEU:O	1:C:648:SER:OG	2.35	0.45
1:D:608:LEU:O	1:D:648:SER:OG	2.35	0.45
1:A:59:THR:OG1	1:A:60:SER:N	2.50	0.45
1:A:318:LYS:HE2	1:A:359:TYR:HB2	1.98	0.45
1:B:318:LYS:HE2	1:B:359:TYR:HB2	1.98	0.45
1:C:73:ARG:HE	1:C:74:GLN:H	1.65	0.45
1:D:318:LYS:HE2	1:D:359:TYR:HB2	1.97	0.45
1:B:501:GLU:OE1	1:B:523:HIS:ND1	2.35	0.45
1:B:115:LYS:HD2	1:B:118:ARG:HH11	1.82	0.45
1:D:59:THR:OG1	1:D:60:SER:N	2.50	0.45
1:C:363:ARG:NH1	1:C:373:LEU:O	2.50	0.45
1:D:73:ARG:HE	1:D:74:GLN:H	1.65	0.45
2:B:901:POV:H21C	2:B:901:POV:H210	1.68	0.45
1:A:115:LYS:HD2	1:A:118:ARG:HH11	1.82	0.44
1:A:379:ASP:OD2	1:A:733:ARG:NH2	2.47	0.44
1:B:608:LEU:O	1:B:648:SER:OG	2.35	0.44
2:C:901:POV:H37	2:C:901:POV:H34A	1.63	0.44
1:A:73:ARG:HE	1:A:74:GLN:H	1.65	0.44
1:A:608:LEU:O	1:A:648:SER:OG	2.35	0.44
1:B:73:ARG:HE	1:B:74:GLN:H	1.65	0.44
1:B:113:ARG:HG3	1:B:116:LYS:H	1.83	0.44
1:C:115:LYS:HD2	1:C:118:ARG:HH11	1.82	0.44
1:D:115:LYS:HD2	1:D:118:ARG:HH11	1.82	0.44
1:B:363:ARG:NH1	1:B:373:LEU:O	2.50	0.44
1:A:363:ARG:NH1	1:A:373:LEU:O	2.50	0.44
1:B:59:THR:OG1	1:B:60:SER:N	2.50	0.44
1:C:113:ARG:HG3	1:C:116:LYS:H	1.83	0.43
1:A:113:ARG:HG3	1:A:116:LYS:H	1.83	0.43
2:C:901:POV:H21C	2:C:901:POV:H210	1.70	0.43
1:D:113:ARG:HG3	1:D:116:LYS:H	1.83	0.43
1:B:346:GLN:NE2	1:B:394:ASN:OD1	2.52	0.43
1:D:363:ARG:NH1	1:D:373:LEU:O	2.50	0.43
1:A:471:HIS:CE1	1:A:473:LEU:HB3	2.54	0.42
1:C:59:THR:OG1	1:C:60:SER:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:LYS:HE2	2:D:902:POV:H2	2.00	0.42
1:C:379:ASP:OD2	1:C:733:ARG:NH2	2.47	0.42
2:D:901:POV:H312	2:D:901:POV:H31F	1.92	0.42
1:B:471:HIS:CE1	1:B:473:LEU:HB3	2.54	0.42
1:D:346:GLN:NE2	1:D:394:ASN:OD1	2.52	0.42
1:A:346:GLN:NE2	1:A:394:ASN:OD1	2.52	0.42
1:C:346:GLN:NE2	1:C:394:ASN:OD1	2.52	0.42
2:C:901:POV:H312	2:C:901:POV:H31F	1.93	0.42
1:D:471:HIS:CE1	1:D:473:LEU:HB3	2.54	0.41
1:C:659:ILE:HD13	2:D:901:POV:H28	2.02	0.41
2:B:901:POV:H37	2:B:901:POV:H34A	1.62	0.41
1:C:471:HIS:CE1	1:C:473:LEU:HB3	2.54	0.41
1:C:741:GLU:O	1:C:744:THR:OG1	2.34	0.41
1:D:233:VAL:O	1:D:237:ALA:N	2.54	0.41
2:A:901:POV:H21C	2:A:901:POV:H210	1.69	0.41
2:C:902:POV:H24A	2:C:902:POV:H33A	2.03	0.41
2:D:902:POV:H33A	2:D:902:POV:H24A	2.03	0.41
1:C:501:GLU:OE1	1:C:523:HIS:ND1	2.35	0.41
1:C:595:ILE:HD13	1:C:595:ILE:HA	1.91	0.40
1:D:501:GLU:OE1	1:D:523:HIS:ND1	2.36	0.40
1:B:149:ARG:HE	1:B:150:ARG:H	1.69	0.40
1:C:233:VAL:O	1:C:237:ALA:N	2.54	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	652/808 (81%)	622 (95%)	29 (4%)	1 (0%)	47 78
1	B	652/808 (81%)	622 (95%)	29 (4%)	1 (0%)	47 78
1	C	652/808 (81%)	622 (95%)	29 (4%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	652/808 (81%)	622 (95%)	29 (4%)	1 (0%)	47 78
All	All	2608/3232 (81%)	2488 (95%)	116 (4%)	4 (0%)	50 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	THR
1	B	476	THR
1	C	476	THR
1	D	476	THR

5.3.2 Protein sidechains (i)

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	588/721 (82%)	581 (99%)	7 (1%)	71 83
1	B	588/721 (82%)	581 (99%)	7 (1%)	71 83
1	C	588/721 (82%)	581 (99%)	7 (1%)	71 83
1	D	588/721 (82%)	581 (99%)	7 (1%)	71 83
All	All	2352/2884 (82%)	2324 (99%)	28 (1%)	72 83

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

Mol	Chain	Res	Type
1	A	197	ASN
1	A	366	LYS
1	A	394	ASN
1	A	469	LEU
1	A	574	MET
1	A	591	LEU
1	A	683	ASN
1	B	197	ASN
1	B	366	LYS
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	469	LEU
1	B	574	MET
1	B	591	LEU
1	B	683	ASN
1	C	197	ASN
1	C	366	LYS
1	C	394	ASN
1	C	469	LEU
1	C	574	MET
1	C	591	LEU
1	C	683	ASN
1	D	197	ASN
1	D	366	LYS
1	D	394	ASN
1	D	469	LEU
1	D	574	MET
1	D	591	LEU
1	D	683	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	A	197	ASN
1	A	346	GLN
1	A	394	ASN
1	A	646	GLN
1	A	683	ASN
1	B	160	HIS
1	B	197	ASN
1	B	346	GLN
1	B	394	ASN
1	B	646	GLN
1	B	683	ASN
1	C	160	HIS
1	C	197	ASN
1	C	346	GLN
1	C	394	ASN
1	C	646	GLN
1	C	683	ASN
1	D	160	HIS
1	D	197	ASN

