Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 11:41 AM EST

PDB ID	:	6DMY
EMDB ID	:	EMD-7968
Title	:	Cryo-EM structure of human Ptch1 and ShhN complex
Authors	:	Yan, N.; Gong, X.; Qian, H.W.
Deposited on	:	2018-06-05
Resolution	:	3.60 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:

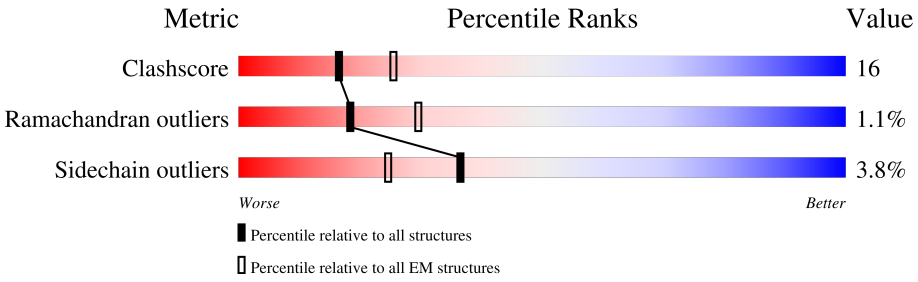
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.60 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	1349	16% 53% 18% • 26%
2	B	177	12% 74% 10% •• 15%
3	C	2	50% 100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9211 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 Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	992	7821	5100	1286	1393	42	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q13635
A	-19	ALA	-	expression tag	UNP Q13635
A	-18	ASP	-	expression tag	UNP Q13635
A	-17	TYR	-	expression tag	UNP Q13635
A	-16	LYS	-	expression tag	UNP Q13635
A	-15	ASP	-	expression tag	UNP Q13635
A	-14	ASP	-	expression tag	UNP Q13635
A	-13	ASP	-	expression tag	UNP Q13635
A	-12	ASP	-	expression tag	UNP Q13635
A	-11	LYS	-	expression tag	UNP Q13635
A	-10	SER	-	expression tag	UNP Q13635
A	-9	GLY	-	expression tag	UNP Q13635
A	-8	PRO	-	expression tag	UNP Q13635
A	-7	ASP	-	expression tag	UNP Q13635
A	-6	GLU	-	expression tag	UNP Q13635
A	-5	VAL	-	expression tag	UNP Q13635
A	-4	ASP	-	expression tag	UNP Q13635
A	-3	ALA	-	expression tag	UNP Q13635
A	-2	SER	-	expression tag	UNP Q13635
A	-1	GLY	-	expression tag	UNP Q13635
A	0	ARG	-	expression tag	UNP Q13635
A	1306	LEU	-	expression tag	UNP Q13635
A	1307	GLU	-	expression tag	UNP Q13635
A	1308	GLY	-	expression tag	UNP Q13635
A	1309	SER	-	expression tag	UNP Q13635
A	1310	ASP	-	expression tag	UNP Q13635
A	1311	GLU	-	expression tag	UNP Q13635
A	1312	VAL	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1313	ASP	-	expression tag	UNP Q13635
A	1314	ALA	-	expression tag	UNP Q13635
A	1315	VAL	-	expression tag	UNP Q13635
A	1316	GLU	-	expression tag	UNP Q13635
A	1317	GLY	-	expression tag	UNP Q13635
A	1318	SER	-	expression tag	UNP Q13635
A	1319	HIS	-	expression tag	UNP Q13635
A	1320	HIS	-	expression tag	UNP Q13635
A	1321	HIS	-	expression tag	UNP Q13635
A	1322	HIS	-	expression tag	UNP Q13635
A	1323	HIS	-	expression tag	UNP Q13635
A	1324	HIS	-	expression tag	UNP Q13635
A	1325	HIS	-	expression tag	UNP Q13635
A	1326	HIS	-	expression tag	UNP Q13635
A	1327	HIS	-	expression tag	UNP Q13635
A	1328	HIS	-	expression tag	UNP Q13635

- Molecule 2 is a protein called Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	151	Total	C	N	O	S	0	0
			1213	757	216	235	5		

There are 3 discrepancies between the modelled and reference sequences:

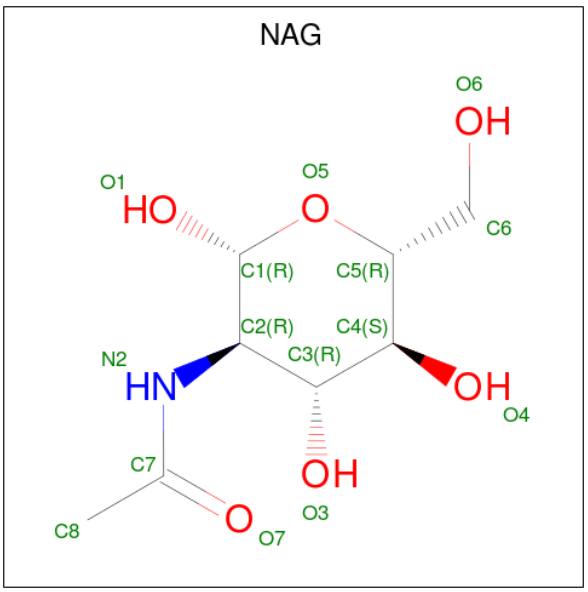
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ALA	-	expression tag	UNP Q15465
B	22	HIS	-	expression tag	UNP Q15465
B	23	MET	-	expression tag	UNP Q15465

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

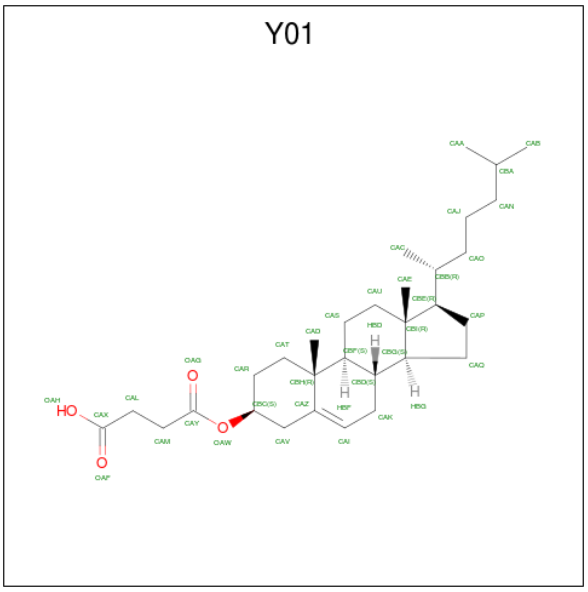
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



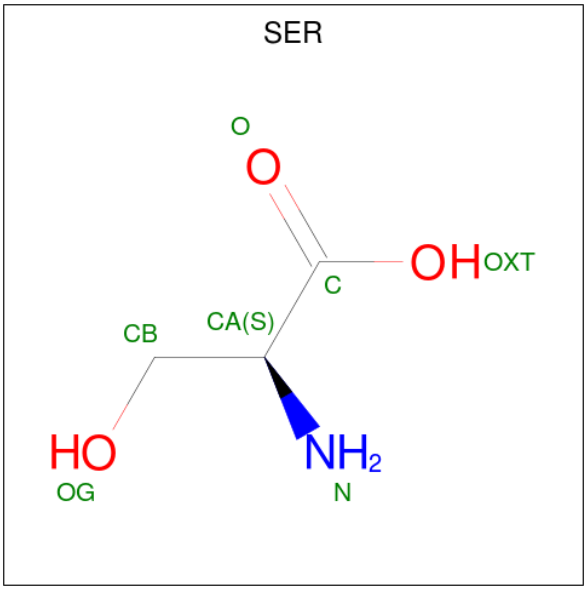
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 70 62 8	0
5	A	1	Total C O 70 62 8	0

- Molecule 6 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C N O 6 3 1 2	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Zn	0
			1	1	

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

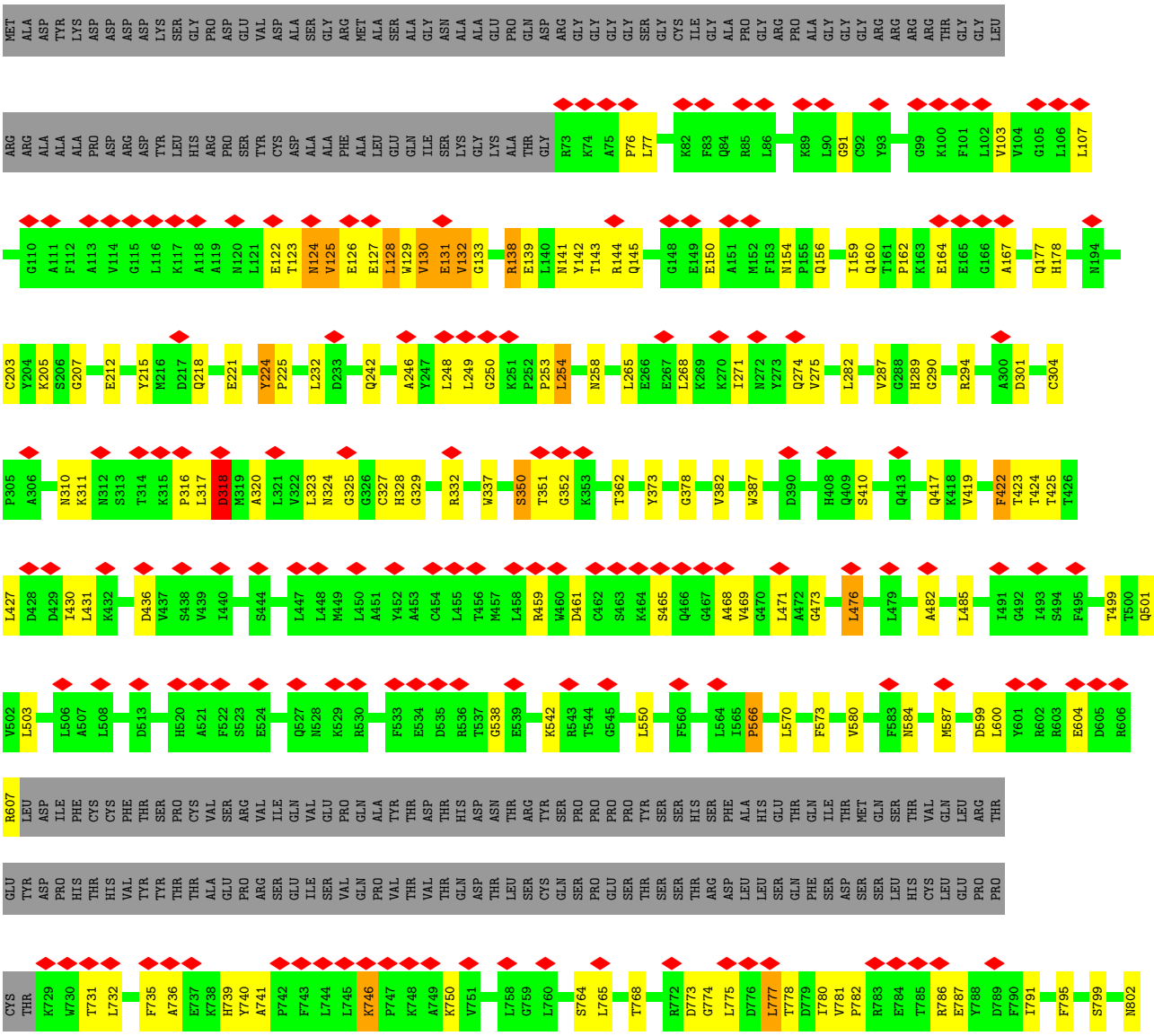
Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total	Ca	0
			2	2	

