Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 02:21 AM JST

PDB ID	:	6AGF
EMDB ID	:	EMD-9617
Title	:	Structure of the human voltage-gated sodium channel Nav1.4 in complex with beta1
Authors	:	Pan, X.J.; li, Z.Q.; Zhou, Q.; Shen, H.Z.; Wu, K.; Huang, X.S.; Chen, J.F.; Zhang, J.R.; Zhu, X.C.; Lei, J.L.; Xiong, W.; Gong, H.P.; Xiao, B.L.; Yan, N.
Deposited on	:	2018-08-11
Resolution	:	3.20 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:

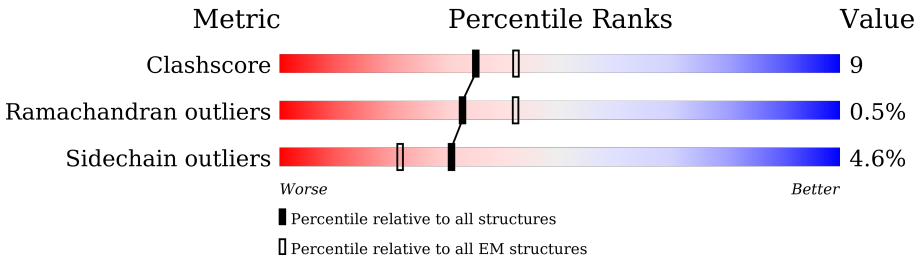
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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	1879	8% 50% 9% · 39%
2	B	218	6% 64% 14% · 21%
3	C	3	33% 67%
4	D	2	100%
4	E	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10980 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 Sodium channel protein type 4 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1138	9163	6071	1443	1571	78	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP P35499
A	-41	ALA	-	expression tag	UNP P35499
A	-40	SER	-	expression tag	UNP P35499
A	-39	TRP	-	expression tag	UNP P35499
A	-38	SER	-	expression tag	UNP P35499
A	-37	HIS	-	expression tag	UNP P35499
A	-36	PRO	-	expression tag	UNP P35499
A	-35	GLN	-	expression tag	UNP P35499
A	-34	PHE	-	expression tag	UNP P35499
A	-33	GLU	-	expression tag	UNP P35499
A	-32	LYS	-	expression tag	UNP P35499
A	-31	GLY	-	expression tag	UNP P35499
A	-30	GLY	-	expression tag	UNP P35499
A	-29	GLY	-	expression tag	UNP P35499
A	-28	ALA	-	expression tag	UNP P35499
A	-27	ARG	-	expression tag	UNP P35499
A	-26	GLY	-	expression tag	UNP P35499
A	-25	GLY	-	expression tag	UNP P35499
A	-24	SER	-	expression tag	UNP P35499
A	-23	GLY	-	expression tag	UNP P35499
A	-22	GLY	-	expression tag	UNP P35499
A	-21	GLY	-	expression tag	UNP P35499
A	-20	SER	-	expression tag	UNP P35499
A	-19	TRP	-	expression tag	UNP P35499
A	-18	SER	-	expression tag	UNP P35499
A	-17	HIS	-	expression tag	UNP P35499
A	-16	PRO	-	expression tag	UNP P35499
A	-15	GLN	-	expression tag	UNP P35499

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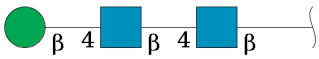
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP P35499
A	-13	GLU	-	expression tag	UNP P35499
A	-12	LYS	-	expression tag	UNP P35499
A	-11	GLY	-	expression tag	UNP P35499
A	-10	PHE	-	expression tag	UNP P35499
A	-9	ASP	-	expression tag	UNP P35499
A	-8	TYR	-	expression tag	UNP P35499
A	-7	LYS	-	expression tag	UNP P35499
A	-6	ASP	-	expression tag	UNP P35499
A	-5	ASP	-	expression tag	UNP P35499
A	-4	ASP	-	expression tag	UNP P35499
A	-3	ASP	-	expression tag	UNP P35499
A	-2	LYS	-	expression tag	UNP P35499
A	-1	GLY	-	expression tag	UNP P35499
A	0	THR	-	expression tag	UNP P35499

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

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

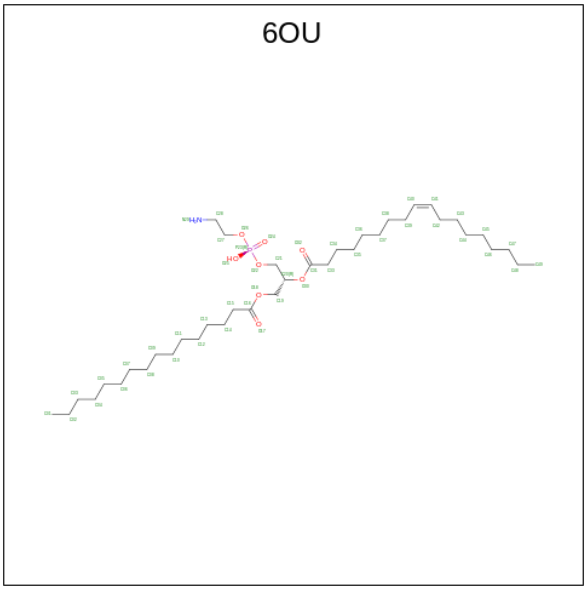


Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

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

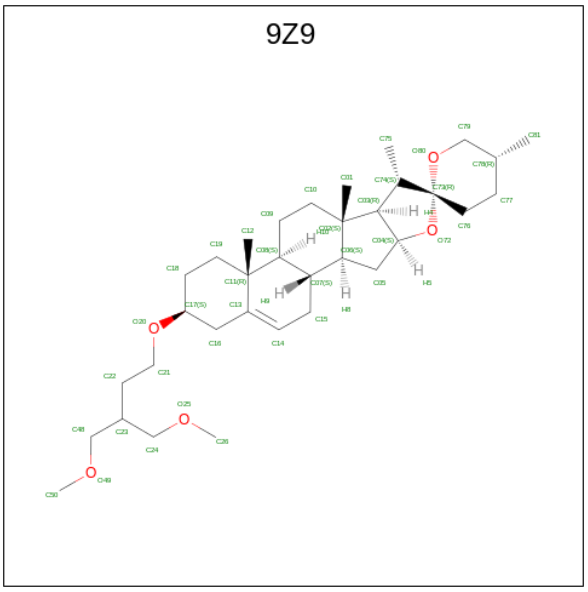
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total 28	C 16	N 2	O 10	0	0
4	E	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



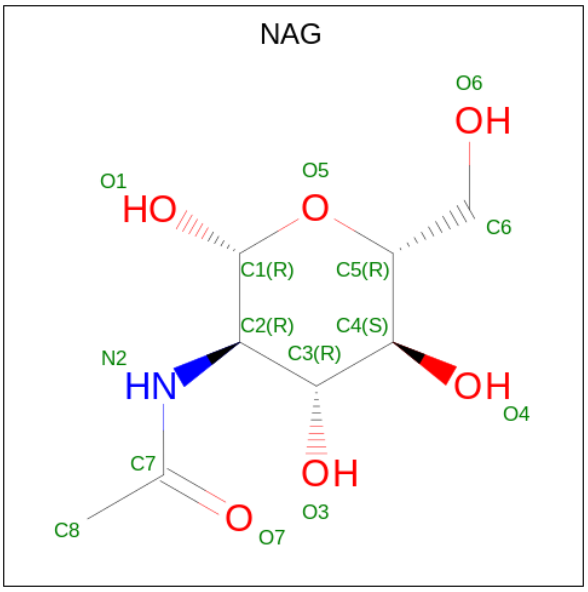
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 239	C 179	N 6	O 48	P 6	0
5	A	1	Total 239	C 179	N 6	O 48	P 6	0
5	A	1	Total 239	C 179	N 6	O 48	P 6	0
5	A	1	Total 239	C 179	N 6	O 48	P 6	0
5	A	1	Total 239	C 179	N 6	O 48	P 6	0
5	A	1	Total 239	C 179	N 6	O 48	P 6	0

- Molecule 6 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	39	34	5	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