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Mol	Chain	Res	Type
1	D	346	GLN
1	D	394	ASN
1	D	646	GLN
1	D	683	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
2	POV	C	902	-	38,38,51	1.15	3 (7%)	44,46,59	1.10	6 (13%)
2	POV	B	902	-	38,38,51	1.16	3 (7%)	44,46,59	1.10	6 (13%)
2	POV	D	901	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	3 (5%)
2	POV	B	901	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	3 (5%)
2	POV	A	901	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	3 (5%)
2	POV	A	902	-	38,38,51	1.16	3 (7%)	44,46,59	1.11	6 (13%)
2	POV	D	902	-	38,38,51	1.16	3 (7%)	44,46,59	1.12	6 (13%)
2	POV	C	901	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	C	902	-	-	22/42/42/55	-
2	POV	B	902	-	-	21/42/42/55	-
2	POV	D	901	-	-	36/55/55/55	-
2	POV	B	901	-	-	33/55/55/55	-
2	POV	A	901	-	-	34/55/55/55	-
2	POV	A	902	-	-	22/42/42/55	-
2	POV	D	902	-	-	22/42/42/55	-
2	POV	C	901	-	-	34/55/55/55	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	POV	O21-C21	2.87	1.42	1.34
2	A	902	POV	O21-C21	2.85	1.42	1.34
2	C	902	POV	O21-C21	2.84	1.42	1.34
2	D	902	POV	O21-C21	2.84	1.42	1.34
2	D	901	POV	O21-C21	2.81	1.42	1.34
2	B	902	POV	O31-C31	2.78	1.41	1.33
2	A	901	POV	O21-C21	2.78	1.42	1.34
2	C	901	POV	O31-C31	2.77	1.41	1.33
2	D	902	POV	O31-C31	2.77	1.41	1.33
2	B	901	POV	O21-C21	2.77	1.42	1.34
2	C	902	POV	O31-C31	2.76	1.41	1.33
2	A	902	POV	O31-C31	2.76	1.41	1.33
2	D	901	POV	O31-C31	2.76	1.41	1.33
2	B	901	POV	O31-C31	2.76	1.41	1.33
2	C	901	POV	O21-C21	2.74	1.42	1.34
2	A	901	POV	O31-C31	2.72	1.41	1.33
2	B	901	POV	O21-C2	-2.38	1.40	1.46
2	A	901	POV	O21-C2	-2.37	1.40	1.46
2	C	901	POV	O21-C2	-2.36	1.40	1.46
2	A	902	POV	O21-C2	-2.36	1.40	1.46
2	B	902	POV	O21-C2	-2.35	1.40	1.46
2	C	902	POV	O21-C2	-2.35	1.40	1.46
2	D	902	POV	O21-C2	-2.35	1.40	1.46
2	D	901	POV	O21-C2	-2.34	1.40	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	901	POV	O21-C21-C22	3.99	120.10	111.50
2	B	901	POV	O21-C21-C22	3.98	120.08	111.50
2	A	901	POV	O21-C21-C22	3.98	120.07	111.50
2	D	901	POV	O21-C21-C22	3.97	120.06	111.50
2	A	902	POV	O21-C21-C22	3.72	119.52	111.50
2	C	902	POV	O21-C21-C22	3.67	119.41	111.50
2	D	902	POV	O21-C21-C22	3.64	119.35	111.50
2	B	902	POV	O21-C21-C22	3.56	119.18	111.50
2	D	902	POV	C14-N-C12	2.61	120.59	109.92
2	B	902	POV	O31-C31-C32	2.55	119.91	111.91
2	A	902	POV	O31-C31-C32	2.54	119.88	111.91
2	A	902	POV	C14-N-C12	2.53	120.26	109.92
2	D	902	POV	O31-C31-C32	2.52	119.81	111.91
2	C	902	POV	C14-N-C12	2.52	120.22	109.92
2	C	902	POV	O31-C31-C32	2.51	119.78	111.91
2	A	901	POV	O31-C31-C32	2.48	119.68	111.91
2	B	902	POV	C14-N-C12	2.48	120.04	109.92
2	D	901	POV	O31-C31-C32	2.46	119.64	111.91
2	C	901	POV	O31-C31-C32	2.46	119.64	111.91
2	B	901	POV	O31-C31-C32	2.43	119.54	111.91
2	D	902	POV	C14-N-C13	-2.33	102.97	108.97
2	A	902	POV	C15-N-C14	-2.31	103.04	108.97
2	C	902	POV	C15-N-C14	-2.28	103.12	108.97
2	D	902	POV	C15-N-C14	-2.27	103.13	108.97
2	B	902	POV	C15-N-C14	-2.27	103.14	108.97
2	B	901	POV	C14-N-C12	2.17	118.79	109.92
2	D	901	POV	C14-N-C12	2.16	118.75	109.92
2	A	901	POV	C14-N-C12	2.16	118.74	109.92
2	C	901	POV	C14-N-C12	2.15	118.70	109.92
2	A	902	POV	C14-N-C13	-2.13	103.50	108.97
2	B	902	POV	C14-N-C13	-2.12	103.53	108.97
2	C	902	POV	C14-N-C13	-2.12	103.53	108.97
2	B	902	POV	C3-C2-C1	-2.09	106.84	111.79
2	A	902	POV	C3-C2-C1	-2.04	106.96	111.79
2	C	902	POV	C3-C2-C1	-2.04	106.97	111.79
2	D	902	POV	C3-C2-C1	-2.02	107.01	111.79

There are no chirality outliers.