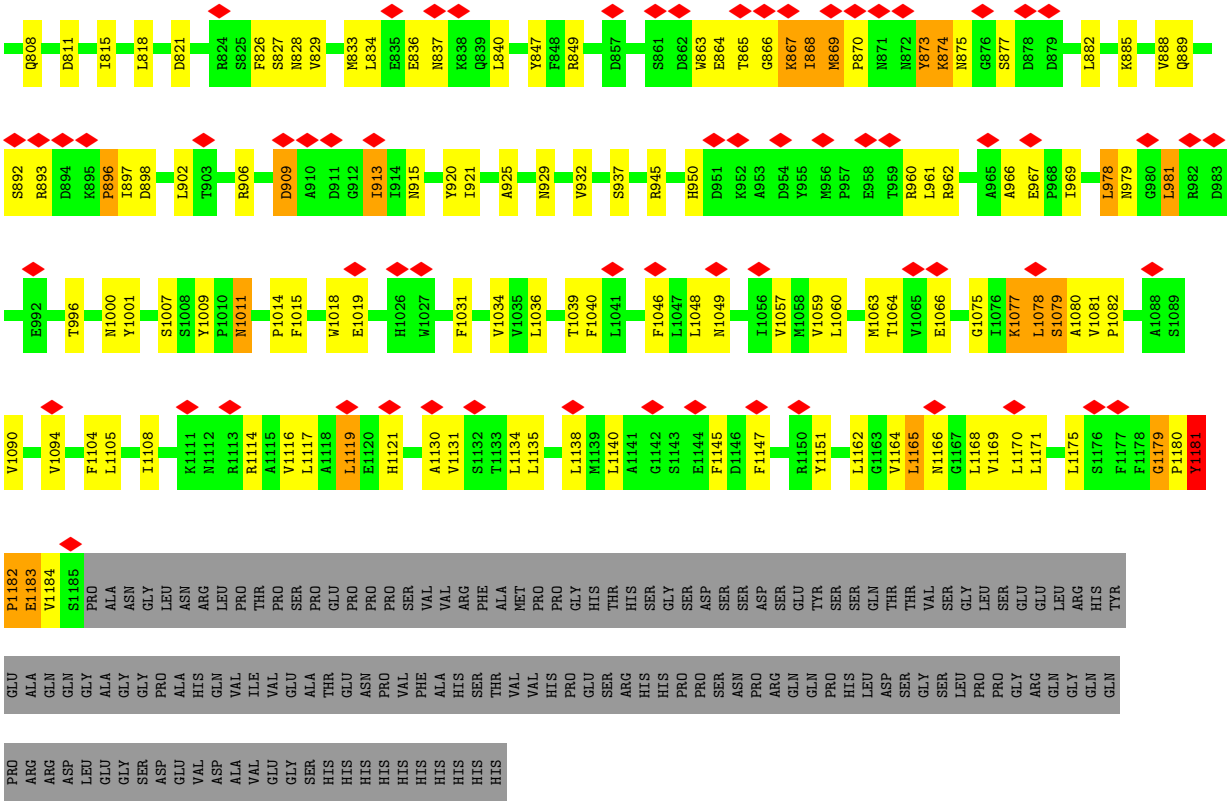
3 Residue-property plots (i)

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: Protein patched homolog 1

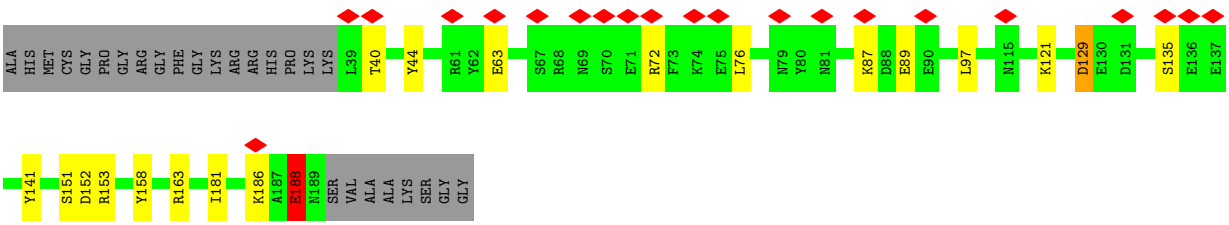
Chain A:





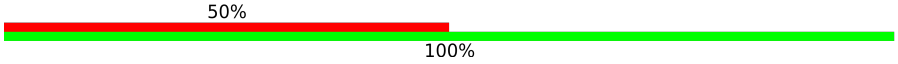
• Molecule 2: Sonic hedgehog protein

Chain B:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	244.38399, 244.38399, 244.38399	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, Y01, CA

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	0.44	1/8014 (0.0%)	0.76	13/10901 (0.1%)
2	B	0.38	0/1239	0.57	0/1672
All	All	0.44	1/9253 (0.0%)	0.73	13/12573 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	915	ASN	C-N	-6.20	1.22	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	LEU	CA-CB-CG	9.73	137.68	115.30
1	A	896	PRO	CA-N-CD	-8.58	99.49	111.50
1	A	323	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	1181	TYR	C-N-CD	-6.09	107.20	120.60
1	A	1179	GLY	N-CA-C	5.52	126.90	113.10
1	A	1119	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	232	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	978	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	909	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	1140	LEU	CA-CB-CG	5.20	127.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	898	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	164	GLU	C-N-CA	5.08	134.39	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	TYR	Peptide
1	A	258	ASN	Peptide
1	A	289	HIS	Peptide
1	A	316	PRO	Peptide
1	A	318	ASP	Peptide
1	A	320	ALA	Peptide
1	A	350	SER	Peptide
1	A	746	LYS	Peptide
1	A	833	MET	Peptide
1	A	913	ILE	Peptide

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	7821	0	7850	279	0
2	B	1213	0	1170	14	0
3	C	28	0	25	0	0
4	A	70	0	65	0	0
5	A	70	0	98	2	0
6	B	6	0	4	1	0
7	B	1	0	0	0	0
8	B	2	0	0	0	0
All	All	9211	0	9212	290	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 16.