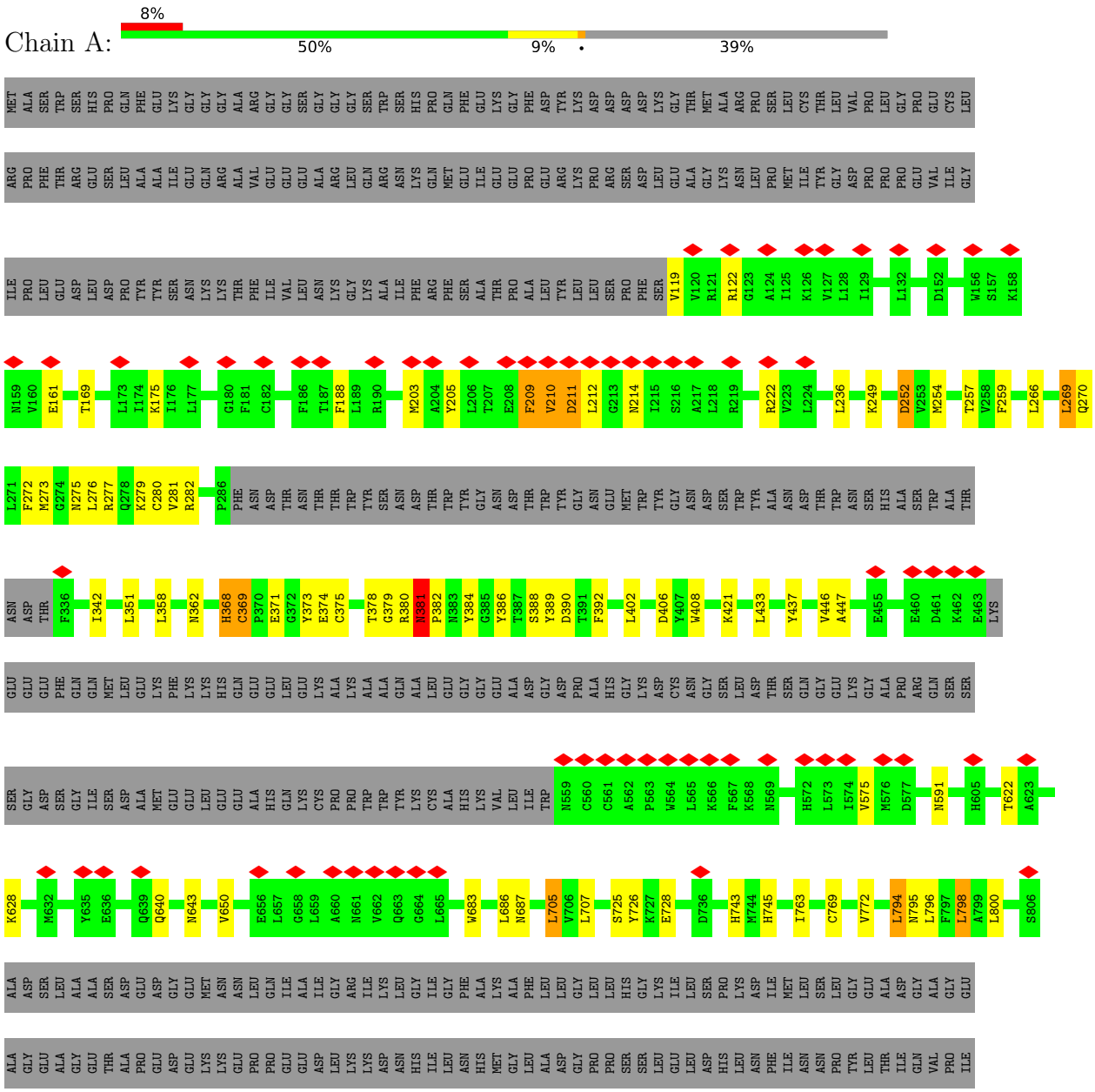


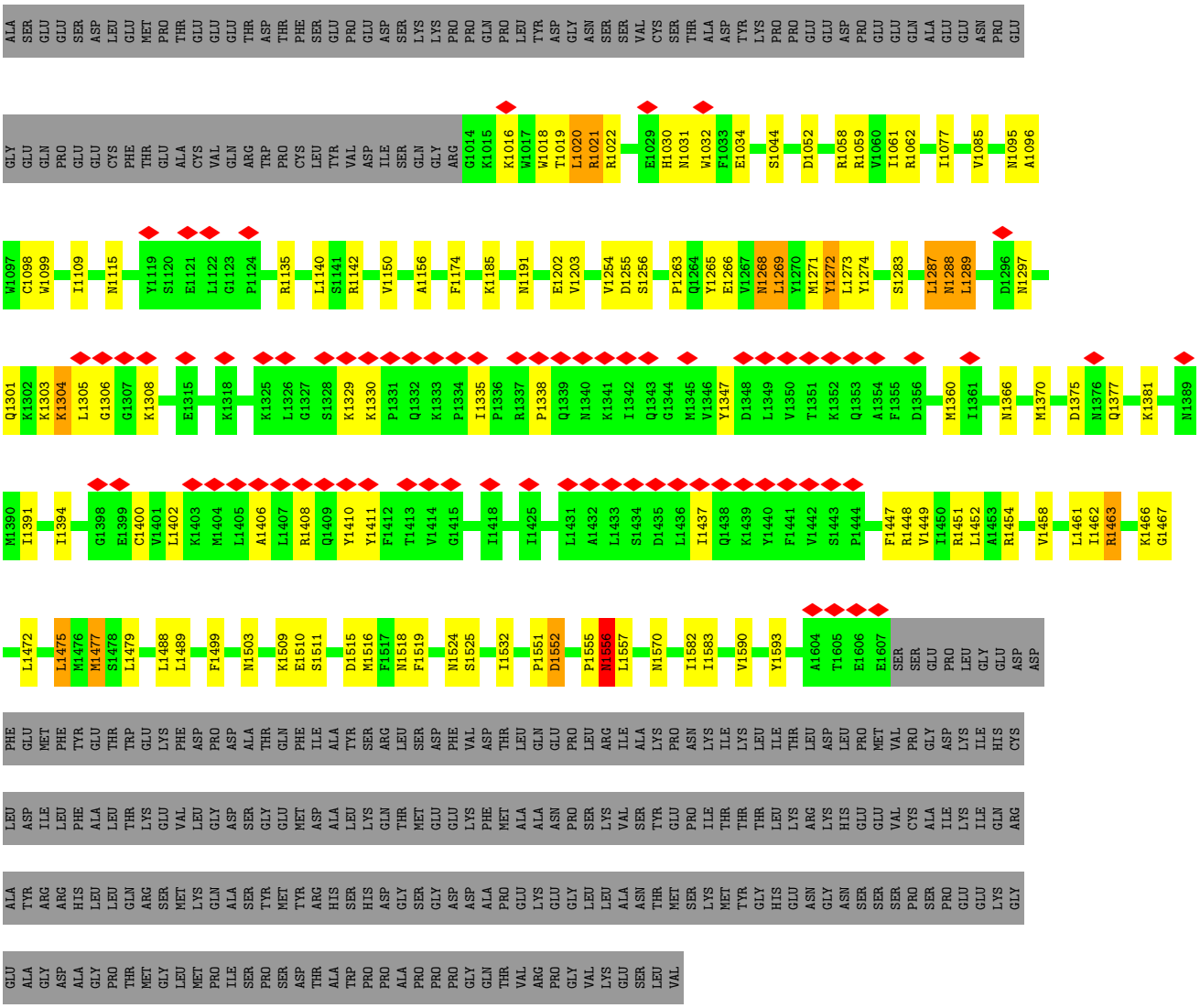
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	B	1	28	16	2	10	0
			Total	C	N	O	
7	B	1	28	16	2	10	0

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.

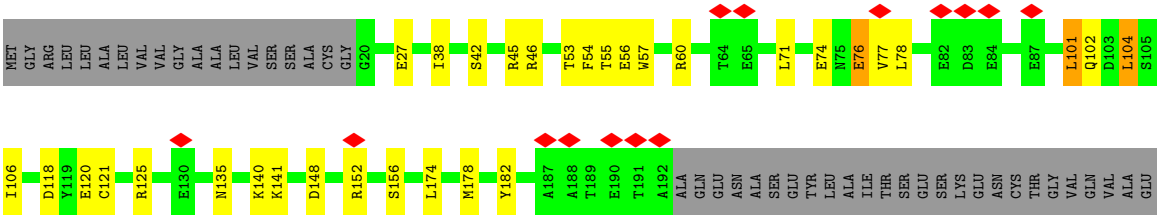
• Molecule 1: Sodium channel protein type 4 subunit alpha





• Molecule 2: Sodium channel subunit beta-1

Chain B:

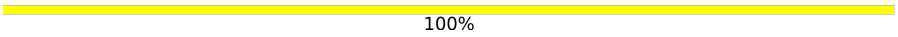


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:



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

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.323	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	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: BMA, NAG, 9Z9, 6OU

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	0.60	0/9386	0.69	0/12728
2	B	0.60	0/1442	0.68	0/1949
All	All	0.60	0/10828	0.69	0/14677