All (224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C1-O11-P-O12
2	A	901	POV	C1-O11-P-O13
2	A	901	POV	C1-O11-P-O14
2	A	901	POV	C11-O12-P-O11
2	A	901	POV	C11-O12-P-O13
2	A	901	POV	C11-O12-P-O14
2	A	901	POV	O12-C11-C12-N
2	A	902	POV	C11-O12-P-O11
2	A	902	POV	O32-C31-O31-C3
2	B	901	POV	C1-O11-P-O12
2	B	901	POV	C1-O11-P-O13
2	B	901	POV	C1-O11-P-O14
2	B	901	POV	C11-O12-P-O11
2	B	901	POV	C11-O12-P-O13
2	B	901	POV	C11-O12-P-O14
2	B	901	POV	O12-C11-C12-N
2	B	902	POV	C11-O12-P-O11
2	C	901	POV	C1-O11-P-O12
2	C	901	POV	C1-O11-P-O13
2	C	901	POV	C1-O11-P-O14
2	C	901	POV	C11-O12-P-O11
2	C	901	POV	C11-O12-P-O13
2	C	901	POV	C11-O12-P-O14
2	C	901	POV	O12-C11-C12-N
2	C	902	POV	C11-O12-P-O11
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C1-O11-P-O14
2	D	901	POV	C11-O12-P-O11
2	D	901	POV	C11-O12-P-O13
2	D	901	POV	C11-O12-P-O14
2	D	901	POV	O12-C11-C12-N
2	D	902	POV	C11-O12-P-O11
2	D	902	POV	O32-C31-O31-C3
2	B	902	POV	O32-C31-O31-C3
2	C	902	POV	O32-C31-O31-C3
2	A	902	POV	C32-C31-O31-C3
2	B	902	POV	C32-C31-O31-C3
2	C	902	POV	C32-C31-O31-C3
2	D	902	POV	C32-C31-O31-C3
2	D	901	POV	C32-C33-C34-C35
2	A	901	POV	C32-C33-C34-C35
2	C	901	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	B	901	POV	C32-C33-C34-C35
2	A	901	POV	C32-C31-O31-C3
2	B	901	POV	C32-C31-O31-C3
2	C	901	POV	C32-C31-O31-C3
2	D	901	POV	C32-C31-O31-C3
2	B	902	POV	C21-C22-C23-C24
2	B	901	POV	O32-C31-O31-C3
2	A	901	POV	O32-C31-O31-C3
2	C	901	POV	O32-C31-O31-C3
2	D	901	POV	O32-C31-O31-C3
2	A	902	POV	C31-C32-C33-C34
2	B	902	POV	C31-C32-C33-C34
2	C	902	POV	C31-C32-C33-C34
2	D	902	POV	C21-C22-C23-C24
2	D	902	POV	C31-C32-C33-C34
2	A	902	POV	C21-C22-C23-C24
2	C	902	POV	C21-C22-C23-C24
2	B	901	POV	C36-C37-C38-C39
2	C	901	POV	C36-C37-C38-C39
2	A	901	POV	C36-C37-C38-C39
2	B	901	POV	C22-C23-C24-C25
2	A	901	POV	C22-C23-C24-C25
2	C	901	POV	C22-C23-C24-C25
2	D	901	POV	C22-C23-C24-C25
2	D	901	POV	C24-C25-C26-C27
2	C	902	POV	C37-C38-C39-C310
2	D	901	POV	C36-C37-C38-C39
2	D	902	POV	C37-C38-C39-C310
2	A	902	POV	C37-C38-C39-C310
2	B	902	POV	C37-C38-C39-C310
2	B	901	POV	C24-C25-C26-C27
2	B	901	POV	C34-C35-C36-C37
2	D	902	POV	C312-C313-C314-C315
2	D	902	POV	C311-C312-C313-C314
2	A	901	POV	C24-C25-C26-C27
2	A	902	POV	C311-C312-C313-C314
2	B	902	POV	C311-C312-C313-C314
2	C	902	POV	C311-C312-C313-C314
2	B	901	POV	C214-C215-C216-C217
2	D	901	POV	C214-C215-C216-C217
2	A	902	POV	C312-C313-C314-C315
2	C	901	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	A	901	POV	C214-C215-C216-C217
2	B	902	POV	C312-C313-C314-C315
2	C	902	POV	C312-C313-C314-C315
2	C	902	POV	C35-C36-C37-C38
2	A	902	POV	C35-C36-C37-C38
2	D	902	POV	C35-C36-C37-C38
2	B	902	POV	C35-C36-C37-C38
2	D	901	POV	C34-C35-C36-C37
2	A	901	POV	C31-C32-C33-C34
2	C	901	POV	C31-C32-C33-C34
2	C	902	POV	C22-C23-C24-C25
2	D	902	POV	C22-C23-C24-C25
2	B	902	POV	C22-C23-C24-C25
2	C	901	POV	C214-C215-C216-C217
2	C	901	POV	C34-C35-C36-C37
2	A	902	POV	C22-C23-C24-C25
2	A	901	POV	C22-C21-O21-C2
2	B	901	POV	C22-C21-O21-C2
2	C	901	POV	C22-C21-O21-C2
2	D	901	POV	C22-C21-O21-C2
2	D	902	POV	C22-C21-O21-C2
2	B	902	POV	O22-C21-O21-C2
2	D	902	POV	O22-C21-O21-C2
2	A	902	POV	C22-C21-O21-C2
2	B	902	POV	C22-C21-O21-C2
2	C	902	POV	C22-C21-O21-C2
2	D	901	POV	C31-C32-C33-C34
2	C	901	POV	O22-C21-O21-C2
2	B	901	POV	C31-C32-C33-C34
2	A	901	POV	C34-C35-C36-C37
2	C	901	POV	C213-C214-C215-C216
2	A	901	POV	C39-C310-C311-C312
2	C	901	POV	C39-C310-C311-C312
2	B	901	POV	C39-C310-C311-C312
2	D	901	POV	C39-C310-C311-C312
2	A	901	POV	C23-C24-C25-C26
2	A	901	POV	O22-C21-O21-C2
2	A	902	POV	O22-C21-O21-C2
2	B	901	POV	O22-C21-O21-C2
2	C	902	POV	O22-C21-O21-C2
2	D	901	POV	O22-C21-O21-C2
2	B	901	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	A	902	POV	C310-C311-C312-C313
2	C	902	POV	C310-C311-C312-C313
2	B	902	POV	C310-C311-C312-C313
2	C	901	POV	C23-C24-C25-C26
2	D	902	POV	C310-C311-C312-C313
2	A	902	POV	O11-C1-C2-C3
2	B	902	POV	O11-C1-C2-C3
2	C	902	POV	O11-C1-C2-C3
2	D	902	POV	O11-C1-C2-C3
2	A	901	POV	C21-C22-C23-C24
2	C	901	POV	C21-C22-C23-C24
2	D	901	POV	C213-C214-C215-C216
2	D	901	POV	C21-C22-C23-C24
2	D	901	POV	C23-C24-C25-C26
2	A	901	POV	C213-C214-C215-C216
2	B	901	POV	C21-C22-C23-C24
2	B	901	POV	C213-C214-C215-C216
2	B	901	POV	C310-C311-C312-C313
2	C	901	POV	C310-C311-C312-C313
2	A	901	POV	C310-C311-C312-C313
2	D	901	POV	C210-C211-C212-C213
2	D	901	POV	C26-C27-C28-C29
2	D	901	POV	C310-C311-C312-C313
2	B	901	POV	C211-C212-C213-C214
2	D	902	POV	C11-O12-P-O13
2	C	901	POV	C33-C34-C35-C36
2	A	902	POV	C12-C11-O12-P
2	B	902	POV	C12-C11-O12-P
2	C	902	POV	C12-C11-O12-P
2	D	902	POV	C12-C11-O12-P
2	A	902	POV	O11-C1-C2-O21
2	B	902	POV	O11-C1-C2-O21
2	C	902	POV	O11-C1-C2-O21
2	D	902	POV	O11-C1-C2-O21
2	A	901	POV	C211-C212-C213-C214
2	A	901	POV	C33-C34-C35-C36
2	C	901	POV	C211-C212-C213-C214
2	B	901	POV	C35-C36-C37-C38
2	B	902	POV	C32-C33-C34-C35
2	D	901	POV	C211-C212-C213-C214
2	C	902	POV	C32-C33-C34-C35
2	A	902	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	902	POV	C1-O11-P-O12
2	B	902	POV	C1-O11-P-O12
2	C	902	POV	C1-O11-P-O12
2	D	902	POV	C1-O11-P-O12
2	D	902	POV	C32-C33-C34-C35
2	D	901	POV	C313-C314-C315-C316
2	D	901	POV	C311-C310-C39-C38
2	C	901	POV	C35-C36-C37-C38
2	A	901	POV	C311-C310-C39-C38
2	C	901	POV	C313-C314-C315-C316
2	B	901	POV	C311-C310-C39-C38
2	A	901	POV	C313-C314-C315-C316
2	B	901	POV	C313-C314-C315-C316
2	A	901	POV	C35-C36-C37-C38
2	D	901	POV	C37-C38-C39-C310
2	B	901	POV	C210-C211-C212-C213
2	B	901	POV	C33-C34-C35-C36
2	D	901	POV	C33-C34-C35-C36
2	D	901	POV	C35-C36-C37-C38
2	C	901	POV	C311-C310-C39-C38
2	B	902	POV	C11-C12-N-C15
2	A	901	POV	C210-C211-C212-C213
2	C	901	POV	C210-C211-C212-C213
2	B	901	POV	C29-C210-C211-C212
2	A	901	POV	C27-C28-C29-C210
2	B	901	POV	C27-C28-C29-C210
2	C	901	POV	C27-C28-C29-C210
2	D	901	POV	C29-C210-C211-C212
2	D	902	POV	C36-C37-C38-C39
2	A	902	POV	C11-C12-N-C13
2	A	902	POV	C11-C12-N-C15
2	B	902	POV	C11-C12-N-C13
2	B	901	POV	O21-C21-C22-C23
2	D	901	POV	O21-C21-C22-C23
2	A	901	POV	O21-C21-C22-C23
2	C	902	POV	C11-C12-N-C13
2	C	902	POV	C11-C12-N-C15
2	D	902	POV	C11-C12-N-C13
2	D	902	POV	C11-C12-N-C15
2	A	901	POV	C37-C38-C39-C310
2	A	901	POV	C29-C210-C211-C212
2	C	901	POV	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C29-C210-C211-C212
2	D	901	POV	C27-C28-C29-C210
2	A	902	POV	C36-C37-C38-C39
2	C	901	POV	C37-C38-C39-C310
2	A	902	POV	C11-O12-P-O13
2	C	902	POV	C11-O12-P-O13
2	D	901	POV	C312-C313-C314-C315
2	A	901	POV	O22-C21-C22-C23
2	B	902	POV	C11-C12-N-C14
2	B	901	POV	O22-C21-C22-C23
2	C	901	POV	O22-C21-C22-C23
2	D	901	POV	O22-C21-C22-C23
2	C	902	POV	C2-C1-O11-P

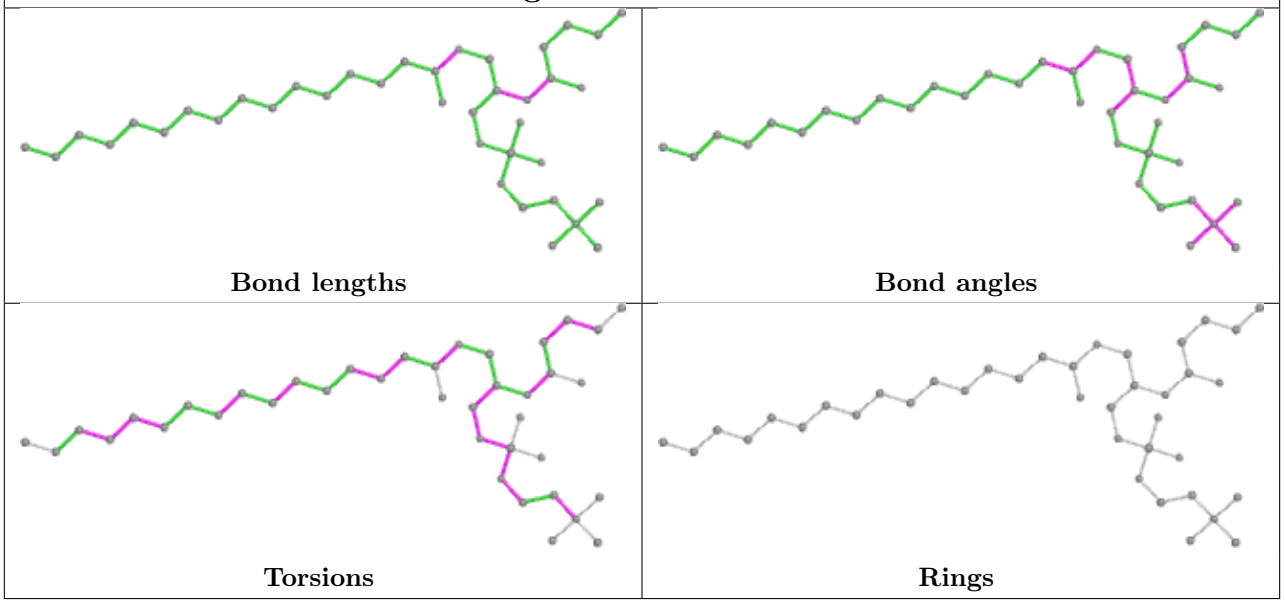
There are no ring outliers.