All (290) 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:775:LEU:HB2	1:A:1079:SER:CB	1.33	1.56
1:A:1114:ARG:CZ	1:A:1182:PRO:HG3	1.34	1.52
1:A:1104:PHE:CD2	1:A:1180:PRO:HG3	1.52	1.42
1:A:1114:ARG:NH1	1:A:1182:PRO:HG3	1.31	1.40
1:A:77:LEU:HD21	1:A:1183:GLU:CG	1.53	1.38
1:A:77:LEU:CD2	1:A:1183:GLU:HG3	1.54	1.38
1:A:906:ARG:CB	1:A:909:ASP:OD2	1.72	1.35
1:A:906:ARG:HB2	1:A:909:ASP:CG	1.48	1.31
1:A:869:MET:HB3	1:A:870:PRO:CD	1.63	1.29
1:A:775:LEU:CD2	1:A:1079:SER:HB2	1.67	1.24
1:A:1104:PHE:CE2	1:A:1180:PRO:CG	2.22	1.23
1:A:775:LEU:CB	1:A:1079:SER:HB3	1.70	1.20
1:A:1108:ILE:HD13	1:A:1184:VAL:CB	1.74	1.17
1:A:122:GLU:O	1:A:124:ASN:ND2	1.80	1.15
1:A:1104:PHE:CE2	1:A:1180:PRO:HG3	1.84	1.12
1:A:896:PRO:HD2	1:A:897:ILE:H	1.11	1.11
1:A:1114:ARG:NH1	1:A:1182:PRO:CG	2.13	1.11
1:A:775:LEU:CB	1:A:1079:SER:CB	2.24	1.10
1:A:1114:ARG:CZ	1:A:1182:PRO:CG	2.29	1.10
1:A:1114:ARG:NH2	1:A:1182:PRO:HG3	1.65	1.10
1:A:775:LEU:HD22	1:A:1079:SER:HB2	1.16	1.09
1:A:866:GLY:O	1:A:868:ILE:CD1	2.01	1.09
1:A:1108:ILE:CD1	1:A:1184:VAL:CB	2.29	1.08
1:A:869:MET:CB	1:A:870:PRO:CD	2.27	1.08
1:A:1114:ARG:HH22	1:A:1182:PRO:CD	1.66	1.08
1:A:866:GLY:O	1:A:868:ILE:HD11	1.54	1.07
1:A:869:MET:CB	1:A:870:PRO:HD3	1.83	1.05
1:A:1104:PHE:HE2	1:A:1180:PRO:CG	1.64	1.05
1:A:1104:PHE:CD2	1:A:1180:PRO:CG	2.39	1.04
1:A:777:LEU:HD23	1:A:795:PHE:CE2	1.91	1.03
1:A:1114:ARG:NH2	1:A:1182:PRO:HD3	1.73	1.03
1:A:1114:ARG:NH2	1:A:1182:PRO:CD	2.21	1.02
1:A:775:LEU:HB2	1:A:1079:SER:HB2	1.41	1.01
1:A:906:ARG:HB2	1:A:909:ASP:OD2	0.85	1.01
1:A:866:GLY:C	1:A:868:ILE:CD1	2.28	1.00
1:A:906:ARG:CB	1:A:909:ASP:CG	2.25	1.00
1:A:1114:ARG:NH2	1:A:1182:PRO:CG	2.24	0.99
1:A:866:GLY:C	1:A:868:ILE:HD13	1.82	0.99
1:A:732:LEU:O	1:A:736:ALA:HB2	1.63	0.98
1:A:1078:LEU:HD22	1:A:1078:LEU:H	1.24	0.98
1:A:129:TRP:CZ2	1:A:775:LEU:HD21	1.99	0.98
1:A:430:ILE:HD12	1:A:781:VAL:HG22	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:O	1:A:1145:PHE:CD1	2.20	0.95
1:A:869:MET:HB3	1:A:870:PRO:HD3	0.94	0.92
1:A:129:TRP:HZ2	1:A:775:LEU:CD2	1.82	0.92
1:A:780:ILE:O	1:A:1145:PHE:HD1	1.51	0.91
1:A:1104:PHE:CE2	1:A:1180:PRO:HG2	2.06	0.91
1:A:1114:ARG:HH12	1:A:1182:PRO:HG3	1.35	0.89
1:A:130:VAL:O	1:A:131:GLU:HB3	1.72	0.88
1:A:896:PRO:HD2	1:A:897:ILE:N	1.89	0.87
1:A:906:ARG:CB	1:A:909:ASP:OD1	2.22	0.86
1:A:1104:PHE:HD2	1:A:1180:PRO:HG3	1.04	0.86
1:A:570:LEU:HD13	1:A:1080:ALA:O	1.74	0.85
1:A:775:LEU:CB	1:A:1079:SER:HB2	2.00	0.84
1:A:775:LEU:HD22	1:A:1079:SER:CB	2.06	0.83
1:A:777:LEU:HD23	1:A:795:PHE:CZ	2.13	0.83
1:A:866:GLY:O	1:A:868:ILE:HD13	1.76	0.82
1:A:1114:ARG:HH12	1:A:1182:PRO:CG	1.86	0.82
1:A:138:ARG:HG2	1:A:139:GLU:N	1.93	0.82
1:A:129:TRP:HZ2	1:A:775:LEU:HD21	1.35	0.82
1:A:775:LEU:HB2	1:A:1079:SER:HB3	0.82	0.82
1:A:873:TYR:HD1	1:A:873:TYR:H	1.26	0.81
1:A:1162:LEU:O	1:A:1166:ASN:HB2	1.81	0.81
1:A:125:VAL:HG12	1:A:431:LEU:CD2	2.12	0.80
1:A:141:ASN:O	1:A:145:GLN:HB2	1.82	0.80
1:A:775:LEU:CG	1:A:1079:SER:HB2	2.11	0.79
1:A:1104:PHE:HE2	1:A:1180:PRO:CD	1.95	0.78
1:A:906:ARG:HB3	1:A:909:ASP:OD1	1.82	0.78
1:A:906:ARG:CA	1:A:909:ASP:OD2	2.32	0.78
1:A:773:ASP:OD1	1:A:1078:LEU:HD23	1.84	0.78
1:A:570:LEU:CD1	1:A:1080:ALA:O	2.31	0.77
1:A:874:LYS:HG3	1:A:875:ASN:N	1.98	0.77
1:A:1077:LYS:O	1:A:1082:PRO:HG2	1.84	0.77
1:A:1114:ARG:HH22	1:A:1182:PRO:HD3	1.40	0.77
1:A:138:ARG:HH21	1:A:138:ARG:HB3	1.49	0.77
1:A:906:ARG:HB2	1:A:909:ASP:OD1	1.82	0.76
1:A:1165:LEU:O	1:A:1169:VAL:HB	1.85	0.76
1:A:1075:GLY:O	1:A:1077:LYS:HD3	1.85	0.76
1:A:777:LEU:HD23	1:A:795:PHE:HE2	1.49	0.76
1:A:777:LEU:HD12	1:A:777:LEU:O	1.85	0.76
1:A:317:LEU:O	1:A:318:ASP:OD1	2.05	0.75
1:A:896:PRO:CD	1:A:897:ILE:H	1.95	0.74
1:A:808:GLN:HB3	1:A:1007:SER:OG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:GLU:OE1	1:A:864:GLU:N	2.14	0.72
1:A:1078:LEU:HD13	1:A:1078:LEU:N	2.05	0.72
1:A:1134:LEU:O	1:A:1138:LEU:HB2	1.90	0.72
1:A:1104:PHE:CE2	1:A:1180:PRO:CD	2.70	0.72
1:A:869:MET:CB	1:A:870:PRO:HD2	2.21	0.71
1:A:1104:PHE:HE2	1:A:1180:PRO:HG2	1.43	0.71
1:A:1108:ILE:HD12	1:A:1184:VAL:CB	2.21	0.70
1:A:469:VAL:HG21	1:A:599:ASP:HB2	1.71	0.70
2:B:129:ASP:OD2	2:B:141:TYR:HE1	1.74	0.70
1:A:867:LYS:C	1:A:868:ILE:HD13	2.12	0.70
1:A:868:ILE:HD13	1:A:868:ILE:N	2.07	0.70
1:A:889:GLN:HG2	1:A:921:ILE:HG21	1.75	0.68
1:A:143:THR:HG21	1:A:1011:ASN:OD1	1.93	0.68
1:A:125:VAL:HG11	1:A:427:LEU:HD21	1.77	0.67
1:A:896:PRO:CD	1:A:897:ILE:N	2.57	0.66
1:A:248:LEU:HD23	1:A:250:GLY:H	1.60	0.66
1:A:775:LEU:HD22	1:A:1079:SER:O	1.96	0.66
1:A:1059:VAL:O	1:A:1063:MET:HB2	1.96	0.66
1:A:775:LEU:CD2	1:A:1079:SER:O	2.44	0.65
1:A:327:CYS:O	1:A:337:TRP:HB2	1.97	0.64
1:A:419:VAL:O	1:A:786:ARG:NH2	2.30	0.64
1:A:1064:THR:HG21	1:A:1090:VAL:HG22	1.80	0.63
1:A:131:GLU:O	1:A:131:GLU:HG2	1.99	0.62
1:A:580:VAL:O	1:A:584:ASN:HB2	1.99	0.62
1:A:746:LYS:HB3	1:A:750:LYS:HE3	1.81	0.62
1:A:129:TRP:HZ2	1:A:775:LEU:HD23	1.63	0.62
1:A:129:TRP:CZ2	1:A:775:LEU:CD2	2.67	0.62
1:A:1166:ASN:O	1:A:1170:LEU:HB3	1.98	0.62
1:A:1078:LEU:HD22	1:A:1078:LEU:N	2.05	0.60
1:A:1171:LEU:O	1:A:1175:LEU:HB2	2.01	0.60
1:A:1031:PHE:HA	1:A:1034:VAL:HG12	1.82	0.60
1:A:864:GLU:H	1:A:864:GLU:CD	2.04	0.60
1:A:869:MET:HB2	1:A:870:PRO:CD	2.30	0.60
1:A:103:VAL:O	1:A:107:LEU:HB2	2.02	0.60
1:A:731:THR:O	1:A:735:PHE:CB	2.50	0.59
1:A:1131:VAL:O	1:A:1135:LEU:HB2	2.02	0.59
1:A:301:ASP:HB3	1:A:304:CYS:HB2	1.85	0.59
1:A:1104:PHE:HE2	1:A:1180:PRO:HD2	1.67	0.59
1:A:1114:ARG:HH22	1:A:1182:PRO:CG	1.99	0.59
1:A:780:ILE:O	1:A:1145:PHE:CE1	2.57	0.58
2:B:129:ASP:OD2	2:B:141:TYR:CE1	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:HA	1:A:130:VAL:HG22	1.84	0.58
1:A:869:MET:HB2	1:A:870:PRO:HD2	1.86	0.58
1:A:124:ASN:O	1:A:128:LEU:HB2	2.04	0.58
1:A:867:LYS:N	1:A:868:ILE:HD13	2.18	0.58
2:B:188:GLU:OE2	2:B:188:GLU:HA	2.03	0.58
1:A:430:ILE:CD1	1:A:781:VAL:HG22	2.28	0.57
1:A:811:ASP:H	1:A:815:ILE:HD12	1.69	0.57
1:A:430:ILE:HD12	1:A:781:VAL:CG2	2.28	0.57
1:A:125:VAL:HG12	1:A:431:LEU:HD21	1.86	0.57
1:A:154:ASN:O	1:A:156:GLN:NE2	2.37	0.57
1:A:205:LYS:HD2	1:A:224:TYR:HD2	1.69	0.56
1:A:849:ARG:HD3	1:A:913:ILE:HG23	1.87	0.56
1:A:1114:ARG:HH12	1:A:1182:PRO:HG2	1.66	0.56
1:A:156:GLN:HG3	1:A:423:THR:HB	1.88	0.56
1:A:221:GLU:OE2	2:B:44:TYR:OH	2.23	0.56
1:A:1147:PHE:O	1:A:1151:TYR:HB2	2.06	0.56
1:A:847:TYR:HD2	1:A:937:SER:HB2	1.71	0.56
1:A:732:LEU:O	1:A:736:ALA:CB	2.47	0.55
1:A:124:ASN:O	1:A:127:GLU:O	2.24	0.55
1:A:815:ILE:HG23	1:A:818:LEU:HD12	1.88	0.55
1:A:144:ARG:NH1	1:A:150:GLU:OE1	2.40	0.55
1:A:290:GLY:O	1:A:294:ARG:NH1	2.39	0.55
1:A:162:PRO:HB3	1:A:167:ALA:HB3	1.89	0.55
1:A:821:ASP:OD2	1:A:1001:TYR:OH	2.21	0.55
1:A:1162:LEU:O	1:A:1166:ASN:CB	2.54	0.55