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9163	0	9343	168	0
2	B	1416	0	1382	29	0
3	C	39	0	34	0	0
4	D	28	0	25	0	0
4	E	28	0	25	2	0
5	A	239	0	0	0	0
6	A	39	0	0	0	0
7	B	28	0	26	0	0
All	All	10980	0	10835	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (188) 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:381:ASN:HD22	1:A:382:PRO:HD3	1.18	1.06
1:A:276:LEU:HD12	1:A:382:PRO:HG2	1.44	0.99
1:A:1509:LYS:HE2	1:A:1518:ASN:HD21	1.29	0.95
1:A:1555:PRO:O	1:A:1556:ASN:CG	2.06	0.94
1:A:1509:LYS:HE2	1:A:1518:ASN:ND2	1.92	0.84
1:A:1304:LYS:CE	1:A:1305:LEU:HD22	2.08	0.83
1:A:1463:ARG:HD2	1:A:1463:ARG:O	1.79	0.82
1:A:421:LYS:HE3	1:A:1516:MET:HE3	1.63	0.80
1:A:1269:LEU:HD22	1:A:1269:LEU:O	1.82	0.79
1:A:1551:PRO:O	1:A:1552:ASP:HB2	1.81	0.78
1:A:342:ILE:HD13	1:A:378:THR:HG21	1.65	0.78
1:A:1515:ASP:OD2	2:B:46:ARG:NH1	2.20	0.75
1:A:1018:TRP:O	1:A:1022:ARG:HG3	1.87	0.74
1:A:1516:MET:O	1:A:1524:ASN:ND2	2.21	0.73
1:A:437:TYR:CZ	1:A:1475:LEU:HB2	2.23	0.73
1:A:380:ARG:O	1:A:380:ARG:HD2	1.89	0.72
1:A:380:ARG:O	1:A:381:ASN:HB2	1.90	0.72
1:A:1268:ASN:OD1	1:A:1271:MET:HG2	1.89	0.72
1:A:1304:LYS:HE2	1:A:1305:LEU:HD22	1.69	0.72
1:A:277:ARG:NH2	1:A:1375:ASP:OD2	2.23	0.72
1:A:381:ASN:HD22	1:A:382:PRO:CD	2.00	0.72
1:A:1254:VAL:O	1:A:1268:ASN:HB3	1.90	0.70
1:A:794:LEU:HD22	1:A:794:LEU:O	1.91	0.70
1:A:381:ASN:ND2	1:A:382:PRO:HD3	2.02	0.70
1:A:1016:LYS:HA	1:A:1019:THR:HG22	1.74	0.70
1:A:1283:SER:O	1:A:1287:LEU:HB2	1.92	0.69
1:A:1304:LYS:HE2	1:A:1305:LEU:CD2	2.24	0.68
1:A:1400:CYS:HG	1:A:1411:TYR:HH	1.42	0.67
1:A:368:HIS:CB	2:B:45:ARG:NH2	2.58	0.66
1:A:1077:ILE:HD11	1:A:1109:ILE:HD11	1.78	0.66
1:A:1555:PRO:O	1:A:1556:ASN:CB	2.43	0.66
1:A:1140:LEU:HD21	1:A:1150:VAL:HG21	1.77	0.66
1:A:368:HIS:HB2	2:B:45:ARG:HH21	1.60	0.65
1:A:342:ILE:HG23	1:A:378:THR:OG1	1.96	0.65
1:A:437:TYR:OH	1:A:1475:LEU:HB2	1.96	0.65
1:A:368:HIS:CB	2:B:45:ARG:HH21	2.11	0.64
1:A:1304:LYS:HD2	1:A:1304:LYS:C	2.18	0.64
2:B:60:ARG:NH2	2:B:118:ASP:OD2	2.29	0.64
1:A:368:HIS:HB2	2:B:45:ARG:NH2	2.13	0.63
1:A:280:CYS:HB3	1:A:369:CYS:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1555:PRO:C	1:A:1556:ASN:OD1	2.36	0.63
1:A:212:LEU:C	1:A:212:LEU:HD13	2.20	0.62
1:A:1463:ARG:HD2	1:A:1463:ARG:C	2.19	0.62
1:A:1518:ASN:O	1:A:1524:ASN:HB3	1.99	0.62
1:A:380:ARG:HH21	1:A:380:ARG:HG3	1.65	0.61
1:A:1555:PRO:C	1:A:1556:ASN:CG	2.58	0.61
1:A:175:LYS:HZ2	1:A:188:PHE:HE1	1.48	0.61
2:B:101:LEU:HD12	2:B:104:LEU:HD21	1.82	0.60
1:A:1458:VAL:O	1:A:1461:LEU:HB3	2.01	0.60
1:A:1019:THR:HG23	2:B:182:TYR:HE1	1.65	0.60
1:A:279:LYS:NZ	1:A:379:GLY:HA3	2.16	0.59
1:A:1202:GLU:HG2	1:A:1203:VAL:HG23	1.84	0.58
1:A:269:LEU:HD21	1:A:390:ASP:HA	1.85	0.58
1:A:1437:ILE:HG21	1:A:1447:PHE:HB2	1.86	0.58
2:B:101:LEU:CD1	2:B:104:LEU:HD23	2.33	0.58
1:A:622:THR:HG22	1:A:650:VAL:HG13	1.86	0.57
1:A:1095:ASN:ND2	1:A:1098:CYS:SG	2.73	0.57
2:B:101:LEU:HD12	2:B:104:LEU:CD2	2.35	0.57
1:A:212:LEU:HD13	1:A:212:LEU:O	2.04	0.57
1:A:1304:LYS:CE	1:A:1305:LEU:CD2	2.79	0.57
1:A:269:LEU:HD23	1:A:389:TYR:O	2.04	0.57
1:A:209:PHE:O	1:A:210:VAL:HG23	2.05	0.56
1:A:1461:LEU:HD12	1:A:1461:LEU:O	2.05	0.56
1:A:406:ASP:OD2	1:A:763:ILE:N	2.37	0.56
1:A:1304:LYS:HE3	1:A:1305:LEU:HD22	1.86	0.56
1:A:421:LYS:CE	1:A:1516:MET:HE3	2.34	0.56
1:A:575:VAL:HG13	1:A:628:LYS:HZ2	1.71	0.55
1:A:1019:THR:HG23	2:B:182:TYR:CE1	2.41	0.55
1:A:1301:GLN:O	1:A:1305:LEU:HB2	2.07	0.54
1:A:380:ARG:HD2	1:A:380:ARG:C	2.27	0.54
2:B:101:LEU:CD1	2:B:104:LEU:CD2	2.86	0.54
2:B:152:ARG:HH21	2:B:156:SER:HG	1.53	0.54
1:A:575:VAL:HG13	1:A:628:LYS:NZ	2.23	0.54
1:A:1059:ARG:HD3	1:A:1062:ARG:HH12	1.72	0.54
1:A:279:LYS:HZ2	1:A:379:GLY:HA3	1.73	0.54
1:A:210:VAL:CG1	1:A:211:ASP:N	2.71	0.53
2:B:53:THR:OG1	2:B:101:LEU:HB2	2.08	0.53
1:A:1271:MET:O	1:A:1273:LEU:N	2.41	0.53
1:A:276:LEU:HD12	1:A:382:PRO:CG	2.30	0.53
1:A:1477:MET:CE	1:A:1477:MET:CA	2.85	0.53
1:A:402:LEU:HD23	1:A:408:TRP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:HIS:HD2	1:A:745:HIS:H	1.56	0.52
1:A:368:HIS:HB3	2:B:45:ARG:NH2	2.25	0.52
2:B:42:SER:O	2:B:125:ARG:NH2	2.43	0.52
2:B:148:ASP:N	2:B:148:ASP:OD1	2.42	0.51
2:B:120:GLU:HG2	2:B:141:LYS:HG2	1.92	0.51
1:A:1174:PHE:O	1:A:1274:TYR:OH	2.28	0.51
1:A:421:LYS:CE	1:A:1516:MET:CE	2.88	0.51
1:A:266:LEU:O	1:A:270:GLN:HG3	2.11	0.51
1:A:380:ARG:HG3	1:A:380:ARG:NH2	2.25	0.51
1:A:640:GLN:NE2	1:A:643:ASN:OD1	2.43	0.51
1:A:259:PHE:CZ	1:A:1462:ILE:HG23	2.46	0.50
1:A:1338:PRO:HG3	1:A:1408:ARG:HE	1.77	0.50
1:A:1360:MET:HE1	1:A:1461:LEU:O	2.12	0.50
2:B:55:THR:HB	2:B:104:LEU:HD22	1.94	0.50
1:A:421:LYS:HE2	1:A:1516:MET:HE2	1.94	0.50
1:A:252:ASP:OD2	1:A:1467:GLY:C	2.51	0.49
1:A:236:LEU:HD11	1:A:705:LEU:HD13	1.94	0.49
1:A:169:THR:HG21	1:A:205:TYR:OH	2.12	0.49
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.44	0.49
1:A:1477:MET:CE	1:A:1477:MET:HA	2.42	0.49
1:A:252:ASP:OD2	1:A:1467:GLY:HA3	2.13	0.49
1:A:446:VAL:HG11	1:A:794:LEU:HD13	1.95	0.48
1:A:683:TRP:HD1	1:A:686:LEU:HB2	1.78	0.48
1:A:1058:ARG:HD3	1:A:1061:ILE:HD12	1.95	0.48
1:A:281:VAL:O	1:A:374:GLU:N	2.45	0.48
1:A:1030:HIS:HE1	1:A:1032:TRP:HD1	1.61	0.48
1:A:1475:LEU:HD22	1:A:1475:LEU:C	2.33	0.48
1:A:1034:GLU:OE1	1:A:1142:ARG:NH1	2.46	0.47
1:A:1191:ASN:HD21	4:E:1:NAG:H62	1.79	0.47
1:A:1451:ARG:HH21	1:A:1454:ARG:HH11	1.62	0.47
2:B:76:GLU:O	2:B:78:LEU:N	2.47	0.47
1:A:794:LEU:HD22	1:A:794:LEU:C	2.34	0.47
1:A:1499:PHE:O	1:A:1503:ASN:ND2	2.47	0.47
1:A:1096:ALA:HA	1:A:1099:TRP:HB2	1.97	0.47
1:A:1059:ARG:NH1	2:B:27:GLU:OE2	2.43	0.47
1:A:1370:MET:HG2	1:A:1454:ARG:HH22	1.80	0.47
1:A:1391:ILE:HA	1:A:1394:ILE:HD12	1.96	0.47
1:A:254:MET:HA	1:A:257:THR:HG22	1.97	0.46
1:A:269:LEU:CD2	1:A:390:ASP:HA	2.45	0.46
1:A:1449:VAL:HA	1:A:1452:LEU:HD13	1.97	0.46
1:A:1475:LEU:HD22	1:A:1475:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.98	0.46
1:A:1191:ASN:ND2	4:E:1:NAG:O5	2.48	0.46
1:A:1185:LYS:HB3	1:A:1256:SER:HB2	1.96	0.46
1:A:1377:GLN:HB2	1:A:1381:LYS:HD3	1.98	0.46
1:A:342:ILE:CG2	1:A:378:THR:OG1	2.63	0.45
1:A:447:ALA:HA	1:A:798:LEU:CD1	2.46	0.45
1:A:351:LEU:HG	1:A:358:LEU:HD12	1.98	0.45
1:A:1016:LYS:CA	1:A:1019:THR:HG22	2.45	0.45
1:A:1306:GLY:O	1:A:1308:LYS:HE2	2.17	0.45
2:B:55:THR:OG1	2:B:56:GLU:N	2.49	0.45
1:A:1016:LYS:HA	1:A:1019:THR:CG2	2.45	0.45
1:A:1475:LEU:C	1:A:1475:LEU:CD2	2.86	0.45
1:A:1271:MET:O	1:A:1274:TYR:N	2.42	0.45
1:A:1020:LEU:C	1:A:1020:LEU:CD2	2.86	0.45
1:A:1156:ALA:HA	1:A:1297:ASN:HD21	1.82	0.45
1:A:1271:MET:C	1:A:1273:LEU:N	2.71	0.45
1:A:1519:PHE:HA	1:A:1525:SER:HB3	1.99	0.45
1:A:252:ASP:OD2	1:A:1467:GLY:CA	2.66	0.44
1:A:800:LEU:HB2	1:A:1288:ASN:OD1	2.17	0.44
1:A:1463:ARG:C	1:A:1463:ARG:CD	2.85	0.44
1:A:212:LEU:C	1:A:212:LEU:CD1	2.86	0.44
1:A:384:TYR:HB2	1:A:386:TYR:CE2	2.53	0.44
1:A:421:LYS:NZ	1:A:1524:ASN:HD21	2.16	0.44
2:B:54:PHE:HB2	2:B:74:GLU:HA	2.00	0.44
1:A:1034:GLU:OE2	1:A:1142:ARG:HD2	2.18	0.44
1:A:1289:LEU:HD22	1:A:1289:LEU:O	2.17	0.44
1:A:1308:LYS:HE2	1:A:1308:LYS:N	2.33	0.44
1:A:1556:ASN:OD1	1:A:1556:ASN:N	2.50	0.44
1:A:1304:LYS:C	1:A:1304:LYS:CD	2.85	0.44
1:A:1304:LYS:HE3	1:A:1305:LEU:CD2	2.48	0.43
1:A:371:GLU:H	1:A:371:GLU:CD	2.22	0.43
1:A:272:PHE:HA	1:A:275:ASN:HD22	1.83	0.43
1:A:384:TYR:HB2	1:A:386:TYR:CD2	2.54	0.43
1:A:161:GLU:HG3	1:A:222:ARG:NH2	2.33	0.43
1:A:1044:SER:HB3	1:A:1135:ARG:NH1	2.34	0.43
1:A:725:SER:HA	1:A:728:GLU:HG2	2.00	0.43
1:A:1021:ARG:CG	1:A:1085:VAL:O	2.67	0.43
1:A:1477:MET:HA	1:A:1477:MET:HE2	2.00	0.43
1:A:1347:TYR:HB3	1:A:1406:ALA:HB1	2.01	0.43
1:A:1451:ARG:NH2	1:A:1454:ARG:HH11	2.16	0.42
2:B:121:CYS:SG	2:B:140:LYS:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HA	1:A:373:TYR:HA	2.01	0.42
1:A:269:LEU:O	1:A:273:MET:HB2	2.19	0.42
1:A:119:VAL:HB	1:A:122:ARG:HD3	2.00	0.42
1:A:1532:ILE:HG21	1:A:1532:ILE:HD13	1.85	0.42
1:A:1265:TYR:CD2	1:A:1266:GLU:HG2	2.54	0.42
1:A:1018:TRP:NE1	1:A:1022:ARG:HD2	2.34	0.42
1:A:277:ARG:CG	1:A:381:ASN:OD1	2.68	0.41
1:A:161:GLU:HG3	1:A:222:ARG:HH22	1.86	0.41
1:A:1304:LYS:HB3	1:A:1304:LYS:HZ3	1.84	0.41
1:A:1590:VAL:HA	1:A:1593:TYR:HD2	1.85	0.41
2:B:38:ILE:HB	2:B:106:ILE:HG22	2.02	0.41
1:A:705:LEU:HA	1:A:705:LEU:HD23	1.80	0.41
1:A:1271:MET:O	1:A:1272:TYR:C	2.59	0.41
1:A:209:PHE:O	1:A:210:VAL:CB	2.69	0.41
1:A:209:PHE:HD1	1:A:209:PHE:HA	1.75	0.41
1:A:726:TYR:HA	1:A:772:VAL:HG11	2.01	0.41
1:A:1510:GLU:HB3	1:A:1511:SER:H	1.70	0.41
2:B:101:LEU:O	2:B:102:GLN:CB	2.68	0.41
2:B:174:LEU:O	2:B:178:MET:N	2.46	0.41
1:A:210:VAL:HG12	1:A:211:ASP:N	2.35	0.41
1:A:270:GLN:O	1:A:1448:ARG:NH1	2.53	0.40
1:A:1335:ILE:HG21	1:A:1410:TYR:CD1	2.56	0.40
1:A:1402:LEU:HD23	1:A:1402:LEU:HA	1.95	0.40
1:A:1255:ASP:HB3	1:A:1263:PRO:HB3	2.02	0.40
2:B:53:THR:HG22	2:B:125:ARG:HA	2.03	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	1130/1879 (60%)	1067 (94%)	58 (5%)	5 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	171/218 (78%)	149 (87%)	20 (12%)	2 (1%)	13 49
All	All	1301/2097 (62%)	1216 (94%)	78 (6%)	7 (0%)	32 67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	VAL
1	A	392	PHE
1	A	1556	ASN
2	B	76	GLU
1	A	381	ASN
1	A	1272	TYR
2	B	77	VAL

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	1009/1637 (62%)	958 (95%)	51 (5%)	24 60
2	B	157/190 (83%)	154 (98%)	3 (2%)	57 81
All	All	1166/1827 (64%)	1112 (95%)	54 (5%)	31 63

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	MET
1	A	209	PHE
1	A	211	ASP
1	A	214	ASN
1	A	249	LYS
1	A	252	ASP
1	A	269	LEU
1	A	362	ASN
1	A	368	HIS

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Mol	Chain	Res	Type
1	A	369	CYS
1	A	375	CYS
1	A	381	ASN
1	A	388	SER
1	A	433	LEU
1	A	591	ASN
1	A	687	ASN
1	A	705	LEU
1	A	707	LEU
1	A	769	CYS
1	A	794	LEU
1	A	795	ASN
1	A	796	LEU
1	A	798	LEU
1	A	1020	LEU
1	A	1021	ARG
1	A	1031	ASN
1	A	1115	ASN
1	A	1268	ASN
1	A	1269	LEU
1	A	1287	LEU
1	A	1288	ASN
1	A	1289	LEU
1	A	1303	LYS
1	A	1304	LYS
1	A	1329	LYS
1	A	1330	LYS
1	A	1366	ASN
1	A	1463	ARG
1	A	1466	LYS
1	A	1472	LEU
1	A	1475	LEU
1	A	1477	MET
1	A	1479	LEU
1	A	1488	LEU
1	A	1489	LEU
1	A	1552	ASP
1	A	1556	ASN
1	A	1557	LEU
1	A	1570	ASN
1	A	1582	ILE
1	A	1583	ILE

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Mol	Chain	Res	Type
2	B	101	LEU
2	B	104	LEU
2	B	135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	275	ASN
1	A	278	GLN
1	A	381	ASN
1	A	687	ASN
1	A	743	HIS
1	A	1031	ASN
1	A	1095	ASN
1	A	1115	ASN
1	A	1297	ASN
1	A	1299	ASN
1	A	1524	ASN
1	A	1570	ASN
1	A	1591	ASN
2	B	135	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

7 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	0.58	0	17,19,21	0.61	0
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	1.29	2 (11%)
3	BMA	C	3	3	11,11,12	1.51	2 (18%)	15,15,17	2.21	5 (33%)
4	NAG	D	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	0.73	1 (5%)
4	NAG	D	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.63	0
4	NAG	E	1	4	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	E	2	4	14,14,15	0.36	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	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	3.51	1.60	1.52
3	C	3	BMA	C2-C3	2.29	1.55	1.52
4	D	1	NAG	O5-C1	-2.27	1.40	1.43
4	D	2	NAG	C1-C2	2.19	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	BMA	C1-O5-C5	4.88	118.81	112.19
3	C	3	BMA	C1-C2-C3	4.72	115.47	109.67
3	C	2	NAG	C1-O5-C5	3.74	117.26	112.19
3	C	3	BMA	O5-C1-C2	3.00	115.40	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	O4-C4-C3	2.23	115.50	110.35
3	C	3	BMA	O2-C2-C3	-2.21	105.70	110.14
3	C	3	BMA	C2-C3-C4	2.06	114.46	110.89
4	D	1	NAG	O4-C4-C3	-2.05	105.62	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

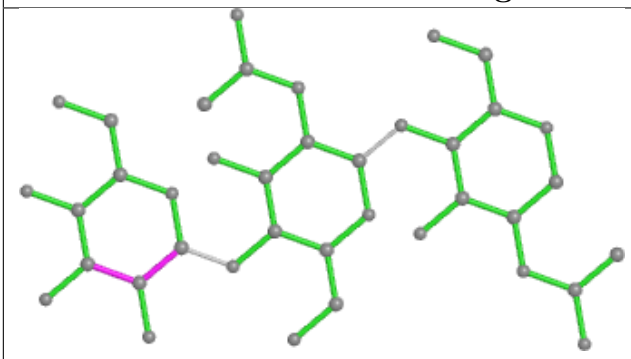
There are no ring outliers.