6 monomers are involved in 19 short contacts:

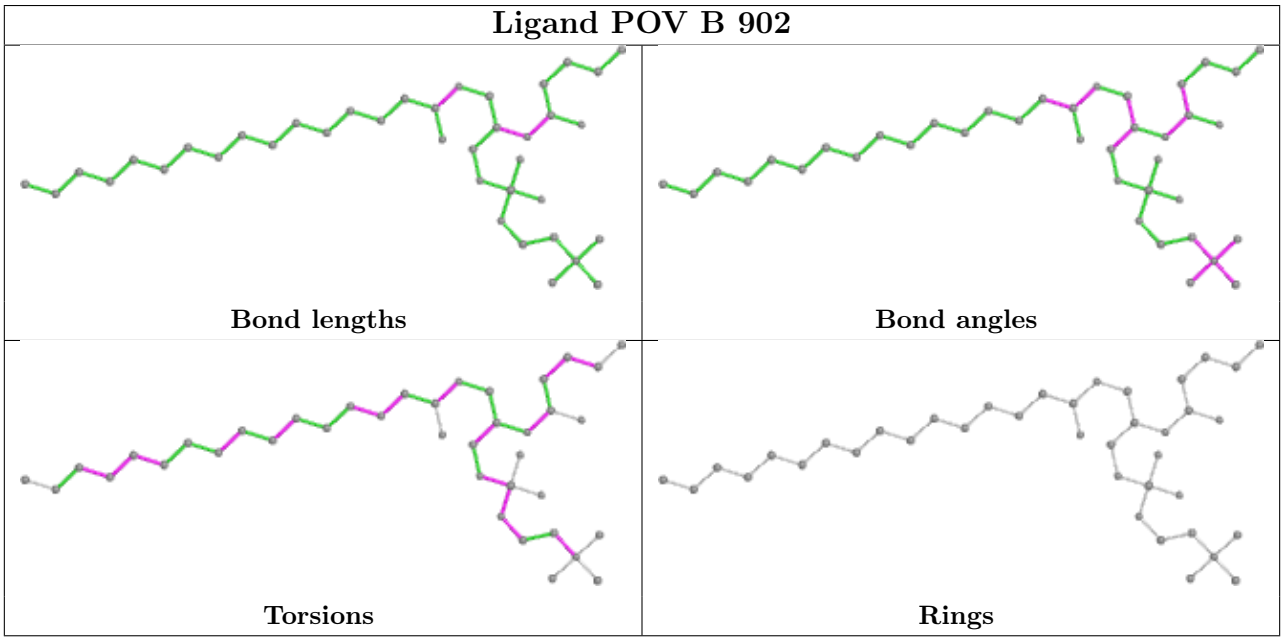
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	902	POV	1	0
2	D	901	POV	5	0
2	B	901	POV	3	0
2	A	901	POV	3	0
2	D	902	POV	3	0
2	C	901	POV	4	0

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 then 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.