1:A:130:VAL:O	1:A:131:GLU:CB	2.44	0.55
1:A:160:GLN:HE21	1:A:417:GLN:HB3	1.71	0.54
1:A:873:TYR:HD1	1:A:873:TYR:N	2.02	0.54
1:A:906:ARG:N	1:A:909:ASP:OD2	2.40	0.54
1:A:422:PHE:HE2	1:A:427:LEU:HB2	1.72	0.54
1:A:215:TYR:O	1:A:218:GLN:HB2	2.07	0.54
1:A:76:PRO:HG3	1:A:1048:LEU:HD22	1.90	0.53
2:B:76:LEU:HB3	2:B:97:LEU:HB3	1.90	0.53
1:A:287:VAL:O	1:A:332:ARG:NH2	2.41	0.53
1:A:138:ARG:HH21	1:A:138:ARG:CB	2.19	0.53
1:A:736:ALA:HA	1:A:739:HIS:HB2	1.91	0.53
1:A:131:GLU:HG3	1:A:566:PRO:HB2	1.91	0.53
1:A:225:PRO:O	1:A:242:GLN:NE2	2.35	0.53
1:A:459:ARG:HB2	1:A:465:SER:HA	1.91	0.52
1:A:143:THR:HG21	1:A:1011:ASN:CG	2.29	0.52
1:A:207:GLY:O	1:A:224:TYR:OH	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:NH2	1:A:329:GLY:O	2.43	0.52
1:A:538:GLY:O	1:A:542:LYS:HB2	2.08	0.52
1:A:1049:ASN:HD22	1:A:1105:LEU:HD21	1.75	0.52
1:A:138:ARG:HB3	1:A:138:ARG:NH2	2.23	0.52
1:A:1130:ALA:HB2	1:A:1164:VAL:HG21	1.92	0.52
1:A:468:ALA:O	1:A:471:LEU:HB2	2.10	0.51
1:A:868:ILE:CG2	1:A:902:LEU:HD12	2.40	0.51
1:A:469:VAL:HG21	1:A:599:ASP:CB	2.41	0.51
1:A:138:ARG:CB	1:A:138:ARG:NH2	2.74	0.51
1:A:125:VAL:CG1	1:A:431:LEU:CD2	2.84	0.51
1:A:274:GLN:HE21	1:A:274:GLN:C	2.13	0.51
1:A:781:VAL:HG11	1:A:787:GLU:HG2	1.92	0.51
1:A:925:ALA:O	1:A:929:ASN:HB2	2.11	0.50
1:A:246:ALA:HB3	1:A:254:LEU:HB3	1.92	0.50
1:A:1181:TYR:N	1:A:1182:PRO:CD	2.71	0.50
1:A:929:ASN:HD21	1:A:950:HIS:H	1.60	0.50
1:A:430:ILE:HD11	1:A:787:GLU:HG3	1.94	0.50
1:A:1015:PHE:O	1:A:1019:GLU:HB2	2.11	0.50
1:A:778:THR:HB	1:A:791:ILE:HG22	1.94	0.49
1:A:885:LYS:HE3	1:A:961:LEU:HD12	1.95	0.49
1:A:774:GLY:HA3	1:A:1077:LYS:HZ3	1.77	0.49
1:A:897:ILE:HG21	1:A:961:LEU:HD23	1.93	0.49
1:A:1078:LEU:H	1:A:1078:LEU:CD2	1.98	0.49
2:B:158:TYR:HB3	2:B:181:ILE:HD11	1.95	0.49
1:A:773:ASP:OD1	1:A:1078:LEU:CD2	2.59	0.49
1:A:430:ILE:HG23	1:A:781:VAL:HG22	1.94	0.49
1:A:1131:VAL:O	1:A:1135:LEU:CB	2.61	0.49
1:A:127:GLU:O	1:A:128:LEU:HD13	2.13	0.48
1:A:91:GLY:HA3	1:A:538:GLY:HA2	1.94	0.48
1:A:127:GLU:O	1:A:128:LEU:HB2	2.13	0.48
1:A:143:THR:HG21	1:A:1011:ASN:ND2	2.28	0.48
1:A:799:SER:OG	1:A:979:ASN:OD1	2.28	0.48
1:A:124:ASN:ND2	1:A:124:ASN:N	2.61	0.48
1:A:124:ASN:N	1:A:124:ASN:HD22	2.12	0.48
1:A:430:ILE:CG2	1:A:781:VAL:HG22	2.44	0.48
1:A:1164:VAL:O	1:A:1168:LEU:HB3	2.13	0.48
1:A:499:THR:HG22	1:A:573:PHE:HD1	1.79	0.47
1:A:945:ARG:HE	1:A:966:ALA:HB1	1.80	0.47
1:A:932:VAL:HG12	5:A:1808:Y01:HAD3	1.95	0.47
1:A:177:GLN:NE2	1:A:410:SER:O	2.48	0.47
1:A:132:VAL:CG2	1:A:133:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:HE2	2:B:89:GLU:HB3	1.97	0.47
1:A:212:GLU:OE1	2:B:153:ARG:NH2	2.42	0.47
1:A:436:ASP:O	1:A:501:GLN:NE2	2.47	0.47
1:A:777:LEU:CD2	1:A:795:PHE:HE2	2.21	0.47
1:A:1179:GLY:HA3	1:A:1180:PRO:HD2	1.44	0.47
1:A:122:GLU:OE1	1:A:128:LEU:HD11	2.15	0.47
2:B:121:LYS:H	2:B:151:SER:HB3	1.80	0.47
1:A:122:GLU:C	1:A:123:THR:HG22	2.36	0.47
1:A:863:TRP:HE1	1:A:877:SER:HB2	1.80	0.47
1:A:1117:LEU:O	1:A:1121:HIS:HB2	2.14	0.47
1:A:141:ASN:O	1:A:145:GLN:CB	2.59	0.46
1:A:888:VAL:HG22	1:A:902:LEU:HB2	1.97	0.46
1:A:1078:LEU:N	1:A:1078:LEU:CD1	2.73	0.46
2:B:152:ASP:OD1	2:B:152:ASP:N	2.46	0.46
1:A:1059:VAL:O	1:A:1063:MET:CB	2.63	0.46
1:A:142:TYR:HD2	1:A:1009:TYR:HH	1.63	0.46
1:A:249:LEU:HD12	2:B:135:SER:HB2	1.98	0.46
1:A:978:LEU:HD13	1:A:981:LEU:HD21	1.97	0.45
1:A:469:VAL:O	1:A:473:GLY:N	2.46	0.45
1:A:570:LEU:HD11	1:A:1080:ALA:O	2.12	0.45
1:A:127:GLU:HA	1:A:130:VAL:CG2	2.46	0.45
1:A:203:CYS:SG	1:A:205:LYS:NZ	2.85	0.45
1:A:328:HIS:CD2	1:A:332:ARG:HG2	2.52	0.45
1:A:781:VAL:HA	1:A:782:PRO:HD3	1.81	0.45
1:A:827:SER:HB3	1:A:840:LEU:HD11	1.99	0.45
1:A:265:LEU:CD1	1:A:275:VAL:HG21	2.47	0.45
1:A:1075:GLY:O	1:A:1077:LYS:CD	2.62	0.45
1:A:1104:PHE:CE2	1:A:1180:PRO:HD2	2.44	0.45
1:A:1181:TYR:O	1:A:1181:TYR:CD1	2.70	0.44
1:A:468:ALA:HA	1:A:471:LEU:HD12	1.98	0.44
1:A:1060:LEU:HD11	1:A:1094:VAL:HG22	1.98	0.44
1:A:485:LEU:HD11	1:A:503:LEU:HD12	2.00	0.44
1:A:836:GLU:HA	1:A:837:ASN:HA	1.65	0.44
1:A:945:ARG:NH2	1:A:967:GLU:O	2.51	0.44
1:A:1181:TYR:O	1:A:1181:TYR:CG	2.70	0.44
1:A:764:SER:HB2	1:A:1066:GLU:HA	1.99	0.44
1:A:778:THR:O	1:A:778:THR:OG1	2.26	0.44
2:B:40:THR:O	2:B:163:ARG:NE	2.40	0.44
1:A:1181:TYR:HA	1:A:1182:PRO:HD2	1.28	0.43
2:B:186:LYS:HE3	6:B:201:SER:OG	2.18	0.43
1:A:423:THR:O	1:A:425:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:TYR:HD2	1:A:1119:LEU:HD11	1.83	0.43
1:A:873:TYR:N	1:A:873:TYR:CD1	2.72	0.43
1:A:350:SER:O	1:A:352:GLY:N	2.52	0.43
1:A:775:LEU:O	1:A:775:LEU:HG	2.18	0.43
1:A:866:GLY:CA	1:A:868:ILE:CD1	2.96	0.43
1:A:274:GLN:NE2	1:A:274:GLN:HA	2.34	0.43
1:A:892:SER:OG	1:A:893:ARG:N	2.51	0.43
1:A:777:LEU:HB3	1:A:795:PHE:HE2	1.84	0.43
1:A:920:TYR:HE1	1:A:969:ILE:HG13	1.84	0.43
1:A:125:VAL:HG11	1:A:427:LEU:CD2	2.48	0.43
1:A:1040:PHE:HB2	1:A:1057:VAL:HG21	2.00	0.43
1:A:867:LYS:CA	1:A:868:ILE:HD13	2.48	0.43
1:A:996:THR:O	1:A:1000:ASN:HB2	2.18	0.43
1:A:1105:LEU:HD23	1:A:1180:PRO:CB	2.49	0.43
1:A:373:TYR:HA	1:A:387:TRP:HE1	1.83	0.43
1:A:741:ALA:HB1	1:A:1116:VAL:HG13	2.00	0.43
1:A:1166:ASN:O	1:A:1170:LEU:CB	2.66	0.43
1:A:125:VAL:HG12	1:A:431:LEU:HD22	1.98	0.42
1:A:866:GLY:C	1:A:868:ILE:HD11	2.15	0.42
1:A:868:ILE:HG21	1:A:902:LEU:HD12	1.99	0.42
1:A:1036:LEU:HA	1:A:1039:THR:HG22	2.00	0.42
1:A:600:LEU:O	1:A:604:GLU:CB	2.68	0.42
1:A:482:ALA:HB2	5:A:1809:Y01:HBA	2.02	0.42
1:A:274:GLN:NE2	1:A:274:GLN:CA	2.82	0.42
1:A:378:GLY:H	1:A:382:VAL:HG21	1.85	0.41
1:A:154:ASN:OD1	1:A:154:ASN:N	2.52	0.41
1:A:123:THR:O	1:A:123:THR:OG1	2.36	0.41
2:B:63:GLU:HG2	2:B:72:ARG:HH22	1.85	0.41
1:A:124:ASN:HB2	1:A:127:GLU:OE2	2.21	0.41
1:A:268:LEU:HD13	1:A:271:ILE:HD13	2.02	0.41
1:A:1014:PRO:HA	1:A:1018:TRP:HE3	1.85	0.41
1:A:1134:LEU:O	1:A:1138:LEU:CB	2.66	0.41
1:A:178:HIS:NE2	1:A:362:THR:OG1	2.43	0.41
1:A:274:GLN:O	1:A:274:GLN:HG3	2.21	0.41
1:A:461:ASP:OD1	1:A:461:ASP:N	2.49	0.41
1:A:550:LEU:HD13	1:A:1046:PHE:HB2	2.03	0.41
1:A:765:LEU:O	1:A:768:THR:OG1	2.27	0.41
1:A:777:LEU:HB3	1:A:795:PHE:CE2	2.56	0.41
1:A:868:ILE:CD1	1:A:868:ILE:N	2.73	0.41
1:A:826:PHE:HA	1:A:829:VAL:HG23	2.02	0.40
1:A:131:GLU:HG3	1:A:566:PRO:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD22	1:A:287:VAL:HG21	2.03	0.40
1:A:777:LEU:HD12	1:A:777:LEU:C	2.42	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	988/1349 (73%)	854 (86%)	123 (12%)	11 (1%)	14	53
2	B	149/177 (84%)	139 (93%)	9 (6%)	1 (1%)	22	61
All	All	1137/1526 (74%)	993 (87%)	132 (12%)	12 (1%)	18	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	MET
2	B	188	GLU
1	A	128	LEU
1	A	131	GLU
1	A	424	THR
1	A	834	LEU
1	A	1182	PRO
1	A	351	THR
1	A	325	GLY
1	A	253	PRO
1	A	1081	VAL
1	A	566	PRO