1 monomer is involved in 2 short contacts:

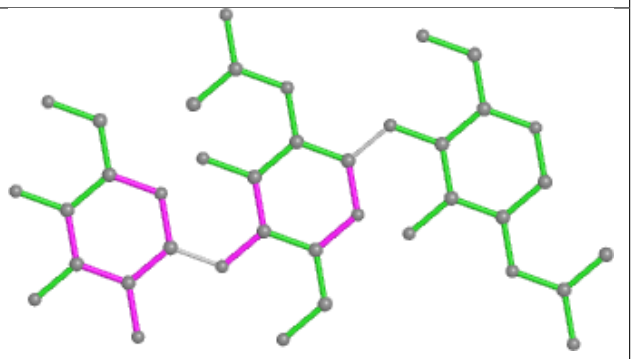
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0

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

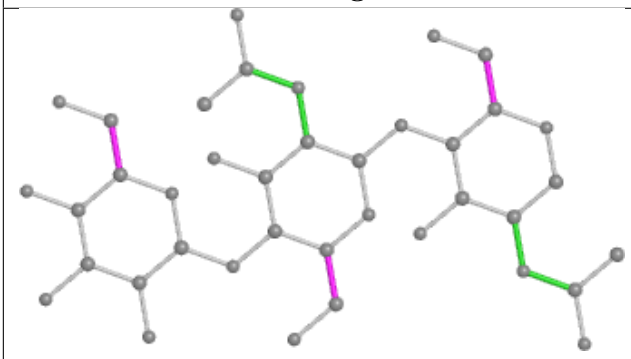
Oligosaccharide Chain C



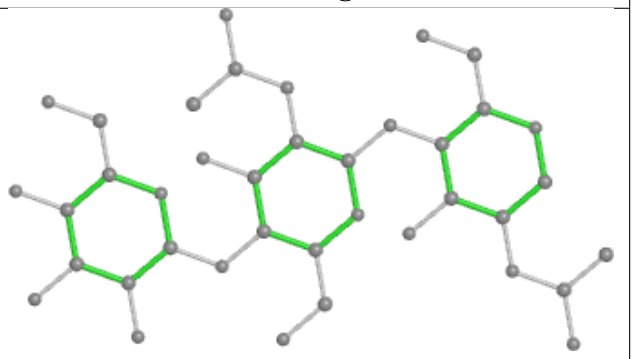
Bond lengths



Bond angles

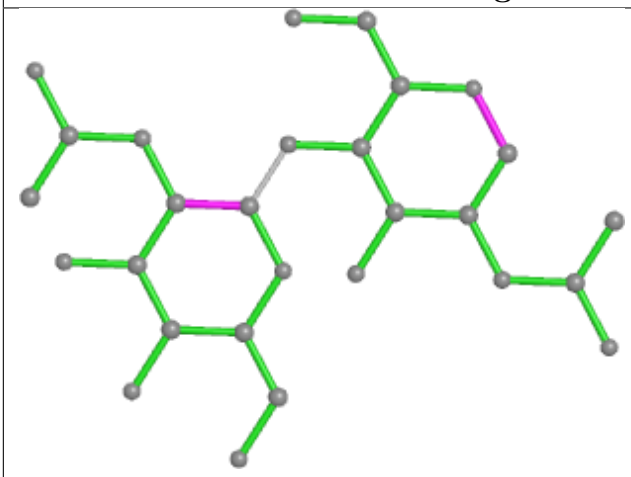


Torsions

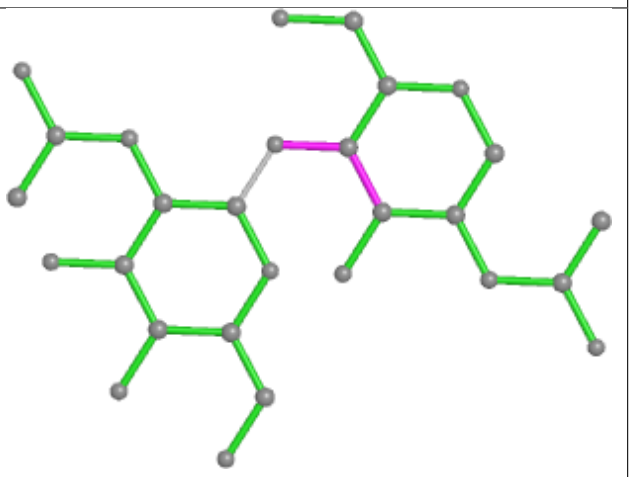


Rings

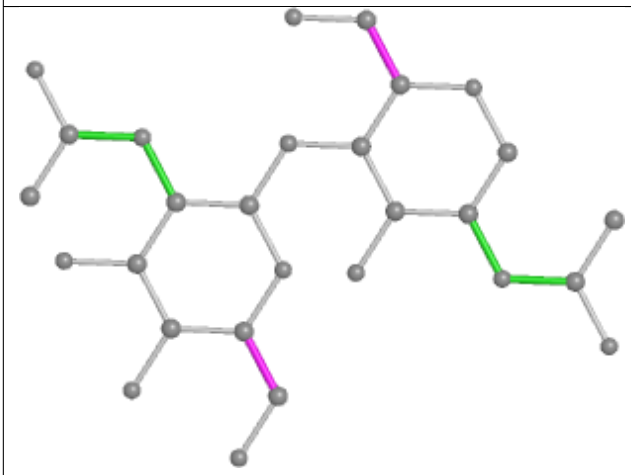
Oligosaccharide Chain D



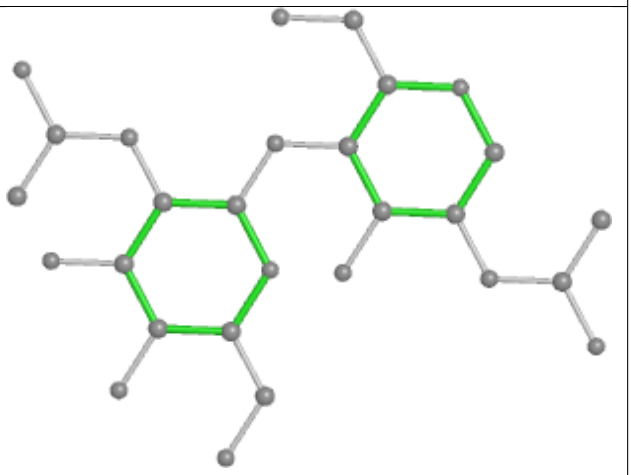
Bond lengths



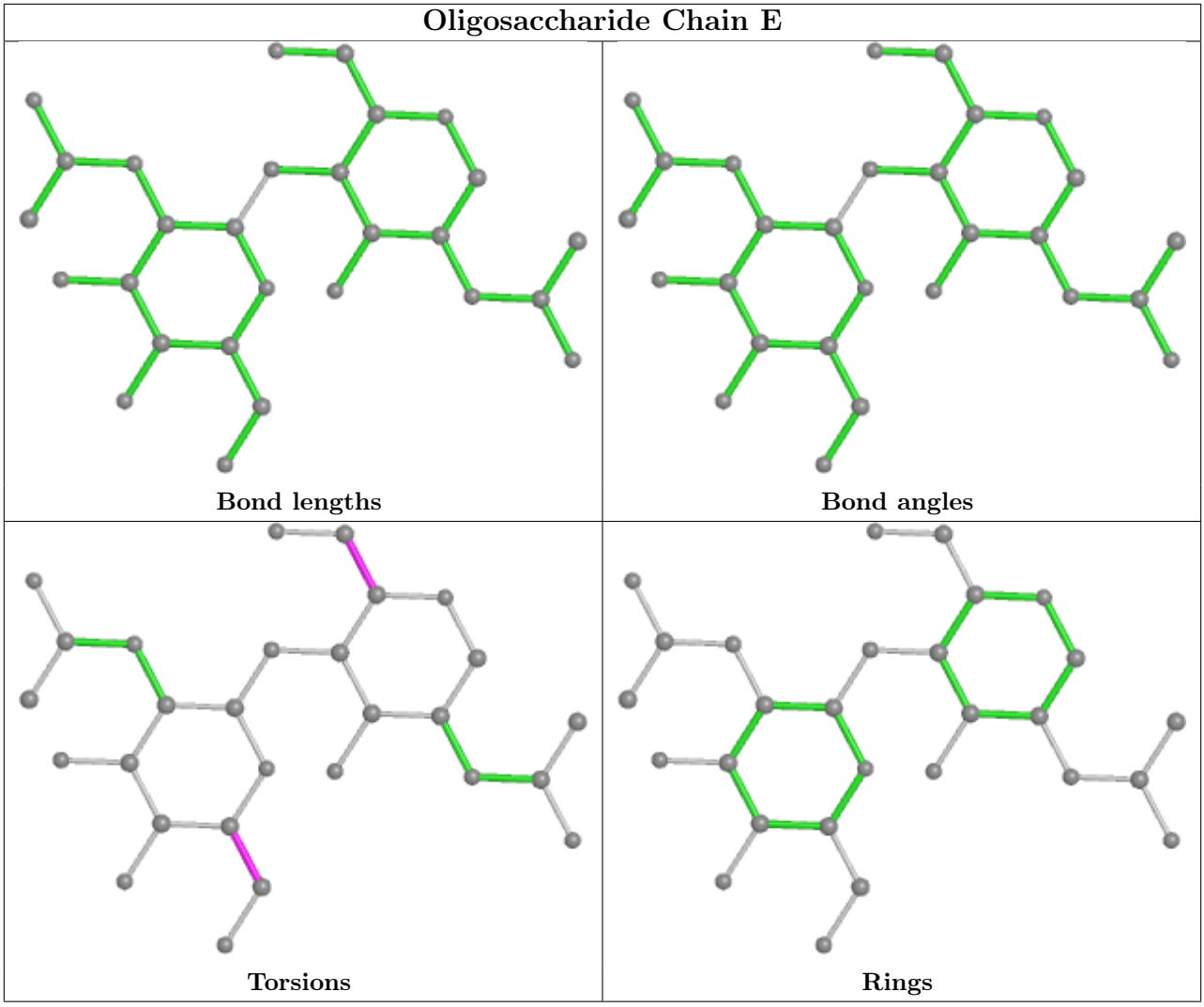
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	6OU	A	1911	-	28,28,48	1.46	6 (21%)	31,33,53	1.32	3 (9%)
6	9Z9	A	1914	-	44,44,44	0.62	1 (2%)	66,68,68	1.03	4 (6%)
5	6OU	A	1913	-	42,42,48	1.26	5 (11%)	45,47,53	1.15	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	6OU	A	1909	-	44,44,48	1.27	5 (11%)	47,49,53	1.25	3 (6%)
5	6OU	A	1908	-	40,40,48	1.30	3 (7%)	43,45,53	1.26	4 (9%)
7	NAG	B	302	2	14,14,15	0.30	0	17,19,21	0.42	0
5	6OU	A	1910	-	44,44,48	1.21	4 (9%)	47,49,53	1.18	3 (6%)
7	NAG	B	301	2	14,14,15	0.53	0	17,19,21	0.68	1 (5%)
5	6OU	A	1912	-	35,35,48	1.37	4 (11%)	38,40,53	1.16	3 (7%)