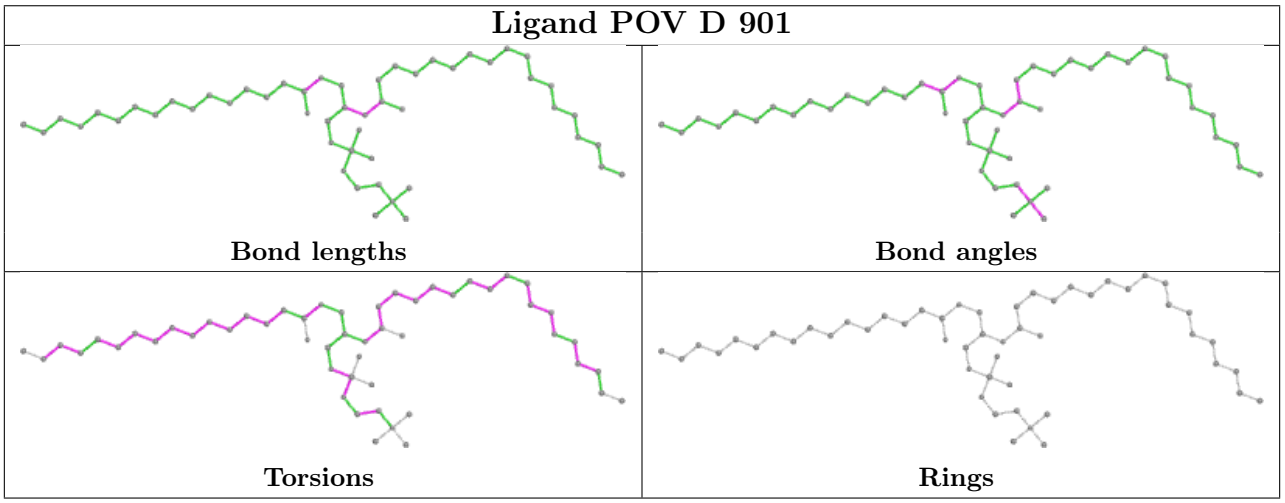
Ligand POV C 902



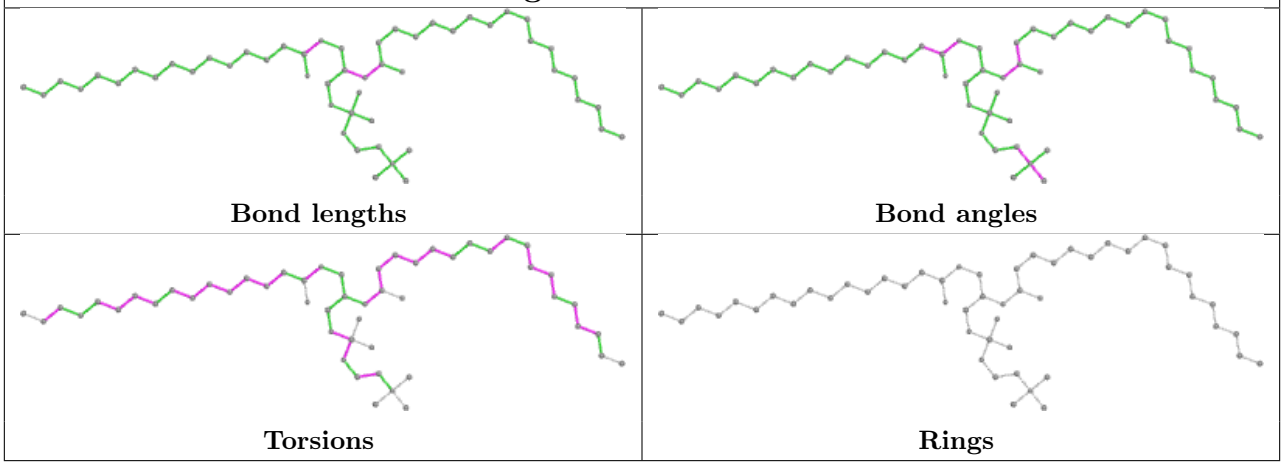
Ligand POV B 902



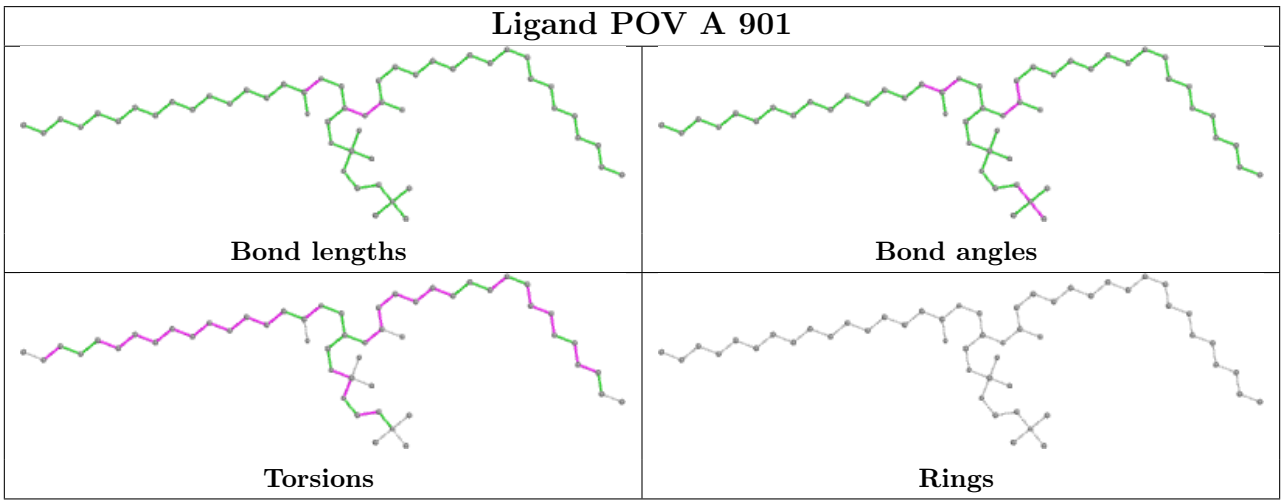
Ligand POV D 901



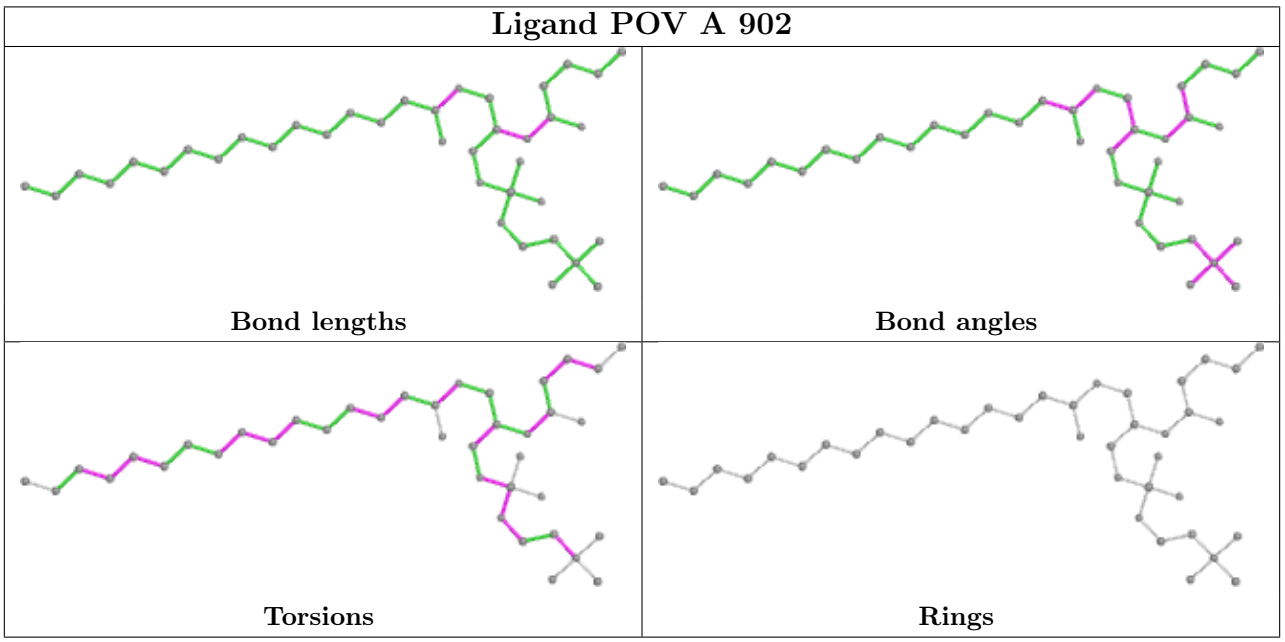
Ligand POV B 901

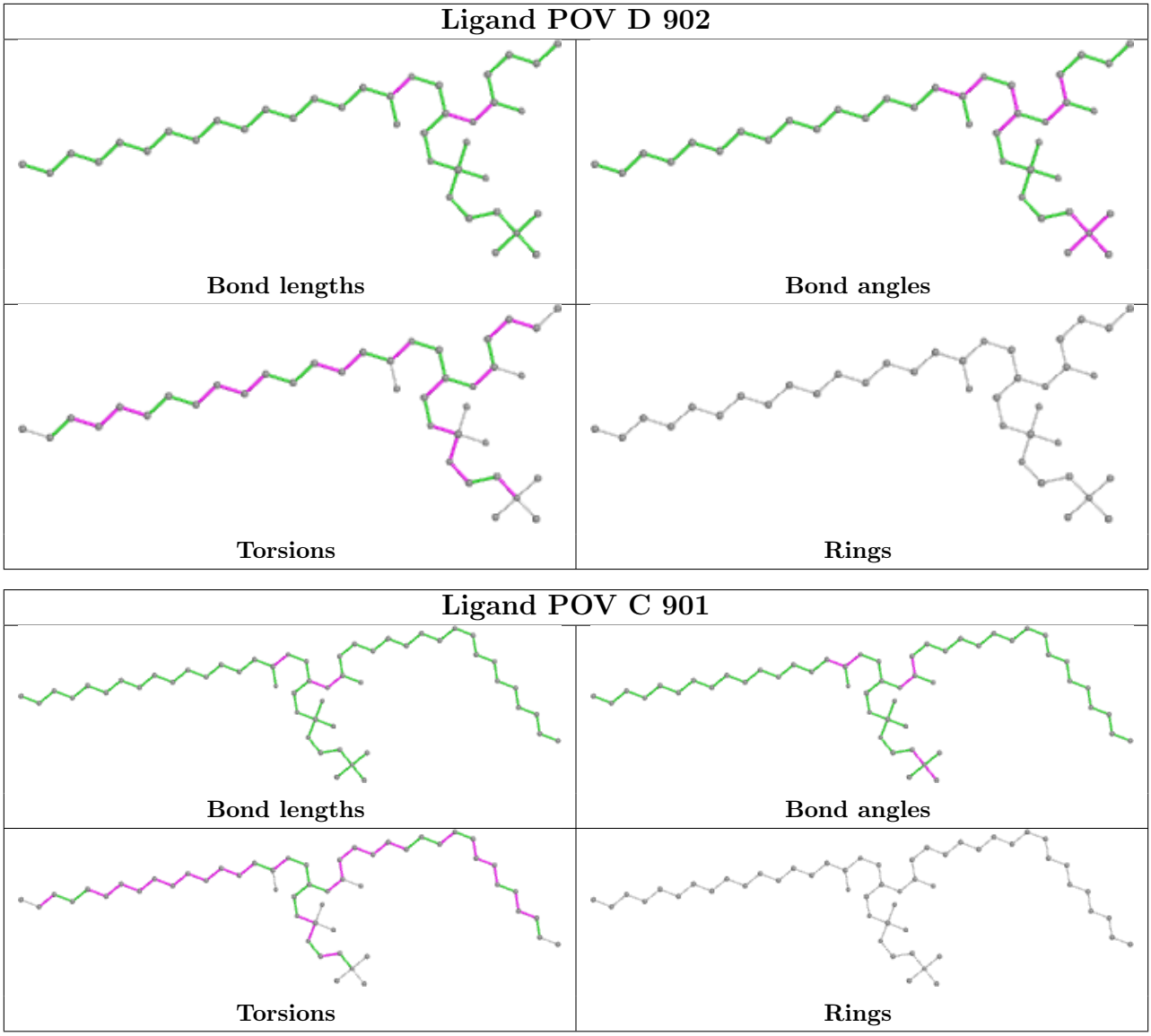


Ligand POV A 901



Ligand POV A 902





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.

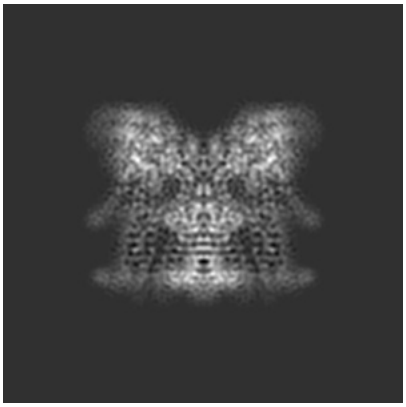
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23855. These allow visual inspection of the internal detail of the map and identification of artifacts.