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	834/1147 (73%)	800 (96%)	34 (4%)	30 64
2	B	129/146 (88%)	127 (98%)	2 (2%)	62 83
All	All	963/1293 (74%)	927 (96%)	36 (4%)	36 66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	125	VAL
1	A	126	GLU
1	A	130	VAL
1	A	132	VAL
1	A	138	ARG
1	A	159	ILE
1	A	254	LEU
1	A	310	ASN
1	A	311	LYS
1	A	324	ASN
1	A	422	PHE
1	A	476	LEU
1	A	587	MET
1	A	607	ARG
1	A	777	LEU
1	A	802	ASN
1	A	828	ASN
1	A	865	THR
1	A	867	LYS
1	A	868	ILE
1	A	873	TYR
1	A	874	LYS
1	A	882	LEU
1	A	960	ARG
1	A	962	ARG
1	A	981	LEU

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Mol	Chain	Res	Type
1	A	1011	ASN
1	A	1077	LYS
1	A	1078	LEU
1	A	1079	SER
1	A	1165	LEU
1	A	1181	TYR
1	A	1183	GLU
2	B	129	ASP
2	B	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	124	ASN
1	A	177	GLN
1	A	274	GLN
1	A	310	ASN
1	A	324	ASN
1	A	328	HIS
1	A	384	HIS
1	A	802	ASN
1	A	828	ASN
1	A	853	GLN
1	A	929	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)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.33	0	17,19,21	0.57	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

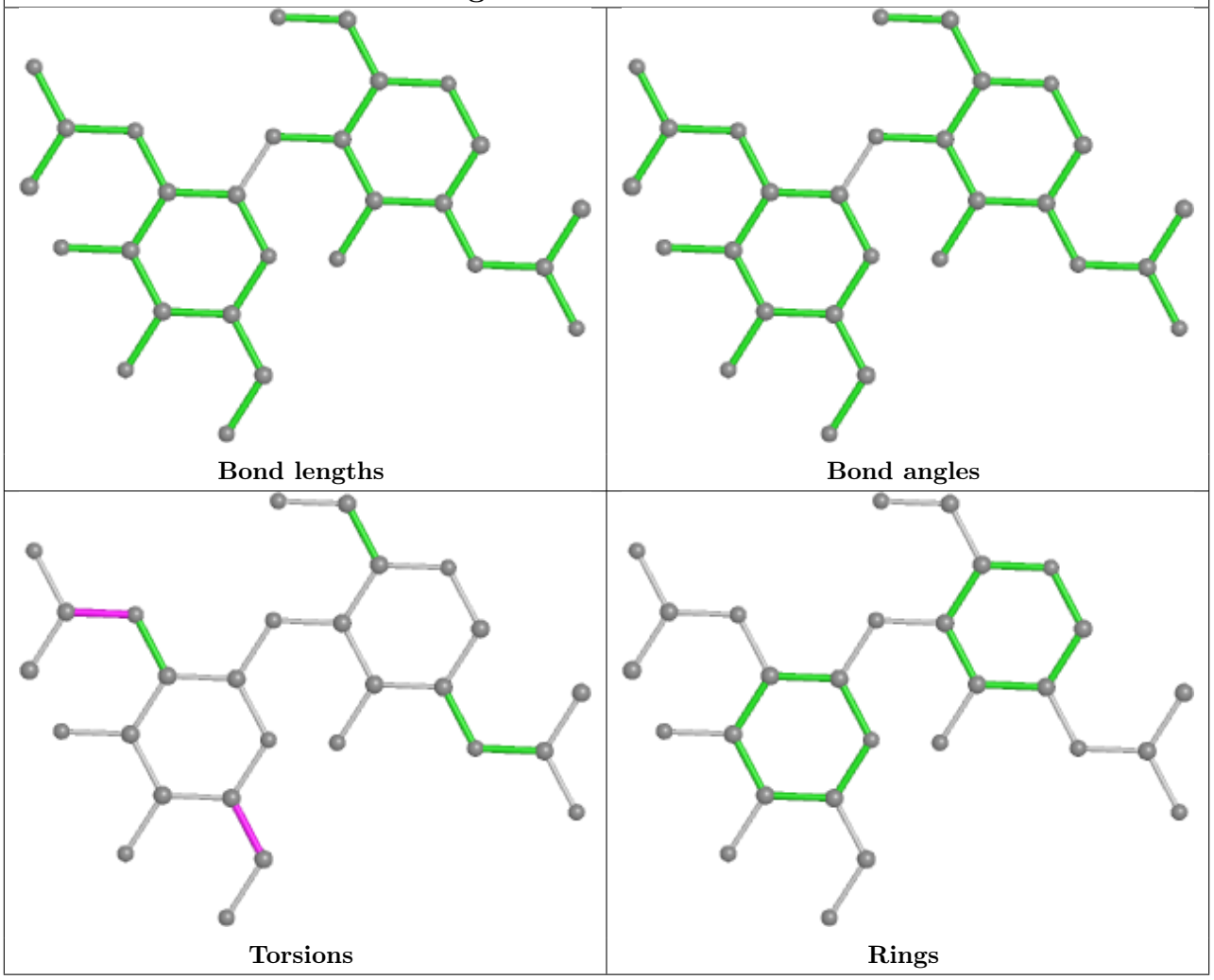
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
4	NAG	A	1802	1	14,14,15	0.40	0	17,19,21	0.55	0
4	NAG	A	1801	1	14,14,15	0.77	1 (7%)	17,19,21	2.33	4 (23%)
6	SER	B	201	-	4,5,6	0.64	0	0,5,7	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	Y01	A	1808	-	38,38,38	1.09	2 (5%)	57,57,57	1.46	8 (14%)
5	Y01	A	1809	-	38,38,38	1.01	2 (5%)	57,57,57	1.90	13 (22%)
4	NAG	A	1807	1	14,14,15	0.42	0	17,19,21	0.55	0
4	NAG	A	1803	1	14,14,15	0.80	1 (7%)	17,19,21	1.17	3 (17%)
4	NAG	A	1804	1	14,14,15	0.35	0	17,19,21	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1802	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	3/6/23/26	0/1/1/1
6	SER	B	201	-	-	2/2/4/6	-
5	Y01	A	1808	-	-	9/19/77/77	0/4/4/4
5	Y01	A	1809	-	-	11/19/77/77	0/4/4/4
4	NAG	A	1807	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1803	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1804	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1809	Y01	OAW-CAY	4.20	1.46	1.34
5	A	1808	Y01	OAW-CAY	3.78	1.45	1.34
4	A	1803	NAG	O5-C1	-2.46	1.39	1.43
4	A	1801	NAG	C1-C2	2.38	1.55	1.52
5	A	1808	Y01	CBH-CBF	-2.27	1.52	1.56
5	A	1809	Y01	CBH-CBF	-2.00	1.52	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1801	NAG	C2-N2-C7	7.75	133.93	122.90
5	A	1809	Y01	CAV-CAZ-CBH	6.42	124.95	116.42
5	A	1809	Y01	CAK-CAI-CAZ	-4.68	116.43	125.06
5	A	1809	Y01	OAW-CAY-CAM	4.09	120.32	111.50
5	A	1808	Y01	CAC-CBB-CAO	-4.06	104.00	110.36
5	A	1809	Y01	CBH-CAZ-CAI	-3.91	116.91	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1801	NAG	C1-C2-N2	3.80	116.99	110.49
5	A	1809	Y01	CBD-CAK-CAI	-3.48	107.74	112.73
5	A	1808	Y01	OAW-CAY-CAM	3.36	118.75	111.50
5	A	1809	Y01	CAC-CBB-CAO	-3.30	105.19	110.36
5	A	1808	Y01	CAM-CAL-CAX	-3.06	107.01	113.60
5	A	1809	Y01	CBF-CBH-CAZ	-3.05	104.88	109.65
4	A	1801	NAG	C1-O5-C5	3.03	116.30	112.19
4	A	1803	NAG	C2-N2-C7	3.02	127.20	122.90
5	A	1808	Y01	CAP-CAQ-CBG	-2.82	99.54	105.13
5	A	1809	Y01	CBC-OAW-CAY	-2.79	110.92	117.79
5	A	1809	Y01	CAK-CBD-CBF	2.78	113.08	109.71
5	A	1808	Y01	CAK-CBD-CBG	-2.51	107.27	110.91
5	A	1808	Y01	CAV-CAZ-CBH	2.43	119.65	116.42
5	A	1808	Y01	CBF-CBD-CBG	-2.41	105.87	109.09
5	A	1809	Y01	OAH-CAX-CAL	2.17	120.99	114.03
4	A	1801	NAG	C8-C7-N2	2.12	119.69	116.10
5	A	1809	Y01	CAT-CBH-CAZ	2.06	112.52	108.75
5	A	1809	Y01	CBC-CAV-CAZ	2.04	114.69	111.52
5	A	1808	Y01	OAH-CAX-CAL	2.04	120.57	114.03
4	A	1803	NAG	C4-C3-C2	2.01	113.96	111.02
5	A	1809	Y01	CAM-CAL-CAX	-2.01	109.28	113.60
4	A	1803	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1809	Y01	OAG-CAY-OAW-CBC
5	A	1809	Y01	CAM-CAY-OAW-CBC
6	B	201	SER	C-CA-CB-OG
4	A	1807	NAG	C4-C5-C6-O6
4	A	1807	NAG	O5-C5-C6-O6
5	A	1808	Y01	CAJ-CAO-CBB-CBE
5	A	1809	Y01	CAJ-CAO-CBB-CBE
5	A	1808	Y01	CAJ-CAO-CBB-CAC
4	A	1801	NAG	C8-C7-N2-C2
4	A	1801	NAG	O7-C7-N2-C2
5	A	1809	Y01	CAJ-CAO-CBB-CAC
4	A	1804	NAG	O5-C5-C6-O6
5	A	1809	Y01	CAO-CAJ-CAN-CBA
4	A	1803	NAG	O5-C5-C6-O6
5	A	1808	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
5	A	1809	Y01	CAX-CAL-CAM-CAY
5	A	1808	Y01	CAC-CBB-CBE-CBI
5	A	1808	Y01	CAC-CBB-CBE-CAP
4	A	1804	NAG	C4-C5-C6-O6
5	A	1809	Y01	CAN-CAJ-CAO-CBB
4	A	1802	NAG	O5-C5-C6-O6
5	A	1808	Y01	CAO-CBB-CBE-CBI
6	B	201	SER	N-CA-CB-OG
5	A	1808	Y01	CAO-CBB-CBE-CAP
4	A	1803	NAG	C4-C5-C6-O6
4	A	1803	NAG	C3-C2-N2-C7
5	A	1809	Y01	CAC-CBB-CBE-CBI
5	A	1809	Y01	CAM-CAL-CAX-OAH
5	A	1808	Y01	CAL-CAM-CAY-OAW
5	A	1809	Y01	CAM-CAL-CAX-OAF
4	A	1801	NAG	C3-C2-N2-C7
5	A	1808	Y01	CAL-CAM-CAY-OAG
5	A	1809	Y01	CAL-CAM-CAY-OAW