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
5	6OU	A	1911	-	-	9/32/32/52	-
6	9Z9	A	1914	-	-	8/12/100/100	0/6/6/6
5	6OU	A	1913	-	-	17/46/46/52	-
5	6OU	A	1909	-	-	23/48/48/52	-
5	6OU	A	1908	-	-	22/44/44/52	-
7	NAG	B	302	2	-	2/6/23/26	0/1/1/1
5	6OU	A	1910	-	-	24/48/48/52	-
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
5	6OU	A	1912	-	-	21/39/39/52	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1912	6OU	O18-C16	3.49	1.43	1.33
5	A	1913	6OU	O18-C16	3.33	1.43	1.33
5	A	1910	6OU	O18-C16	3.30	1.43	1.33
5	A	1909	6OU	O18-C16	3.23	1.42	1.33
5	A	1911	6OU	O18-C16	3.21	1.42	1.33
5	A	1908	6OU	O30-C31	3.12	1.43	1.34
5	A	1912	6OU	O30-C31	3.11	1.43	1.34
5	A	1908	6OU	O18-C16	3.04	1.42	1.33
5	A	1909	6OU	O30-C31	2.92	1.42	1.34
5	A	1913	6OU	O30-C31	2.85	1.42	1.34
5	A	1911	6OU	O30-C31	2.72	1.42	1.34
5	A	1910	6OU	O30-C20	-2.67	1.39	1.46
5	A	1910	6OU	O30-C31	2.52	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1913	6OU	O30-C20	-2.50	1.40	1.46
5	A	1908	6OU	O30-C20	-2.46	1.40	1.46
5	A	1913	6OU	P23-O22	2.41	1.69	1.59
5	A	1911	6OU	O30-C20	-2.35	1.40	1.46
5	A	1912	6OU	P23-O22	2.34	1.68	1.59
5	A	1909	6OU	O30-C20	-2.28	1.40	1.46
5	A	1911	6OU	P23-O22	2.23	1.68	1.59
5	A	1909	6OU	P23-O22	2.19	1.68	1.59
5	A	1909	6OU	P23-O26	2.15	1.68	1.59
5	A	1910	6OU	P23-O22	2.14	1.68	1.59
5	A	1911	6OU	P23-O26	2.13	1.67	1.59
5	A	1912	6OU	P23-O26	2.08	1.67	1.59
5	A	1913	6OU	P23-O26	2.06	1.67	1.59
6	A	1914	9Z9	O80-C79	-2.05	1.40	1.43
5	A	1911	6OU	P23-O25	-2.00	1.45	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1914	9Z9	O80-C73-C76	4.60	115.05	110.77
5	A	1909	6OU	O30-C31-C33	4.52	121.23	111.50
5	A	1908	6OU	O30-C31-C33	4.26	120.69	111.50
5	A	1911	6OU	O30-C31-C33	3.99	120.11	111.50
5	A	1910	6OU	O30-C31-C33	3.86	119.82	111.50
5	A	1912	6OU	O30-C31-C33	3.76	119.61	111.50
5	A	1913	6OU	O30-C31-C33	3.74	119.57	111.50
5	A	1909	6OU	O18-C16-C15	3.18	121.88	111.91
6	A	1914	9Z9	C77-C78-C79	3.08	112.84	108.56
5	A	1908	6OU	O18-C16-C15	2.86	120.89	111.91
5	A	1910	6OU	O18-C16-C15	2.75	120.54	111.91
5	A	1911	6OU	O25-P23-O24	-2.70	98.87	112.24
5	A	1913	6OU	O18-C16-C15	2.62	120.12	111.91
5	A	1909	6OU	O25-P23-O24	-2.59	99.41	112.24
5	A	1913	6OU	O25-P23-O24	-2.57	99.51	112.24
5	A	1908	6OU	C21-C20-C19	-2.51	105.86	111.79
5	A	1911	6OU	O18-C16-C15	2.49	119.72	111.91
5	A	1912	6OU	O18-C16-C15	2.43	119.53	111.91
6	A	1914	9Z9	C79-O80-C73	2.38	118.23	113.72
5	A	1912	6OU	O25-P23-O24	-2.26	101.08	112.24
5	A	1908	6OU	O25-P23-O24	-2.23	101.22	112.24
5	A	1910	6OU	O25-P23-O24	-2.22	101.28	112.24
7	B	301	NAG	C1-O5-C5	2.17	115.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1914	9Z9	O80-C73-O72	-2.02	104.14	109.78

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1908	6OU	C21-O22-P23-O24
5	A	1908	6OU	C21-O22-P23-O25
5	A	1908	6OU	C33-C31-O30-C20
5	A	1909	6OU	O30-C20-C21-O22
5	A	1909	6OU	C27-O26-P23-O24
5	A	1909	6OU	C27-O26-P23-O25
5	A	1909	6OU	O26-C27-C28-N29
5	A	1910	6OU	C21-O22-P23-O24
5	A	1910	6OU	C21-O22-P23-O26
5	A	1910	6OU	O32-C31-O30-C20
5	A	1910	6OU	C33-C31-O30-C20
5	A	1911	6OU	O26-C27-C28-N29
5	A	1911	6OU	C33-C31-O30-C20
5	A	1912	6OU	C21-O22-P23-O24
5	A	1912	6OU	C21-O22-P23-O26
5	A	1912	6OU	C27-O26-P23-O24
5	A	1912	6OU	C27-O26-P23-O25
5	A	1913	6OU	C33-C31-O30-C20
6	A	1914	9Z9	C22-C21-O20-C17
6	A	1914	9Z9	C48-C23-C24-O25
6	A	1914	9Z9	C24-C23-C48-O49
5	A	1910	6OU	O17-C16-O18-C19
5	A	1910	6OU	C15-C16-O18-C19
5	A	1908	6OU	O32-C31-O30-C20
5	A	1912	6OU	O32-C31-O30-C20
5	A	1913	6OU	O32-C31-O30-C20
5	A	1912	6OU	C15-C16-O18-C19
5	A	1911	6OU	O32-C31-O30-C20
5	A	1912	6OU	O17-C16-O18-C19
7	B	302	NAG	C4-C5-C6-O6
5	A	1912	6OU	C33-C31-O30-C20
7	B	302	NAG	O5-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
5	A	1909	6OU	C03-C04-C05-C06
5	A	1913	6OU	C31-C33-C34-C35
7	B	301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1908	6OU	C21-O22-P23-O26
5	A	1909	6OU	C21-O22-P23-O26
5	A	1909	6OU	C27-O26-P23-O22
5	A	1912	6OU	C27-O26-P23-O22
5	A	1909	6OU	C15-C16-O18-C19
5	A	1910	6OU	C02-C03-C04-C05
5	A	1909	6OU	C33-C31-O30-C20
5	A	1913	6OU	C08-C09-C10-C11
5	A	1909	6OU	O32-C31-O30-C20
5	A	1910	6OU	C20-C21-O22-P23
5	A	1913	6OU	C11-C12-C13-C14
5	A	1913	6OU	C33-C34-C35-C36
5	A	1912	6OU	C13-C14-C15-C16
5	A	1908	6OU	C08-C09-C10-C11
5	A	1909	6OU	C34-C35-C36-C37
5	A	1913	6OU	C04-C05-C06-C07
5	A	1913	6OU	C06-C07-C08-C09
5	A	1909	6OU	O17-C16-O18-C19
5	A	1913	6OU	C15-C16-O18-C19
5	A	1908	6OU	C33-C34-C35-C36
5	A	1909	6OU	C06-C07-C08-C09
6	A	1914	9Z9	C21-C22-C23-C24
5	A	1912	6OU	C11-C12-C13-C14
5	A	1910	6OU	C03-C04-C05-C06
5	A	1909	6OU	C33-C34-C35-C36
6	A	1914	9Z9	O20-C21-C22-C23
5	A	1910	6OU	C13-C14-C15-C16
5	A	1908	6OU	C12-C13-C14-C15
6	A	1914	9Z9	C22-C23-C24-O25
6	A	1914	9Z9	C22-C23-C48-O49
5	A	1913	6OU	O17-C16-O18-C19
5	A	1910	6OU	C31-C33-C34-C35
5	A	1910	6OU	C12-C13-C14-C15
5	A	1910	6OU	C05-C06-C07-C08
5	A	1910	6OU	C36-C37-C38-C39
5	A	1910	6OU	C06-C07-C08-C09
5	A	1912	6OU	C10-C11-C12-C13
5	A	1909	6OU	C19-C20-C21-O22
5	A	1910	6OU	C09-C10-C11-C12
5	A	1912	6OU	C12-C13-C14-C15
5	A	1908	6OU	O18-C19-C20-C21
5	A	1911	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	A	1910	6OU	C33-C34-C35-C36
5	A	1908	6OU	C15-C16-O18-C19
5	A	1912	6OU	C19-C20-O30-C31
5	A	1909	6OU	C08-C09-C10-C11
5	A	1910	6OU	C35-C36-C37-C38
5	A	1908	6OU	O18-C19-C20-O30
5	A	1908	6OU	C04-C05-C06-C07
5	A	1912	6OU	C31-C33-C34-C35
5	A	1913	6OU	C40-C41-C42-C43
5	A	1908	6OU	C19-C20-C21-O22
5	A	1913	6OU	C19-C20-C21-O22
5	A	1911	6OU	C20-C21-O22-P23
6	A	1914	9Z9	C23-C24-O25-C26
5	A	1908	6OU	O17-C16-O18-C19
5	A	1908	6OU	O30-C20-C21-O22
5	A	1913	6OU	C09-C10-C11-C12
5	A	1909	6OU	C20-C19-O18-C16
5	A	1912	6OU	O18-C19-C20-C21
5	A	1913	6OU	O30-C20-C21-O22
5	A	1908	6OU	C27-O26-P23-O22
5	A	1908	6OU	C27-O26-P23-O24
5	A	1909	6OU	C21-O22-P23-O24
5	A	1908	6OU	C34-C35-C36-C37
5	A	1909	6OU	C28-C27-O26-P23
5	A	1912	6OU	O18-C19-C20-O30
5	A	1908	6OU	C36-C37-C38-C39
5	A	1913	6OU	C12-C13-C14-C15
5	A	1910	6OU	C34-C35-C36-C37
5	A	1911	6OU	C21-O22-P23-O26
5	A	1908	6OU	C10-C11-C12-C13
5	A	1909	6OU	C38-C39-C40-C41
5	A	1910	6OU	O18-C19-C20-O30
5	A	1912	6OU	C14-C15-C16-O18
5	A	1909	6OU	C40-C41-C42-C43
5	A	1910	6OU	O18-C19-C20-C21
5	A	1912	6OU	C36-C37-C38-C39
5	A	1910	6OU	C40-C41-C42-C43
5	A	1908	6OU	C38-C39-C40-C41
5	A	1913	6OU	C38-C39-C40-C41
5	A	1909	6OU	C02-C03-C04-C05
5	A	1912	6OU	C14-C15-C16-O17
5	A	1910	6OU	C10-C11-C12-C13