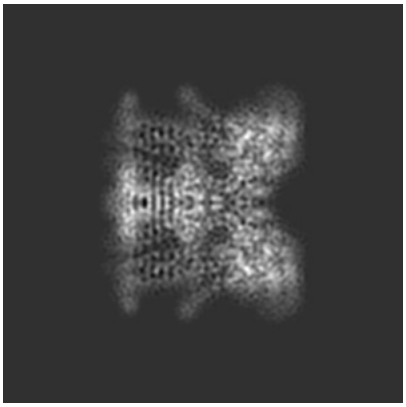
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

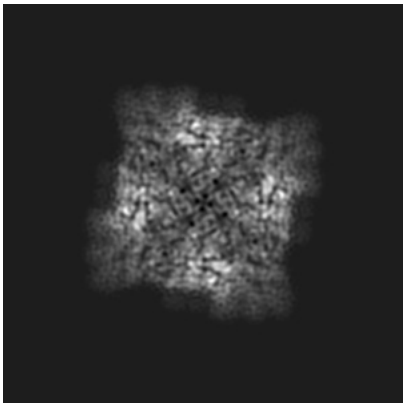
6.1.1 Primary map



X



Y



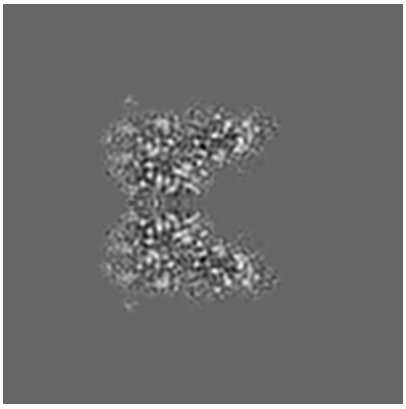
Z

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

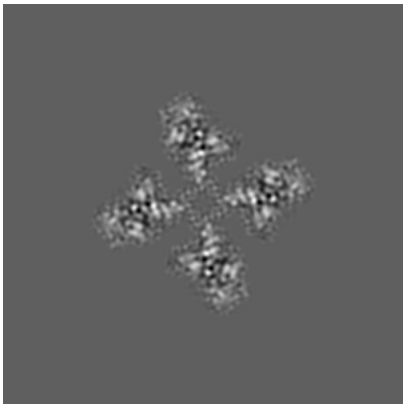
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128



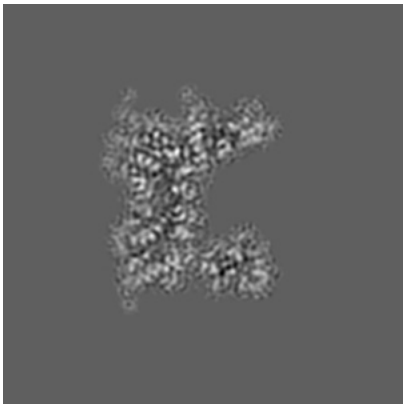
Z Index: 128

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

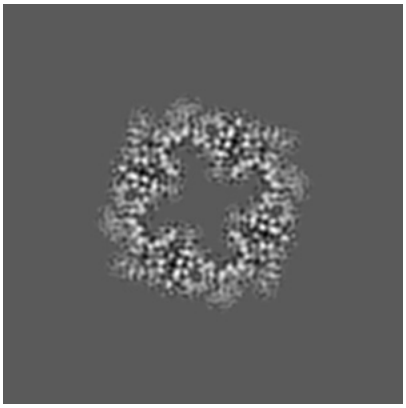
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134



Y Index: 134

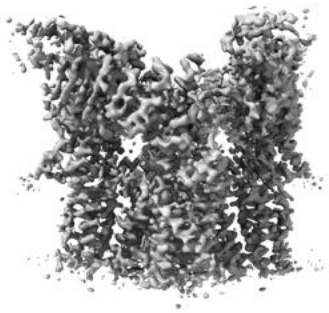


Z Index: 157

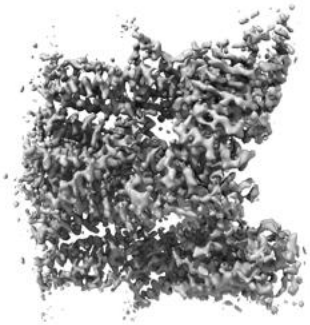
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

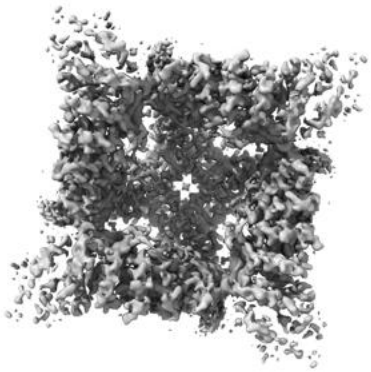
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0225. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

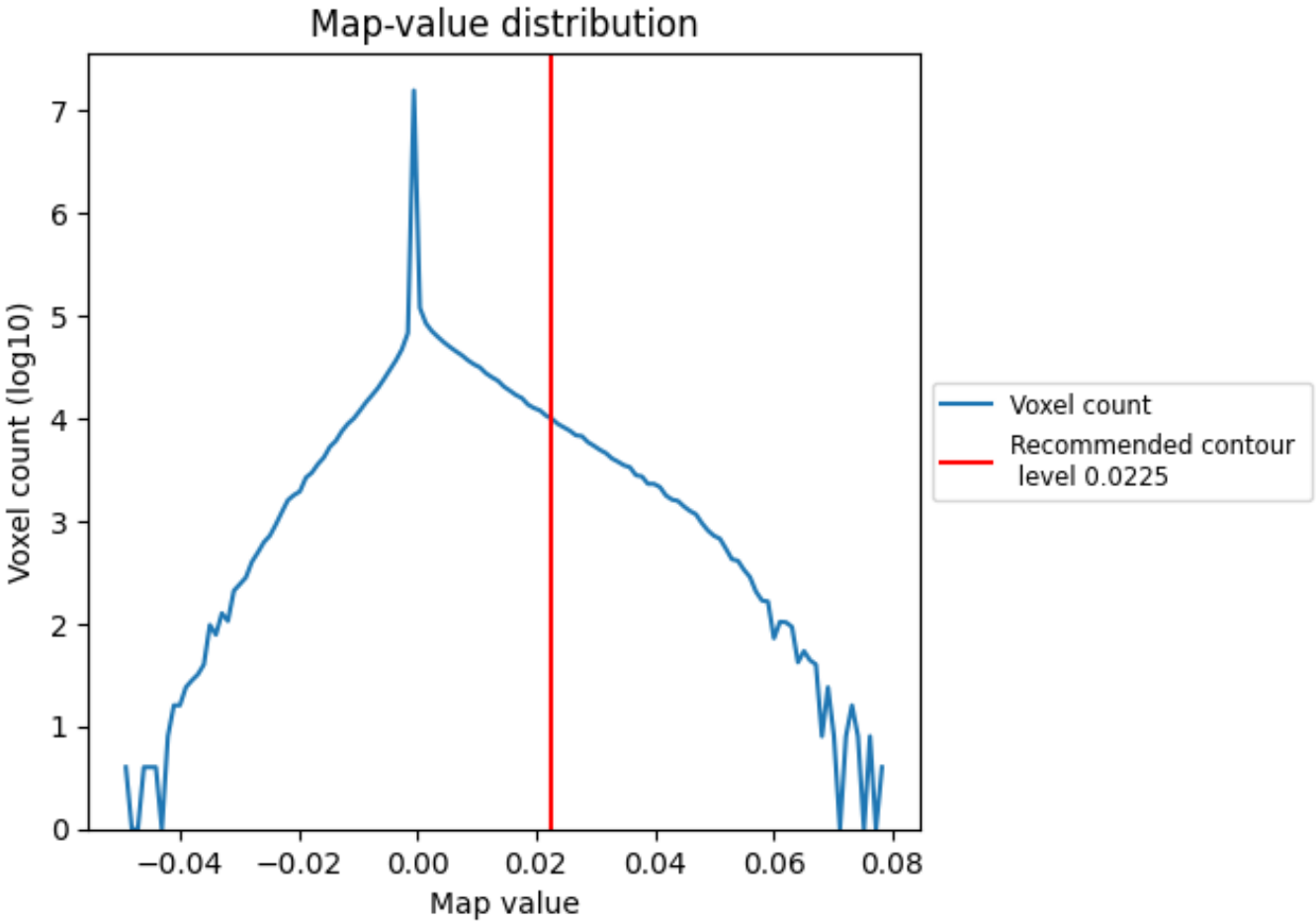
6.5 Mask visualisation (i)