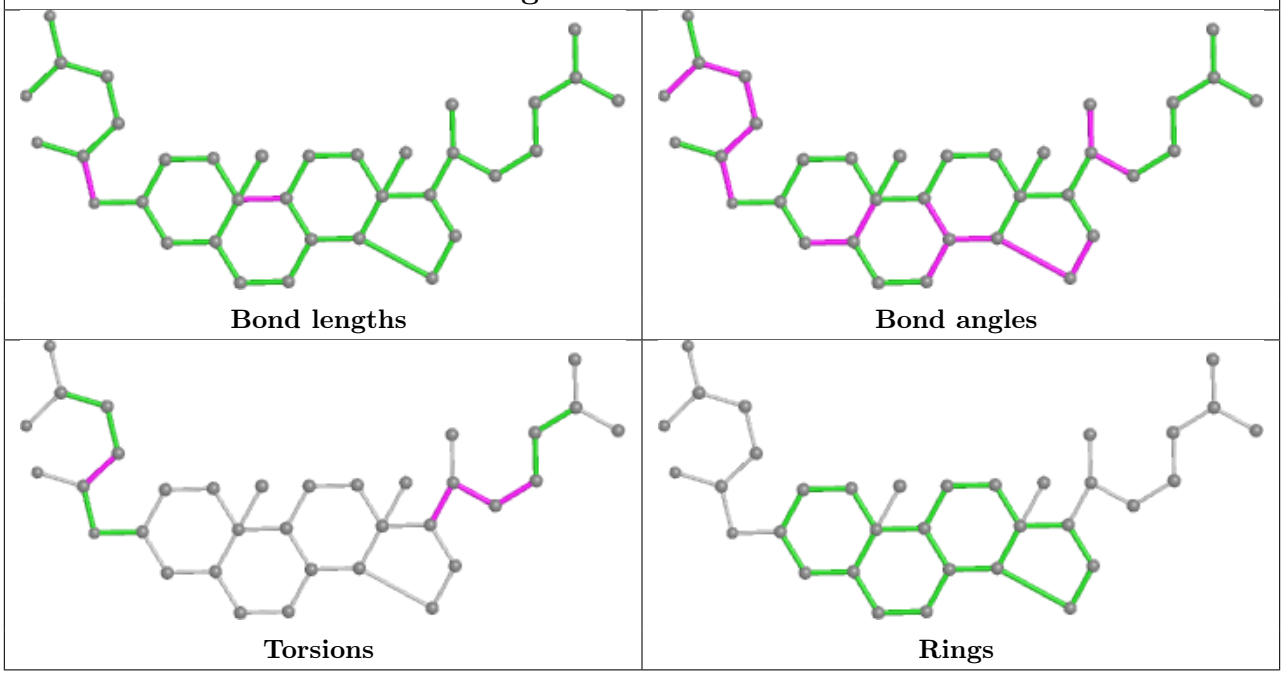
There are no ring outliers.

3 monomers are involved in 3 short contacts:

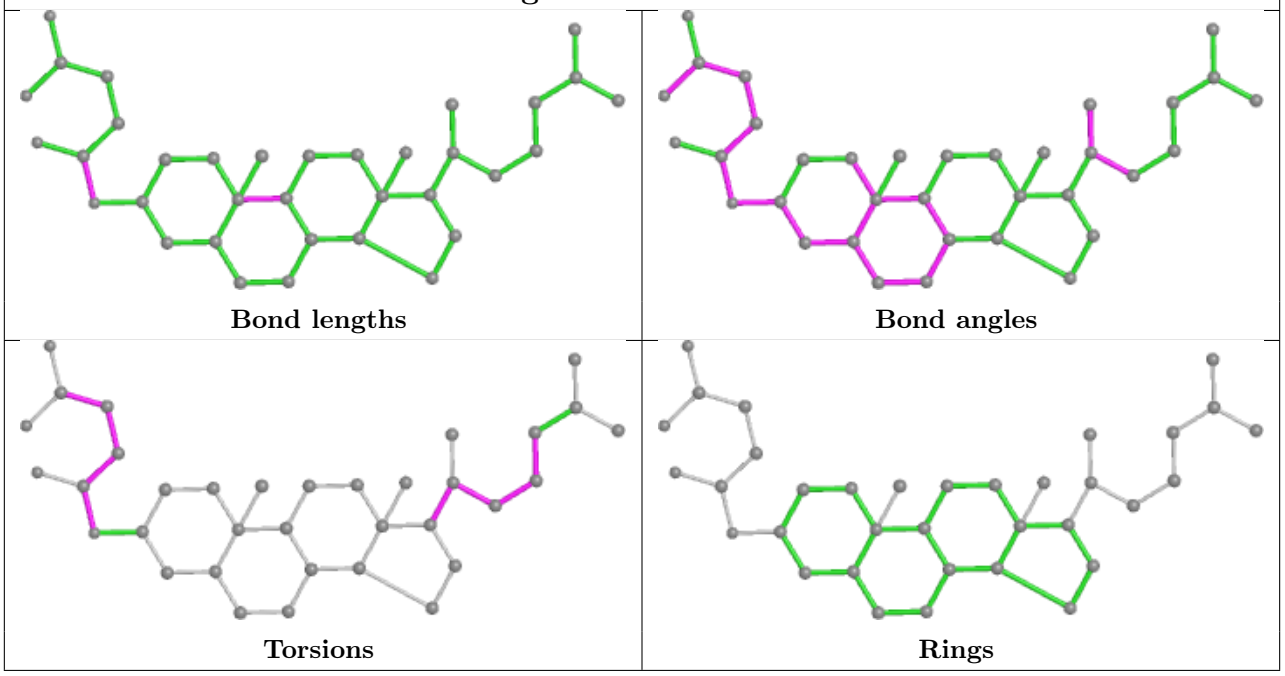
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	201	SER	1	0
5	A	1808	Y01	1	0
5	A	1809	Y01	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 Y01 A 1808



Ligand Y01 A 1809



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.

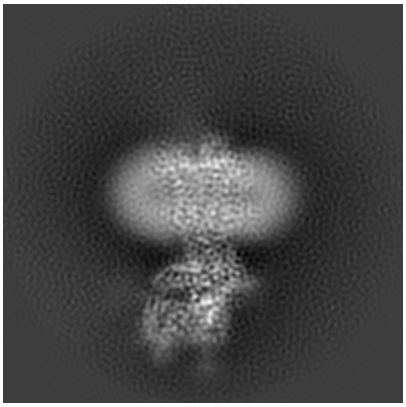
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7968. These allow visual inspection of the internal detail of the map and identification of artifacts.

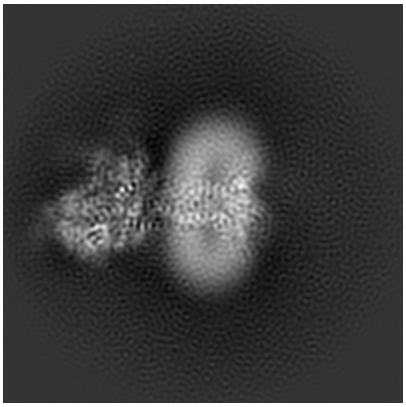
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

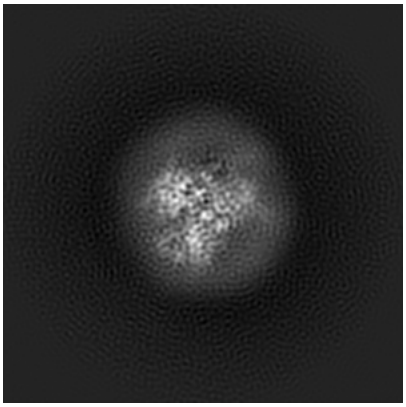
6.1.1 Primary map



X



Y

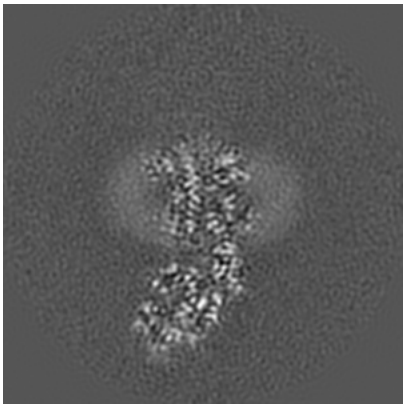


Z

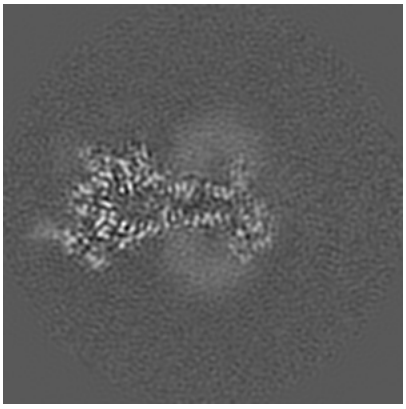
The images above show the map projected in three orthogonal directions.

6.2 Central slices

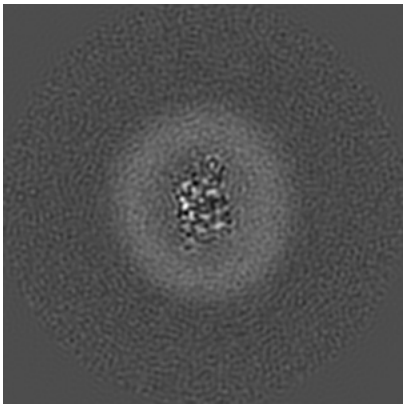
6.2.1 Primary map



X Index: 112



Y Index: 112

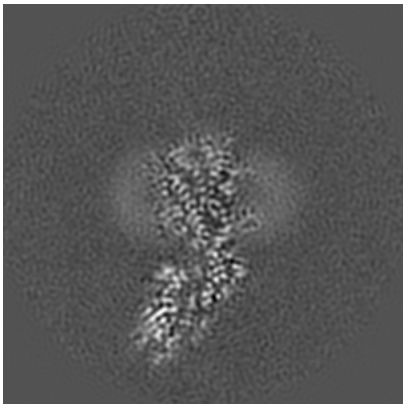


Z Index: 112

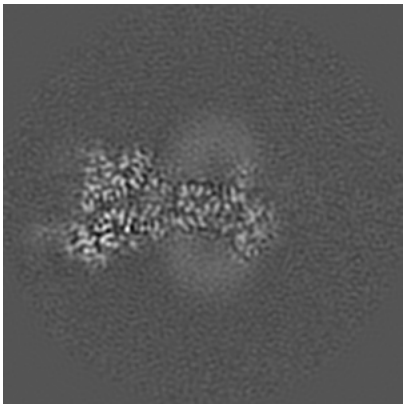
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

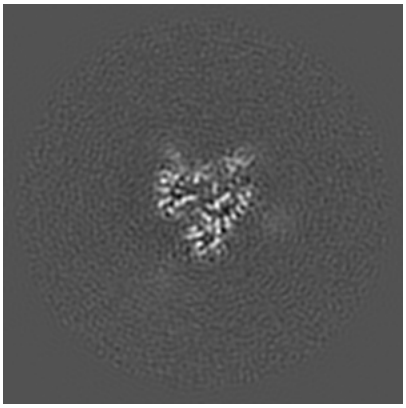
6.3.1 Primary map



X Index: 106



Y Index: 115



Z Index: 66

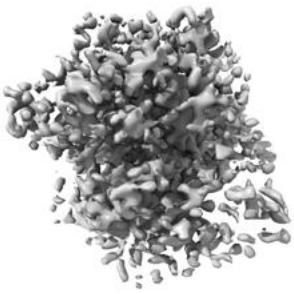
The images above show the largest variance slices of the map in three orthogonal directions.