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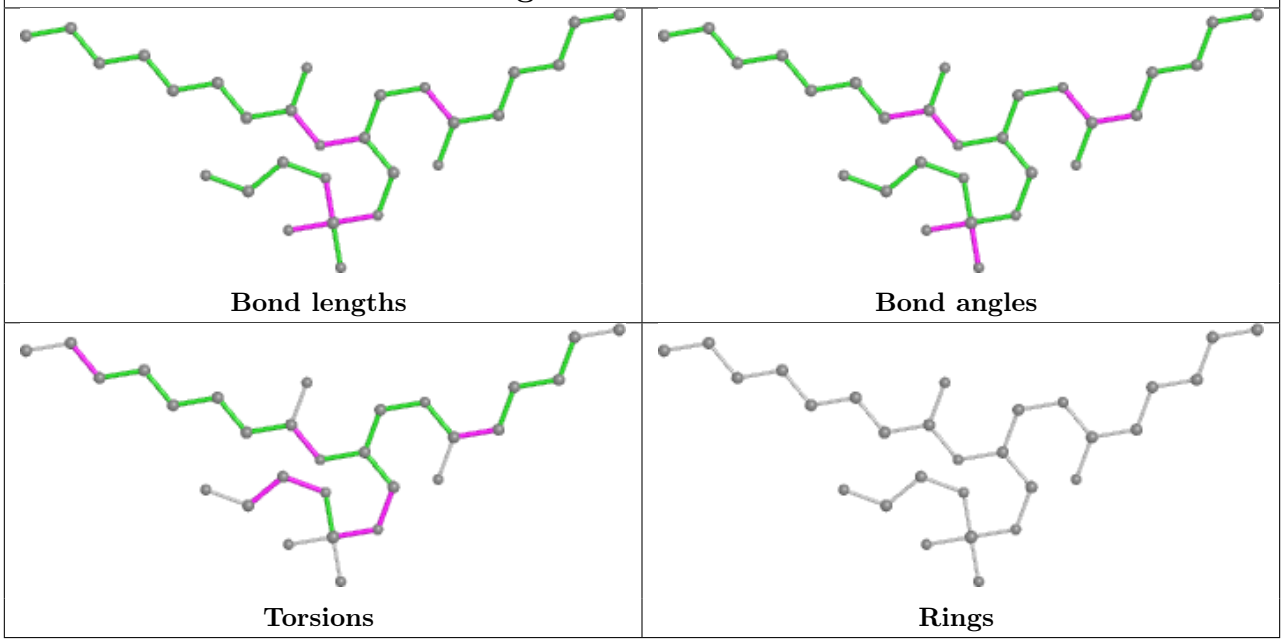
Mol	Chain	Res	Type	Atoms
5	A	1913	6OU	C27-O26-P23-O25
5	A	1908	6OU	O26-C27-C28-N29
5	A	1910	6OU	O26-C27-C28-N29
5	A	1912	6OU	C08-C09-C10-C11
5	A	1911	6OU	C28-C27-O26-P23
5	A	1911	6OU	C14-C15-C16-O18
5	A	1909	6OU	C35-C36-C37-C38
5	A	1911	6OU	C14-C15-C16-O17

There are no ring outliers.

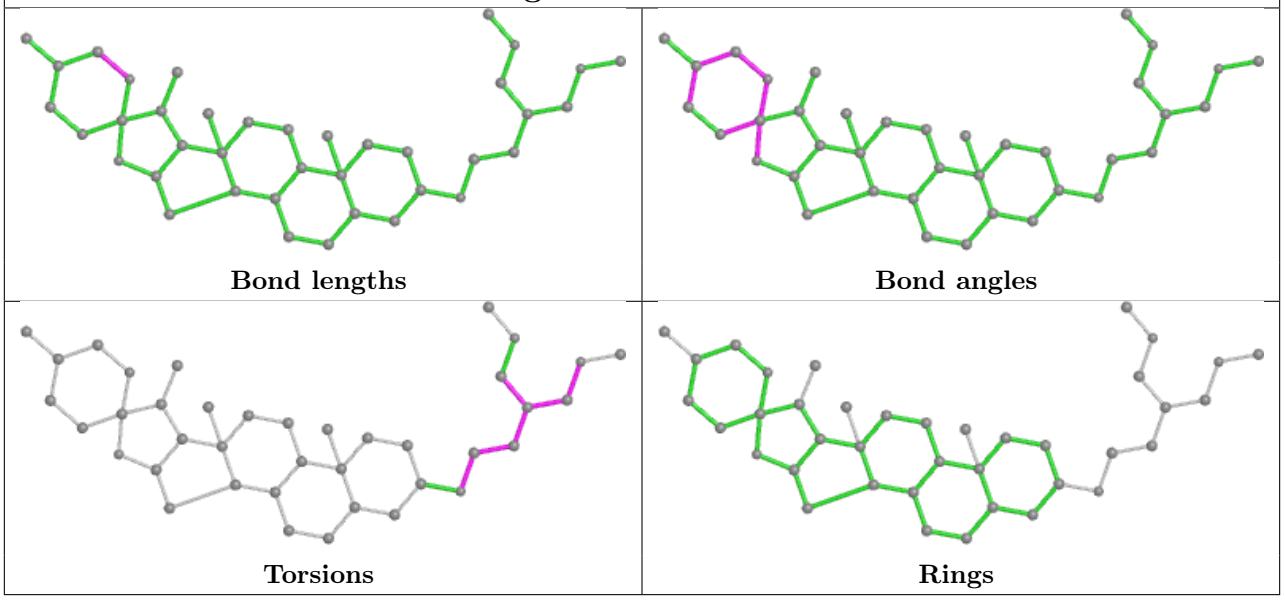
No monomer is involved in short contacts.