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

7 Map analysis

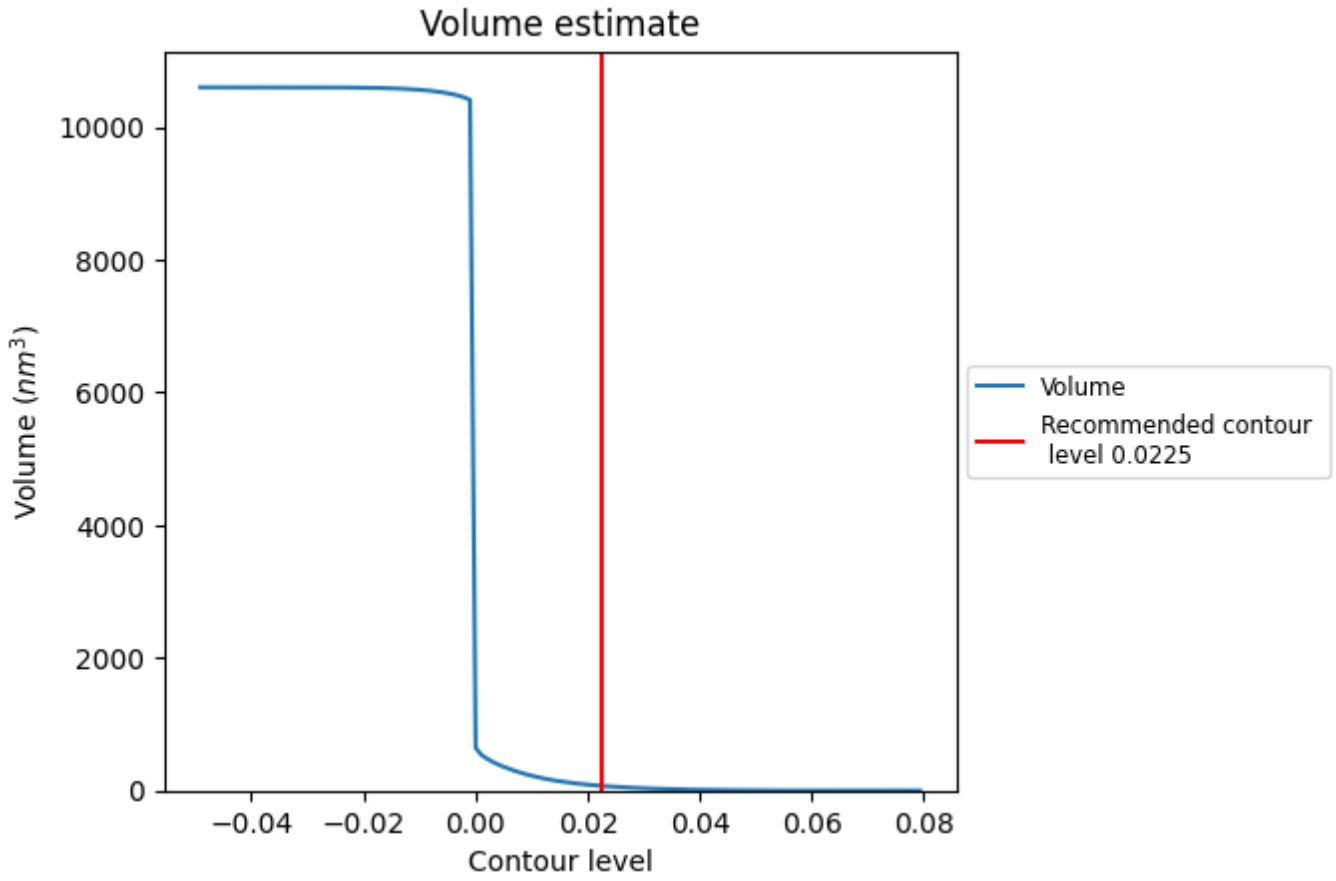
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

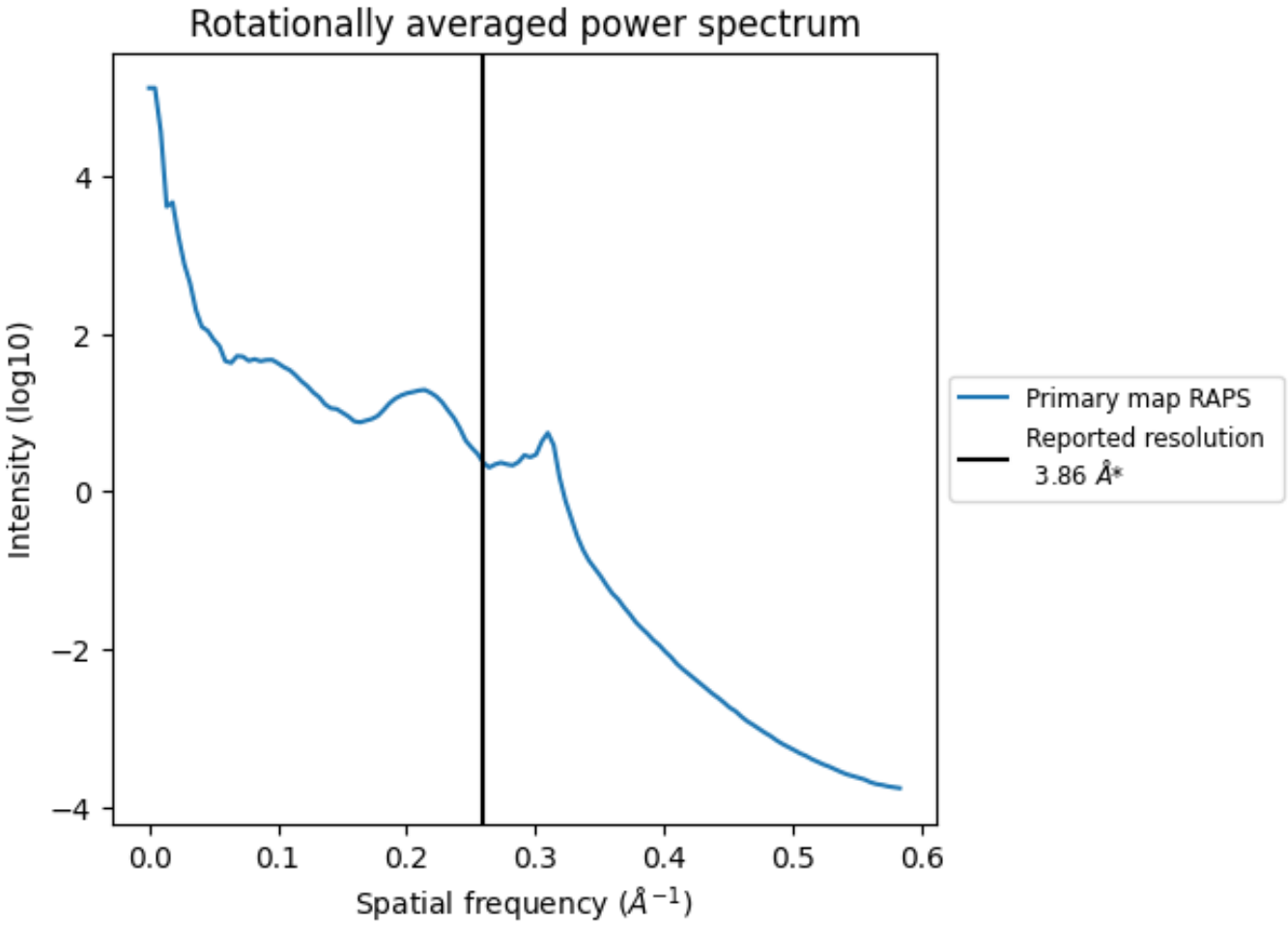
7.2 Volume estimate (i)



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 64 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)



*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

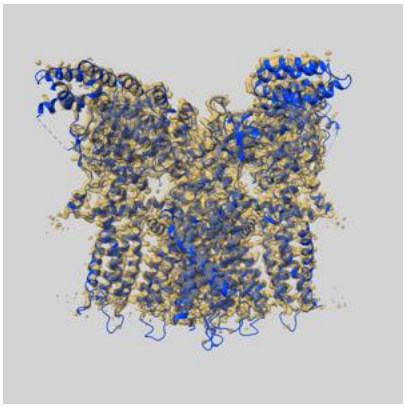
8 Fourier-Shell correlation

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

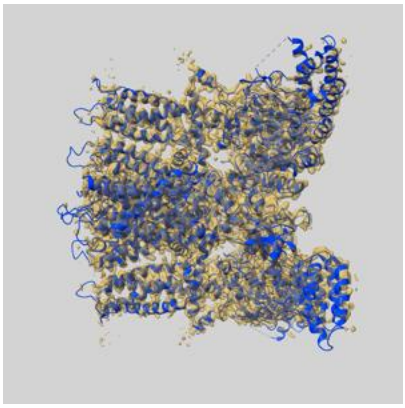
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23855 and PDB model 7MIL. Per-residue inclusion information can be found in section 3 on page 7.