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

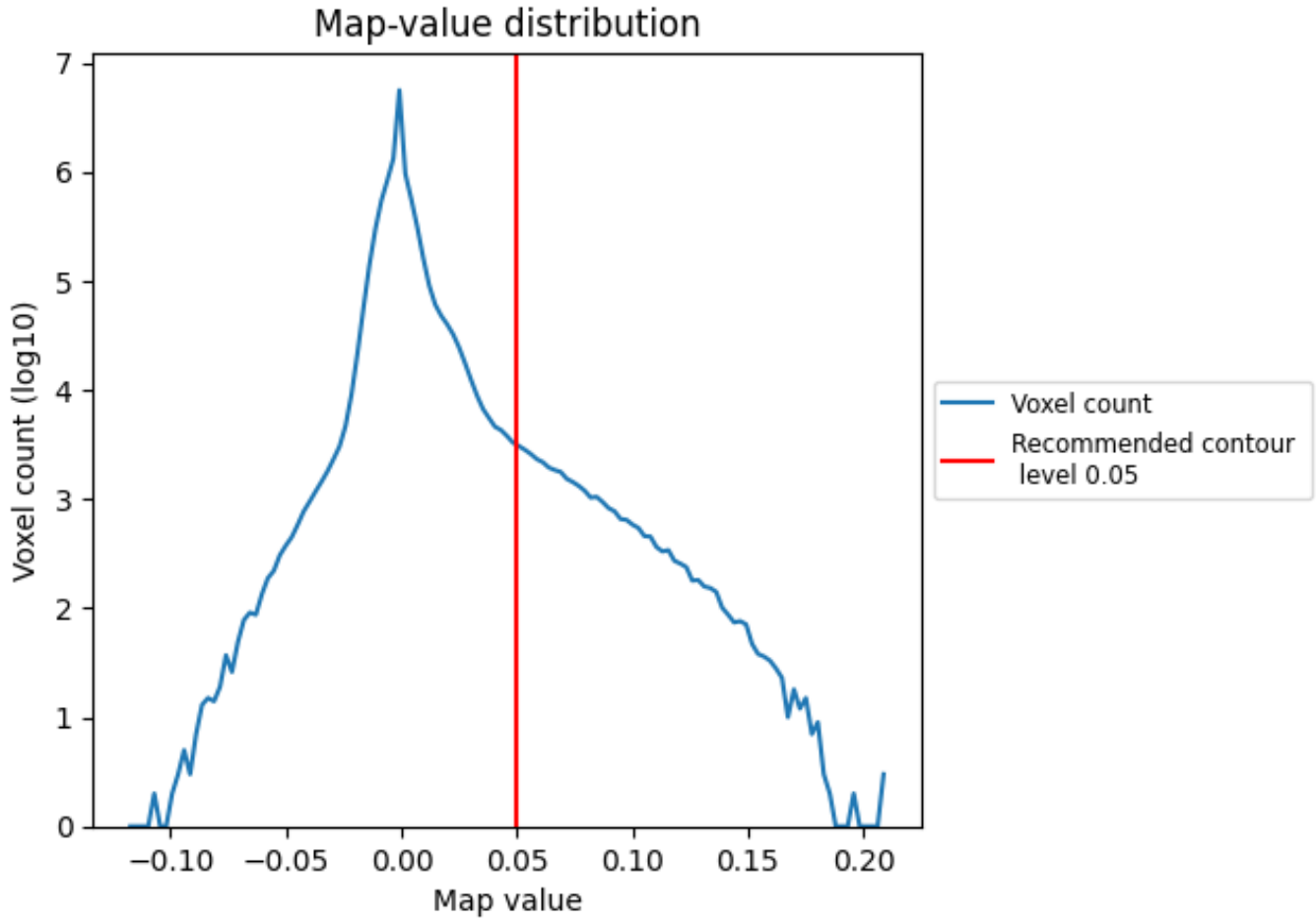
6.5 Mask visualisation (i)

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

7 Map analysis

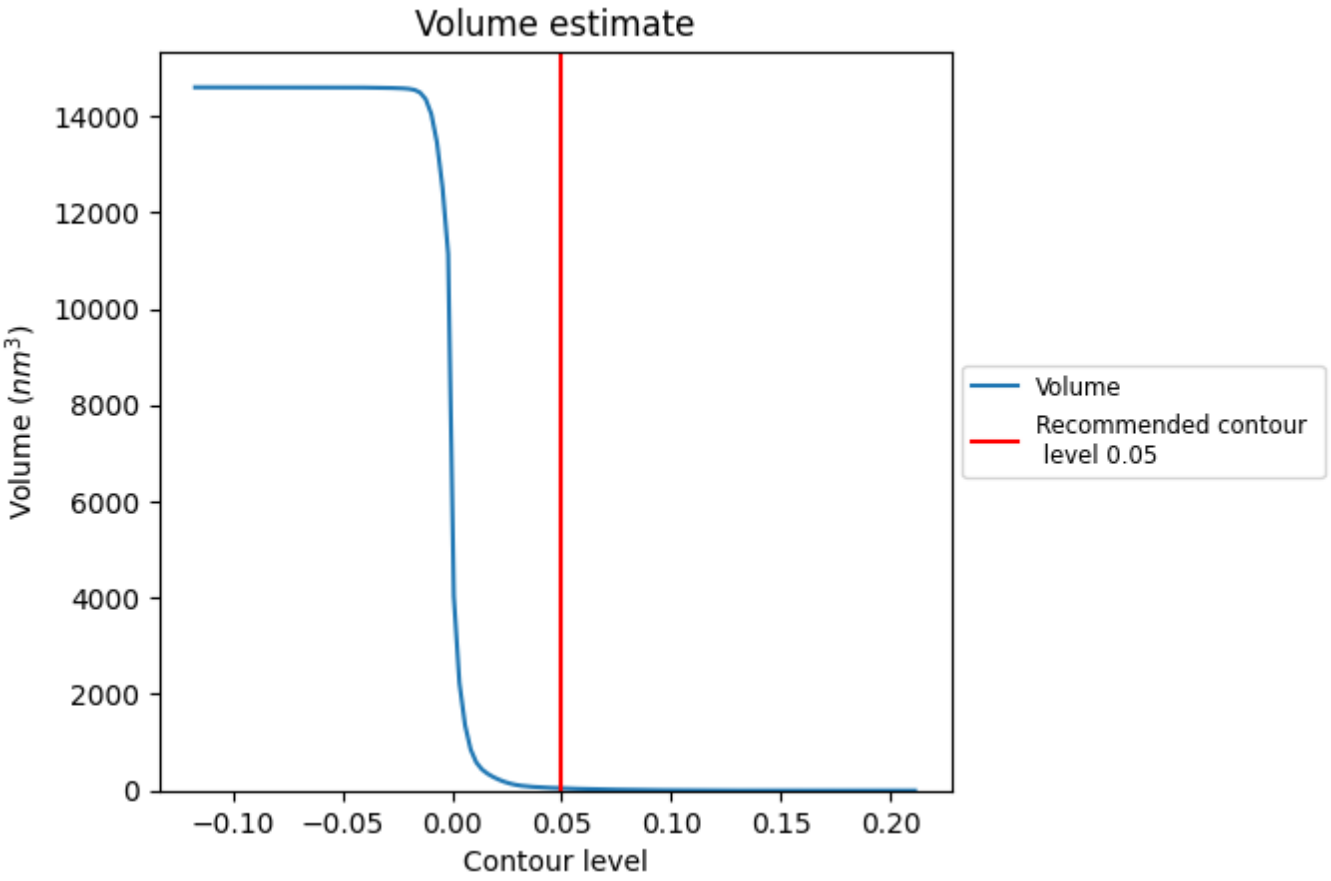
This section contains the results of statistical analysis of the map.

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.