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

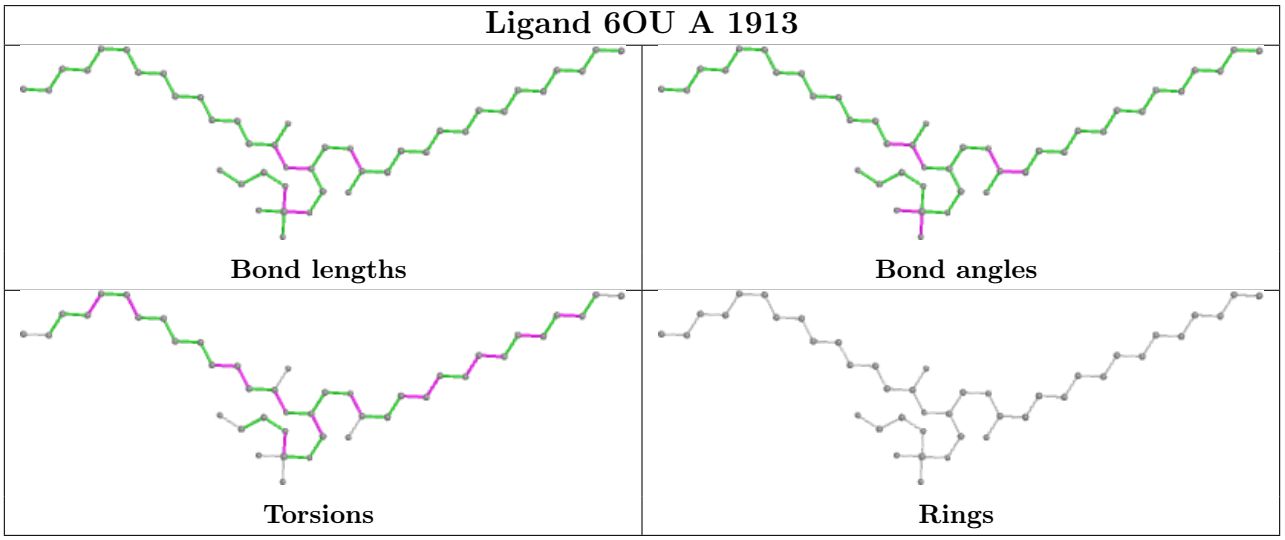
Ligand 6OU A 1911



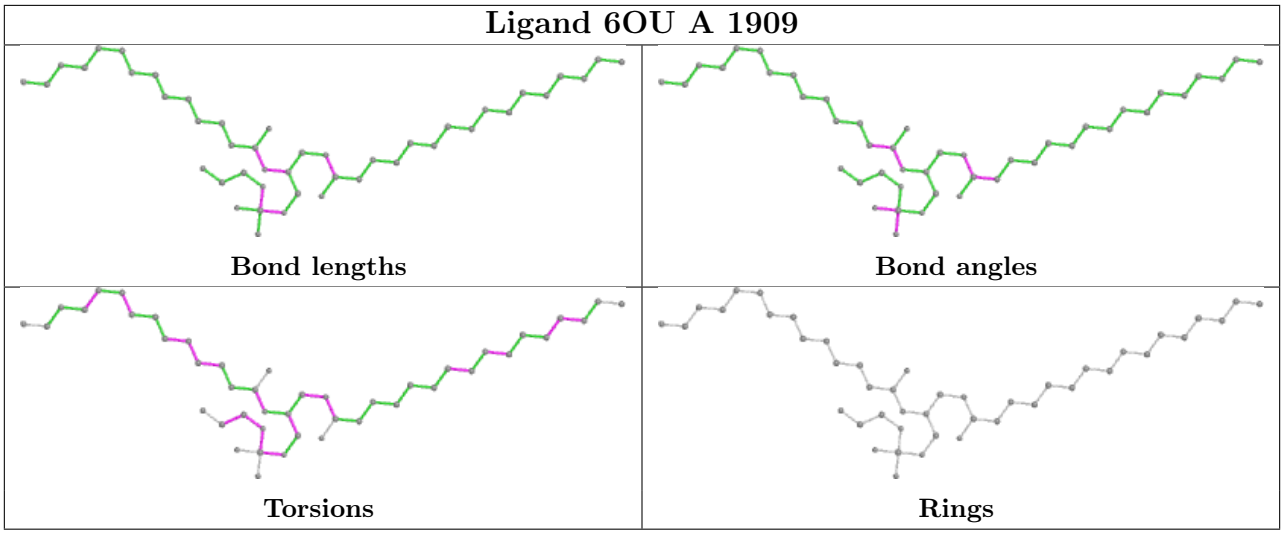
Ligand 9Z9 A 1914



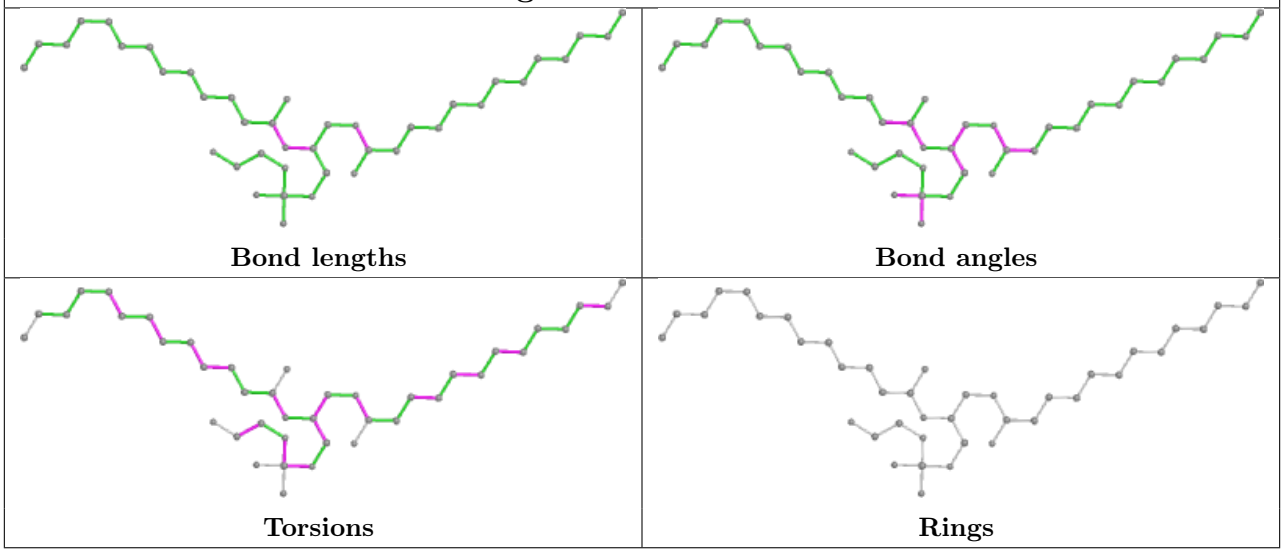
Ligand 6OU A 1913



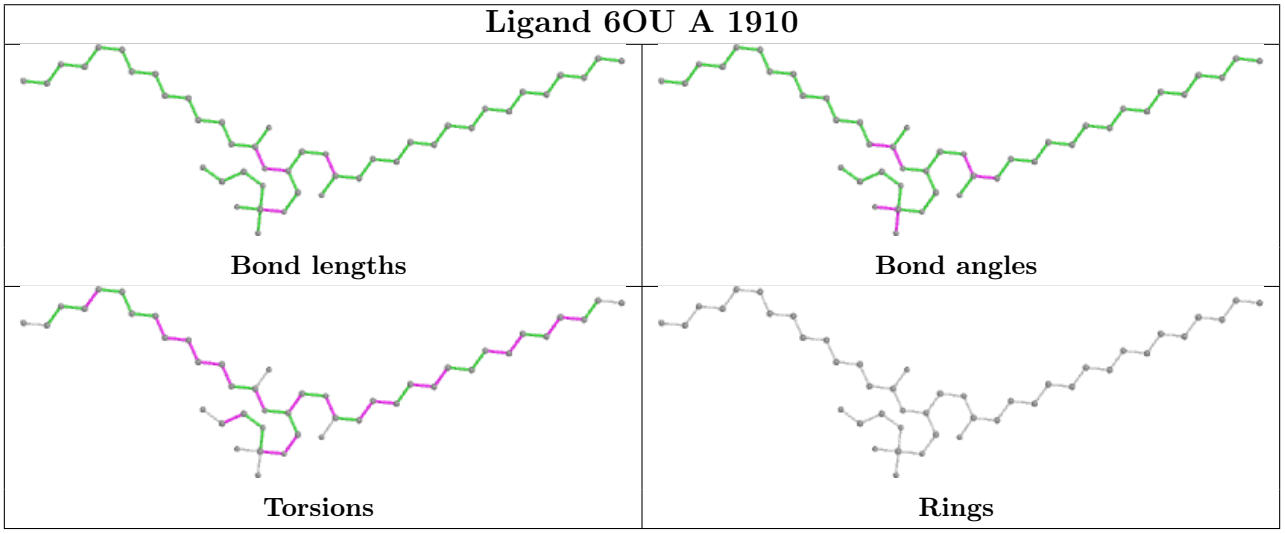
Ligand 6OU A 1909



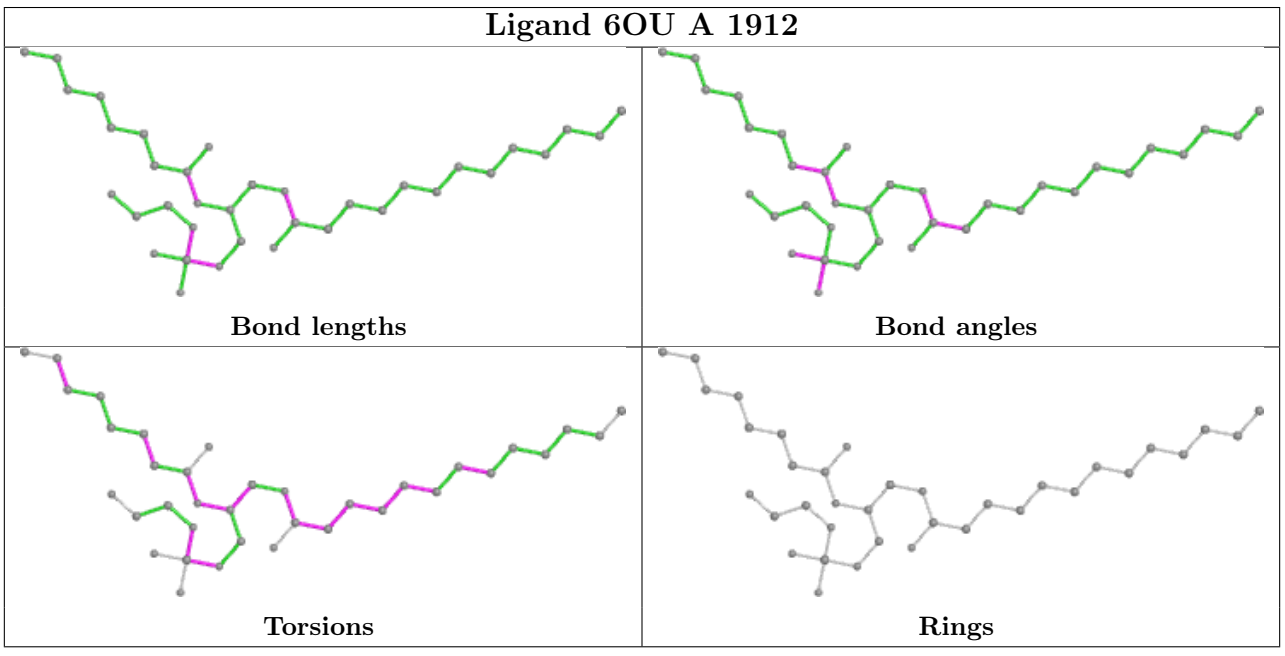
Ligand 6OU A 1908



Ligand 6OU A 1910



Ligand 6OU A 1912



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.

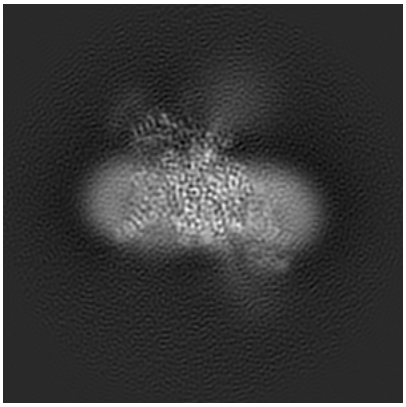
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9617. These allow visual inspection of the internal detail of the map and identification of artifacts.

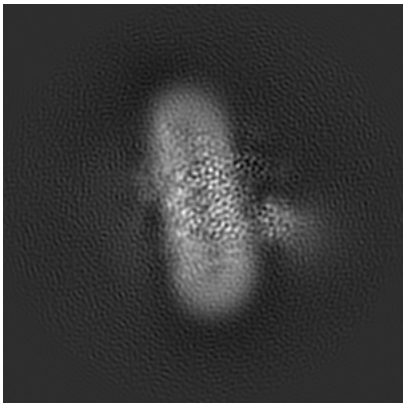
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

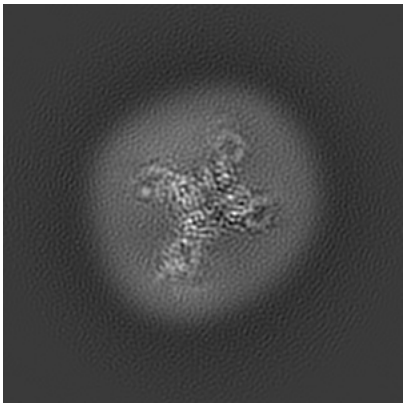
6.1.1 Primary map



X



Y

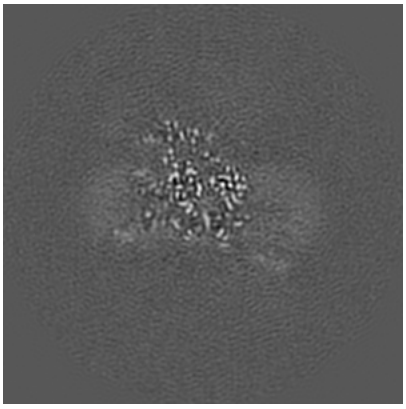


Z

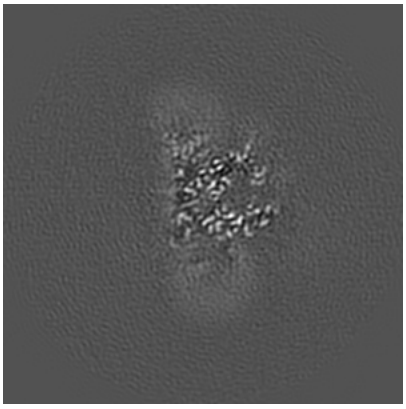
The images above show the map projected in three orthogonal directions.

6.2 Central slices

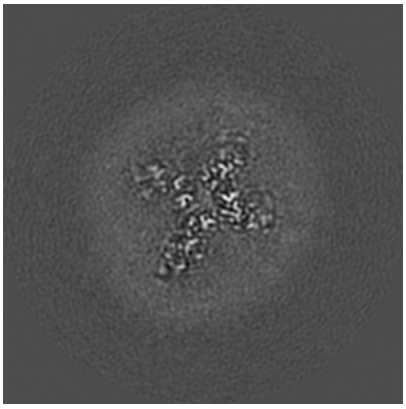
6.2.1 Primary map



X Index: 120



Y Index: 120

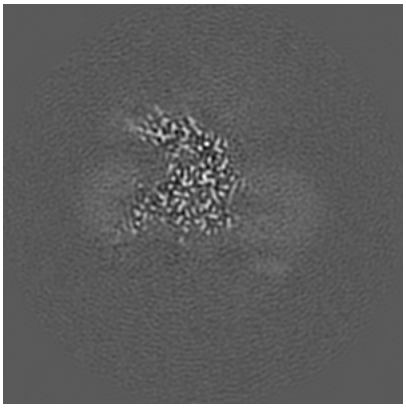


Z Index: 120

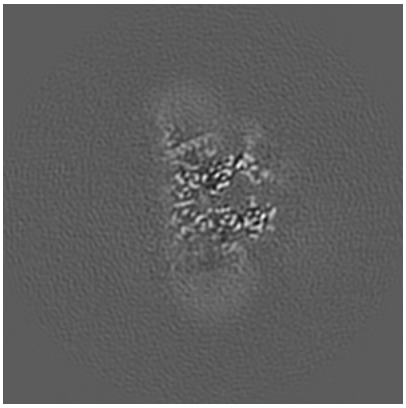
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

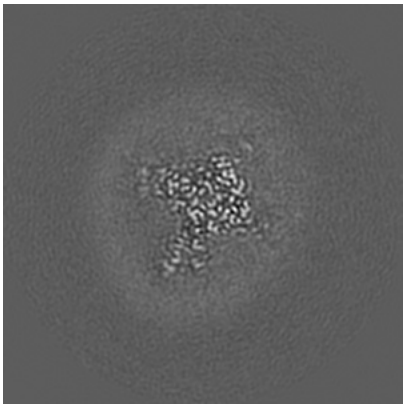
6.3.1 Primary map



X Index: 112



Y Index: 122



Z Index: 128

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.