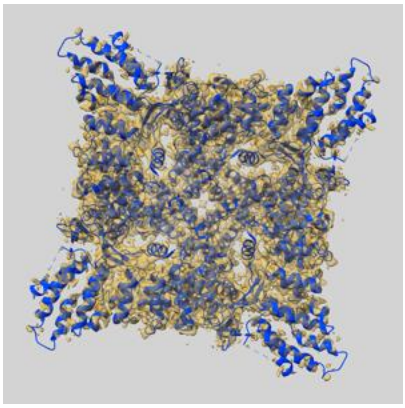
9.1 Map-model overlay



X



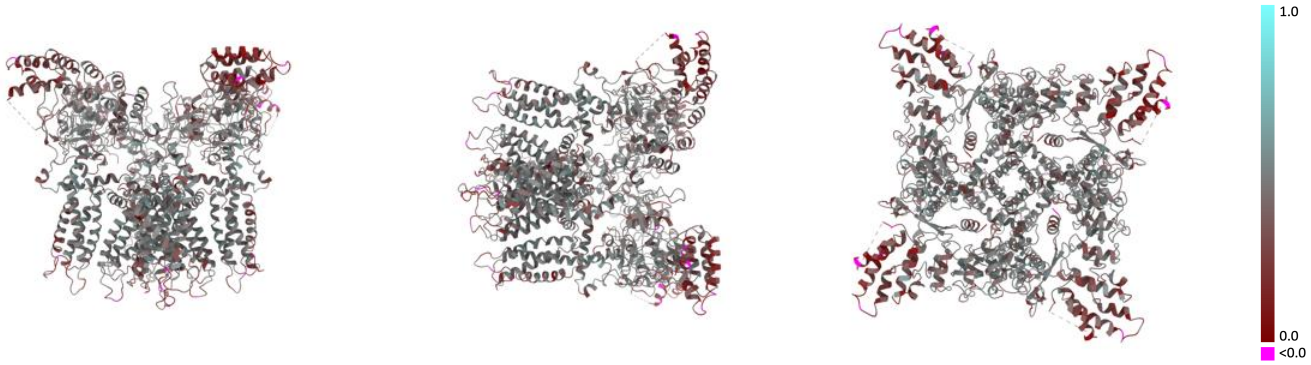
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0225 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.

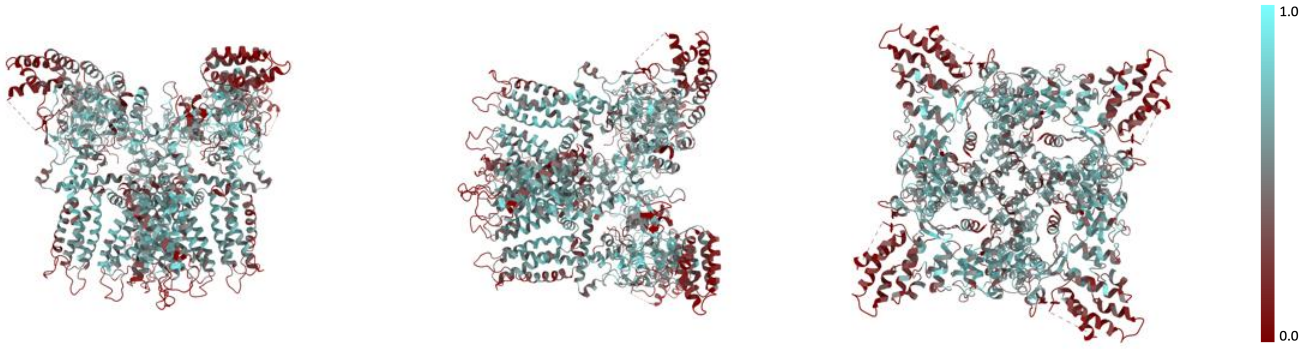
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

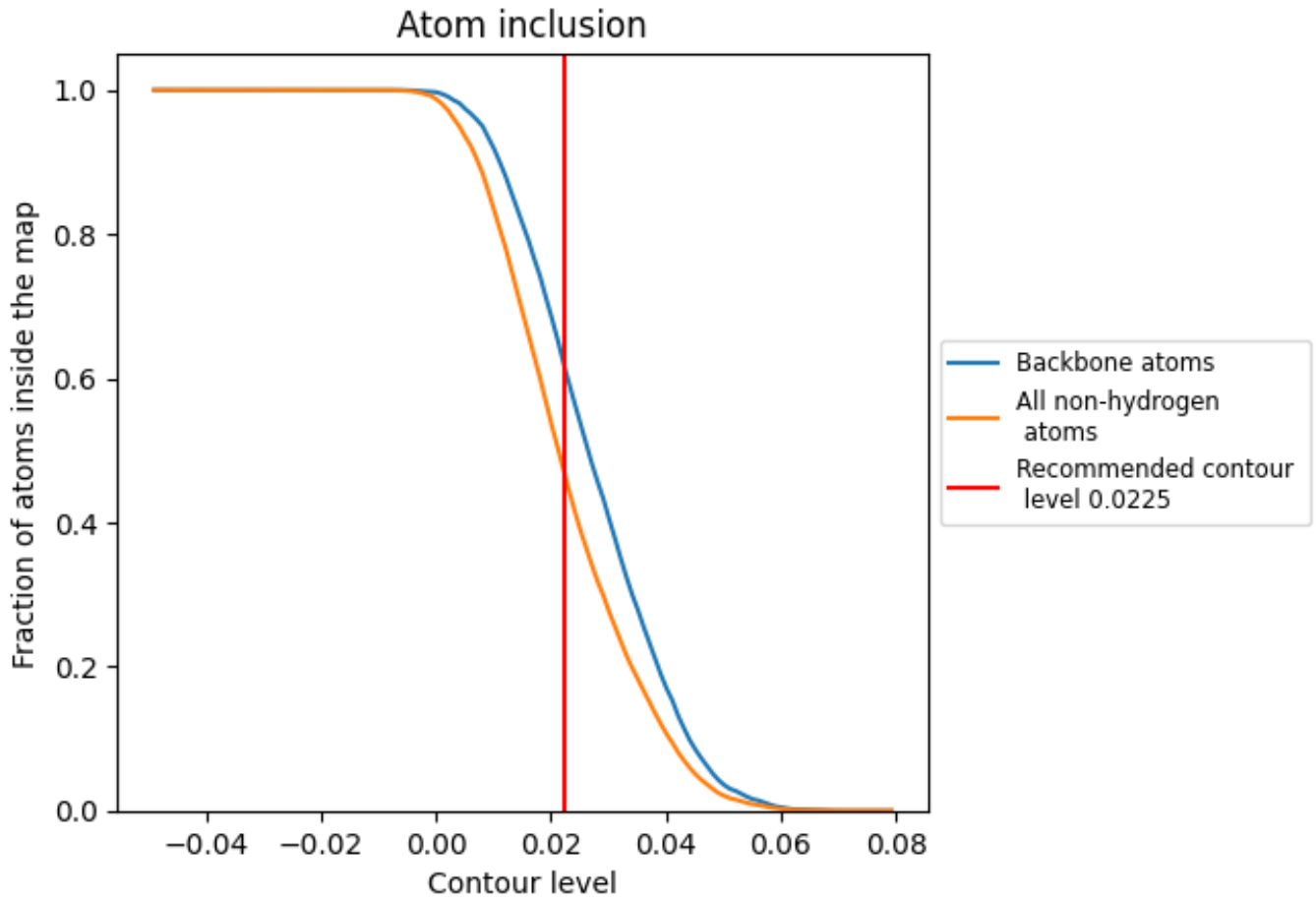
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0225).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 46% 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 (0.0225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4621	0.4080
A	0.4641	0.4120
B	0.4564	0.3990
C	0.4655	0.4150
D	0.4626	0.4060