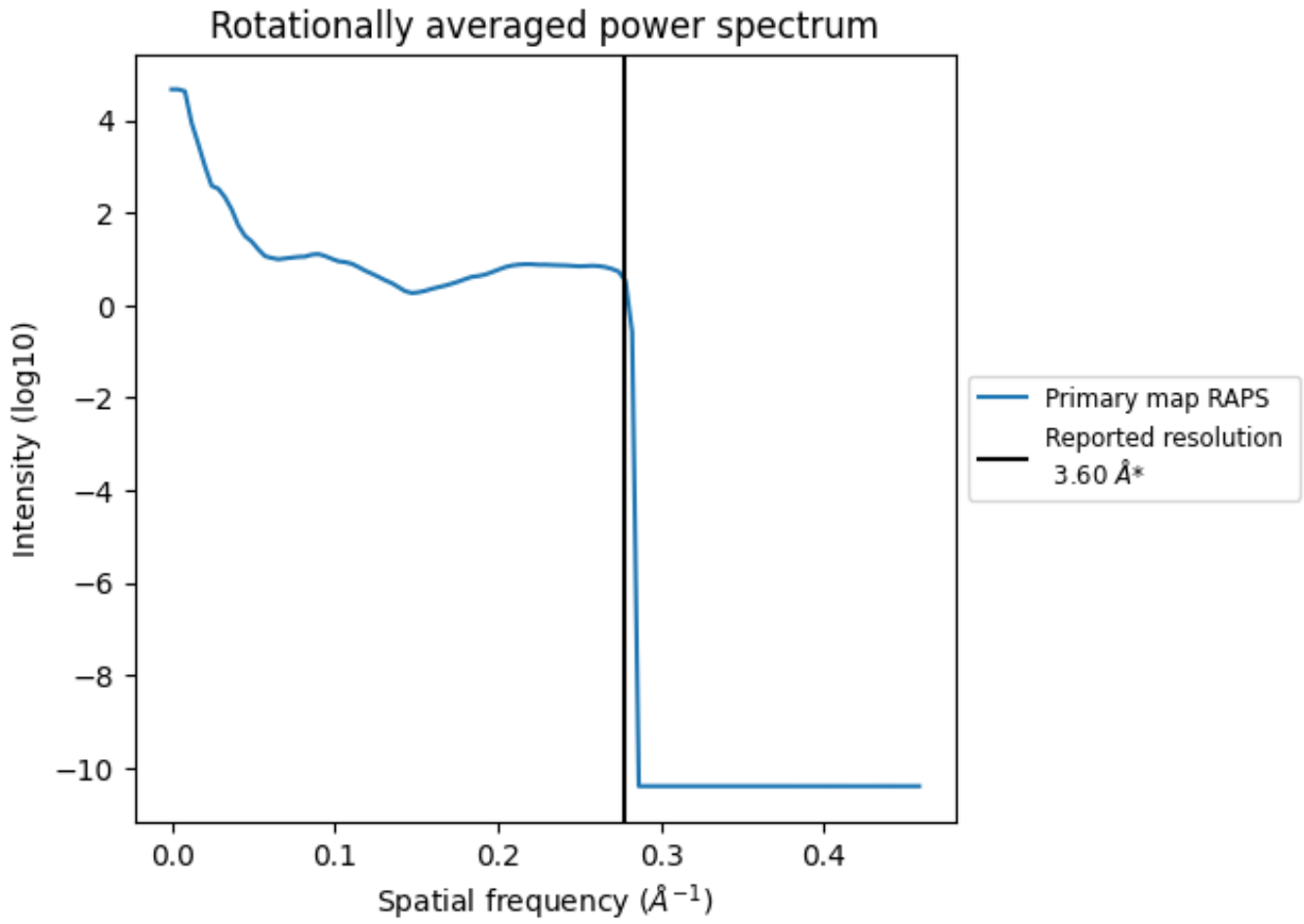
7.2 Volume estimate



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 43 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 0.278 Å^{-1}

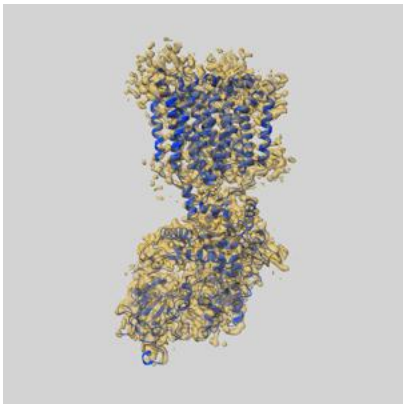
8 Fourier-Shell correlation

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

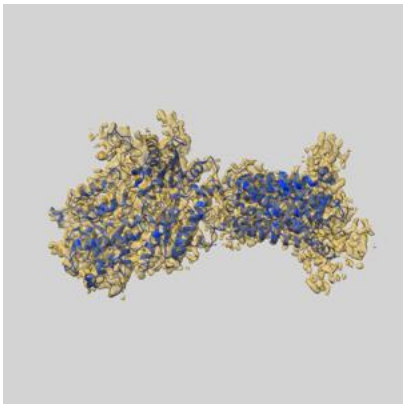
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7968 and PDB model 6DMY. Per-residue inclusion information can be found in section 3 on page 8.

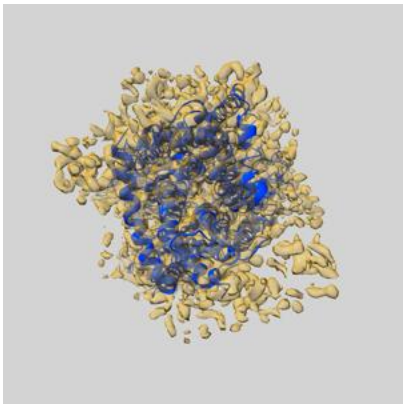
9.1 Map-model overlay



X



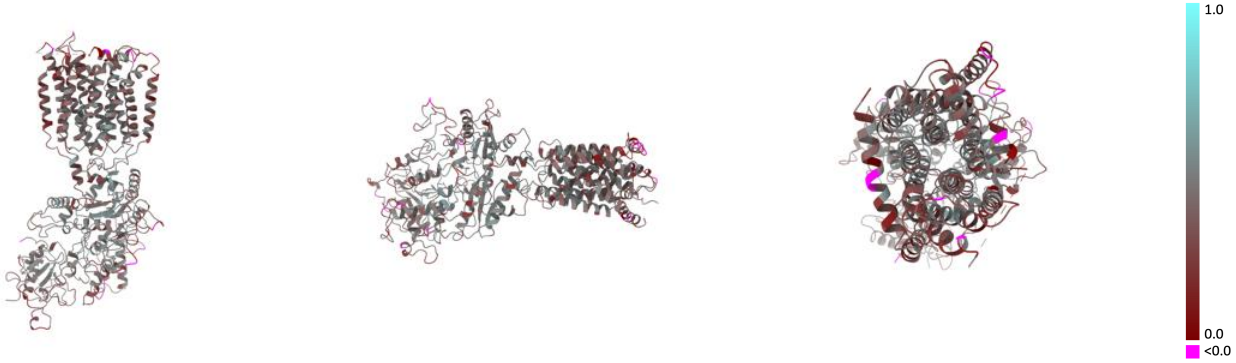
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

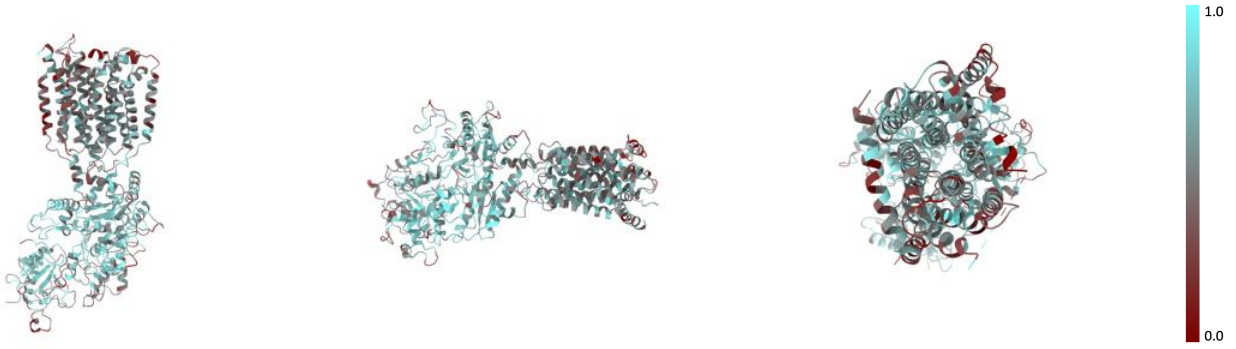
9.2 Q-score mapped to coordinate model (i)



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.

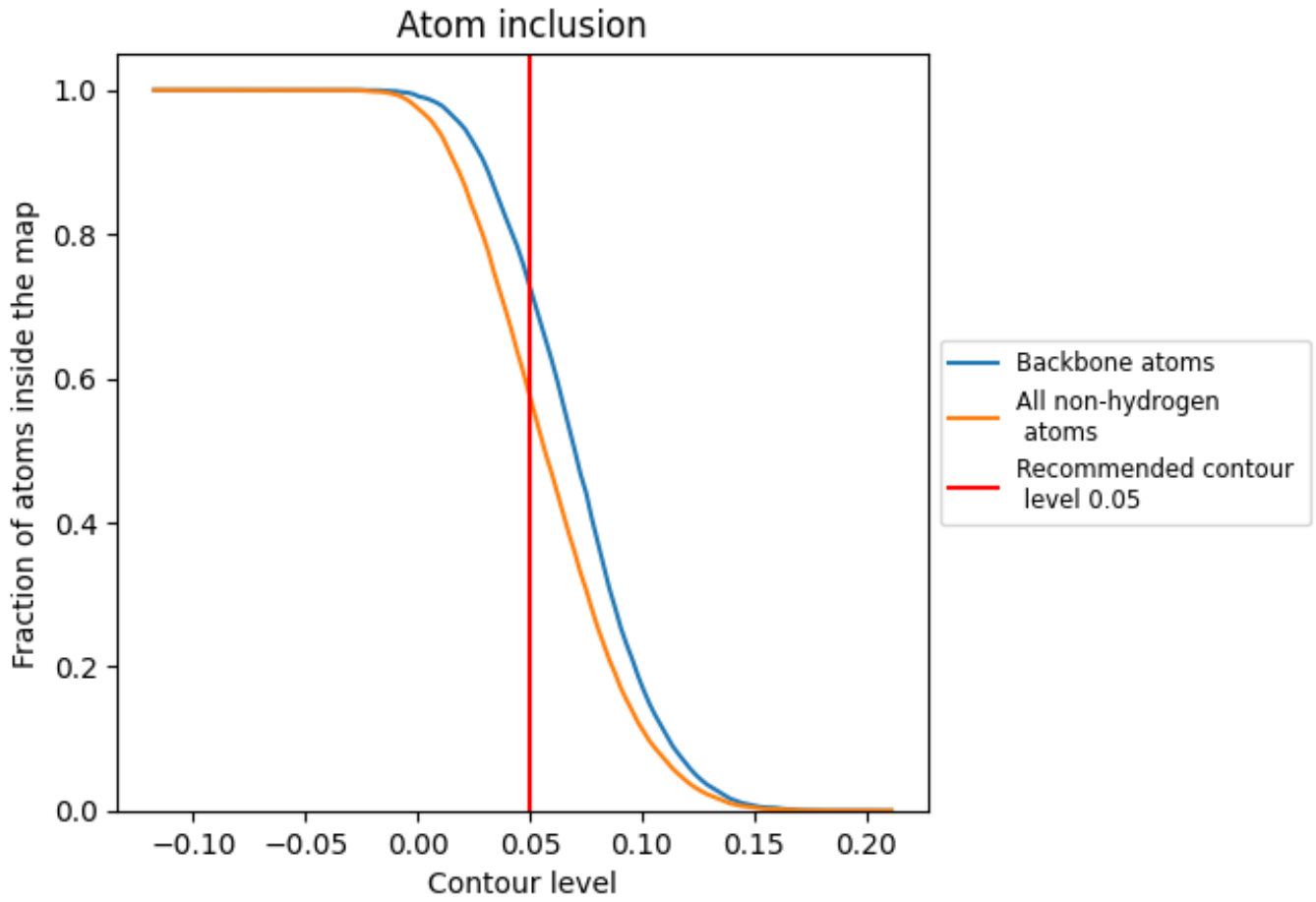
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5767	0.3880
A	0.5718	0.3890
B	0.6166	0.3850
C	0.2500	0.2060