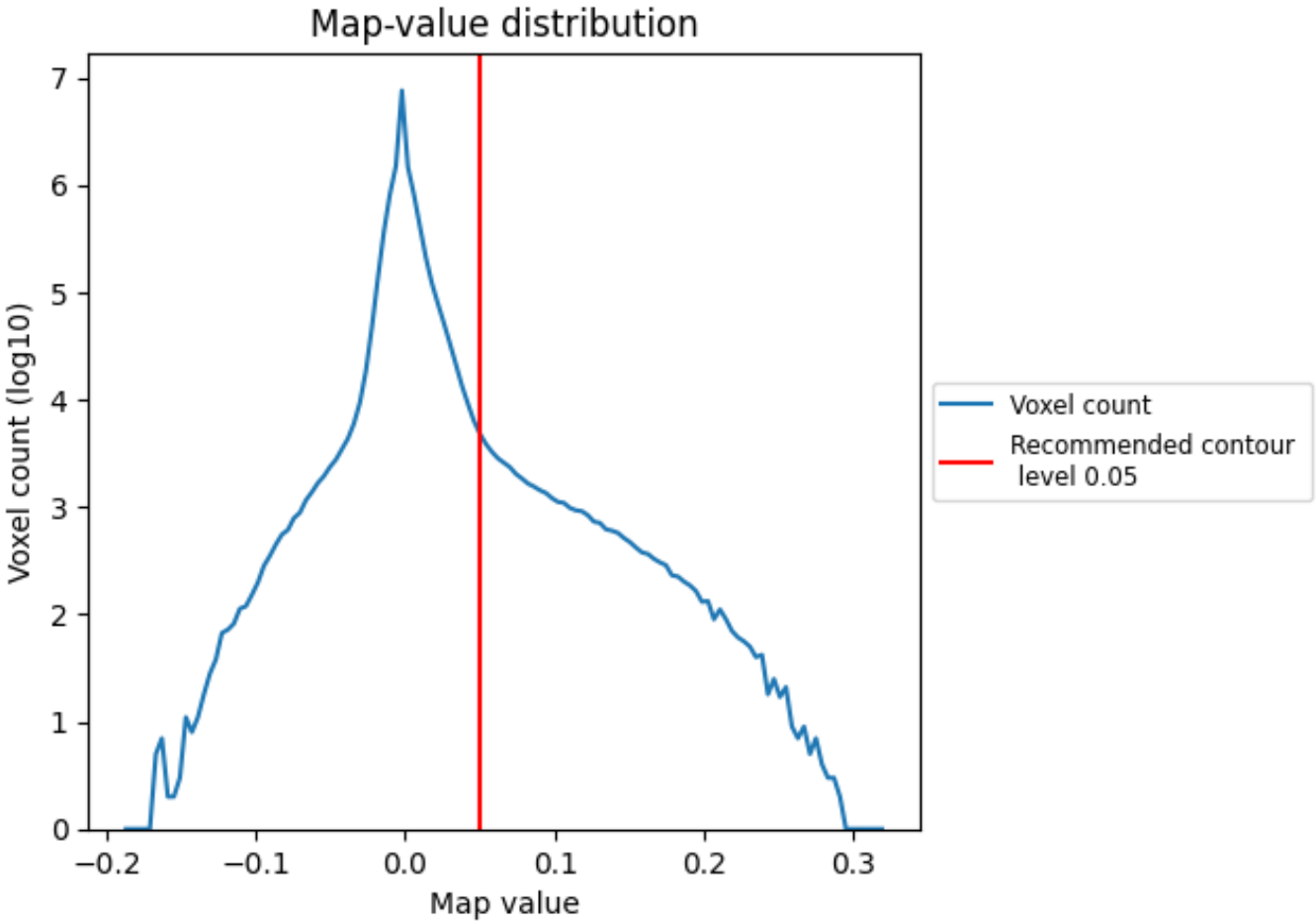
6.5 Mask visualisation (i)

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

7 Map analysis

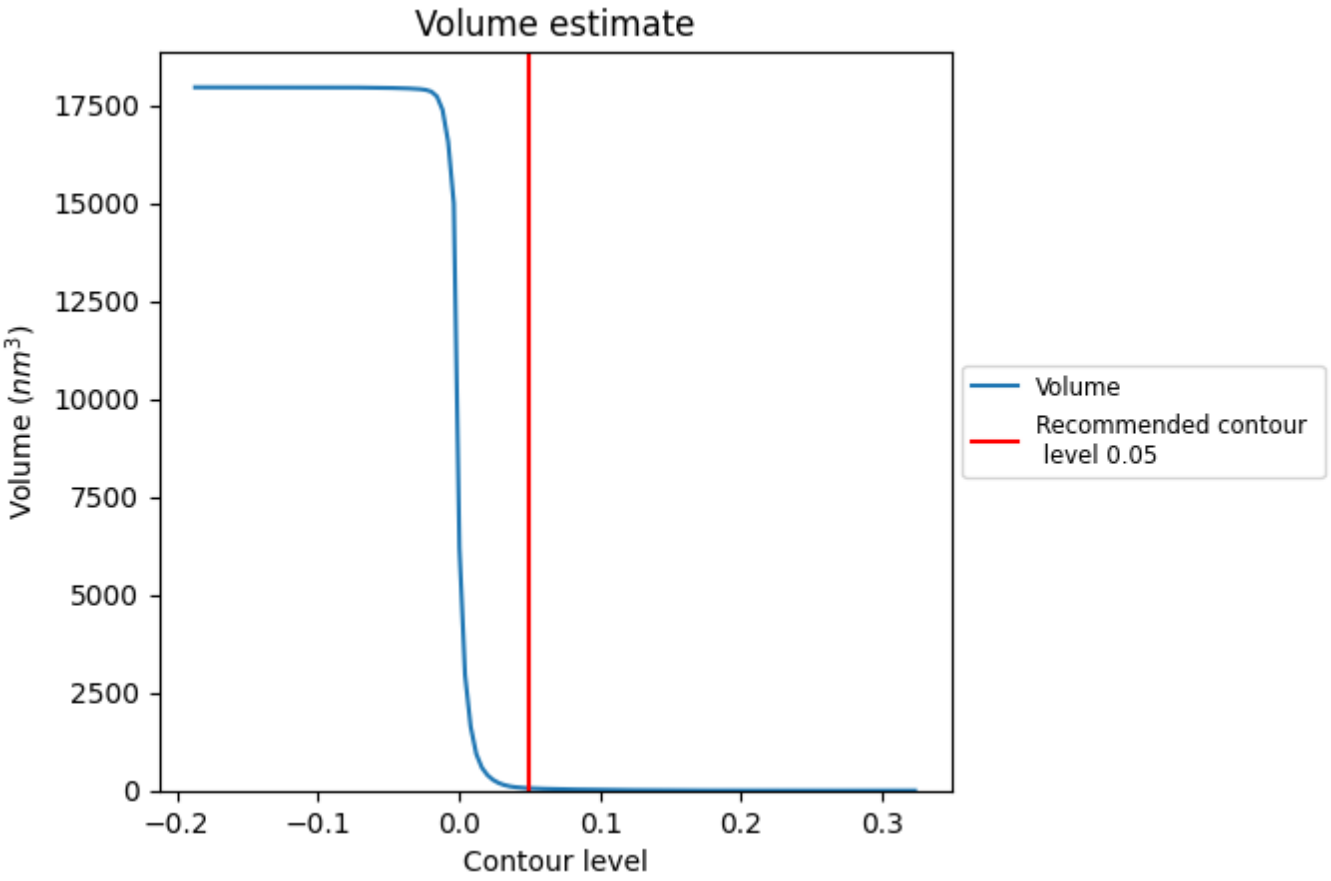
This section contains the results of statistical analysis of the map.

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.

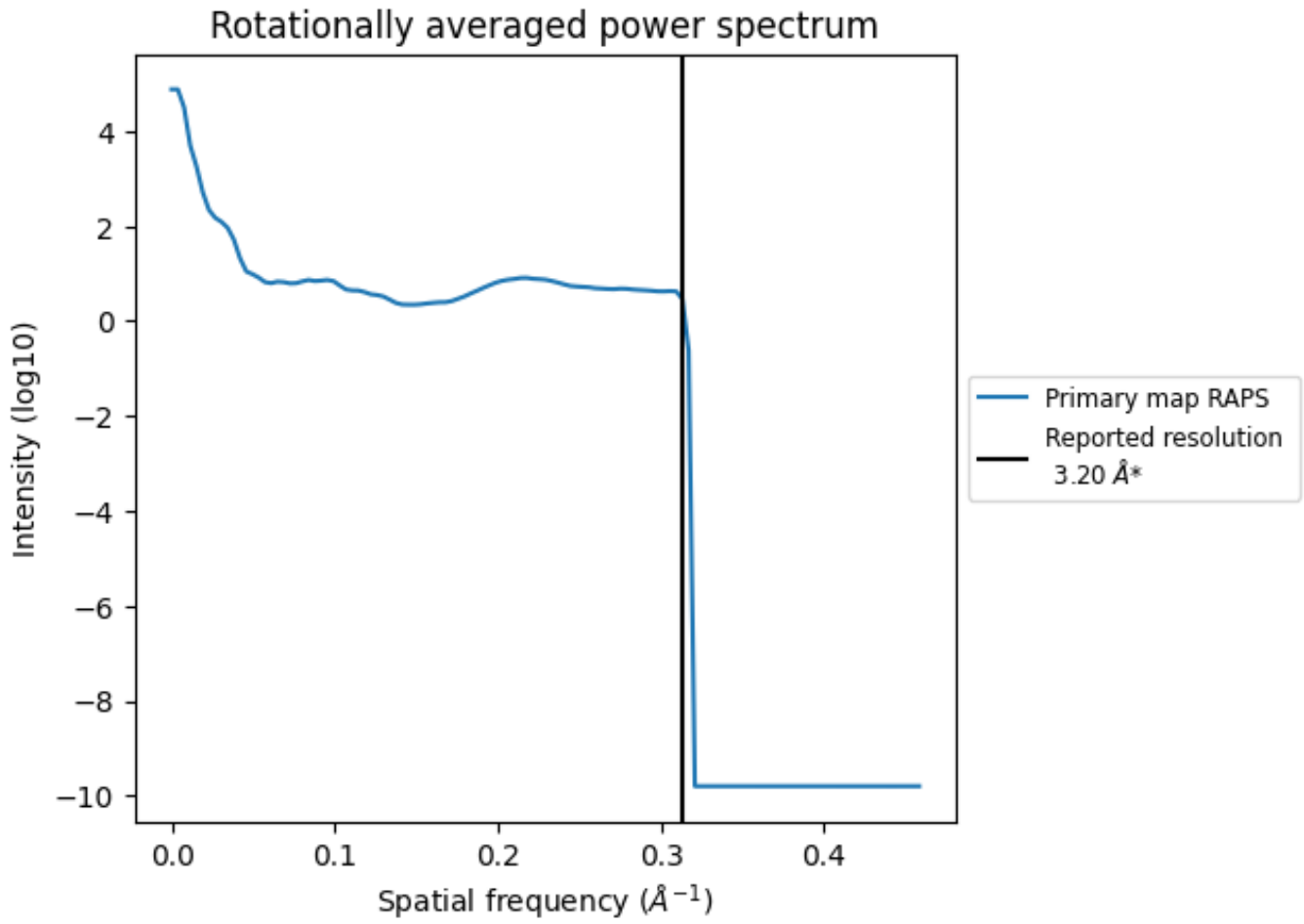
7.2 Volume estimate



The volume at the recommended contour level is 59 nm^3; this corresponds to an approximate mass of 53 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 0.312 Å^{-1}

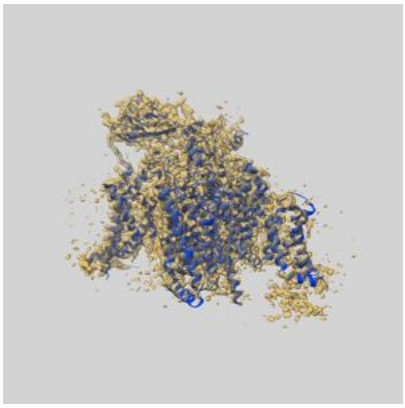
8 Fourier-Shell correlation

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

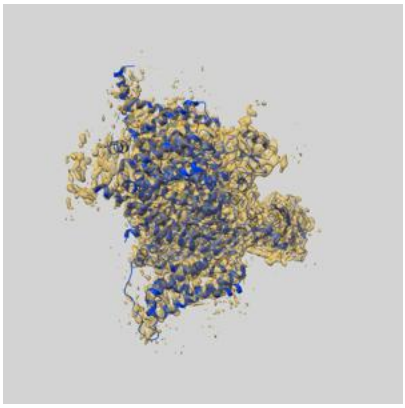
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9617 and PDB model 6AGF. Per-residue inclusion information can be found in section 3 on page 7.

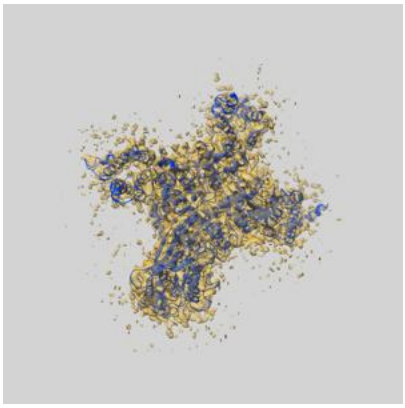
9.1 Map-model overlay



X



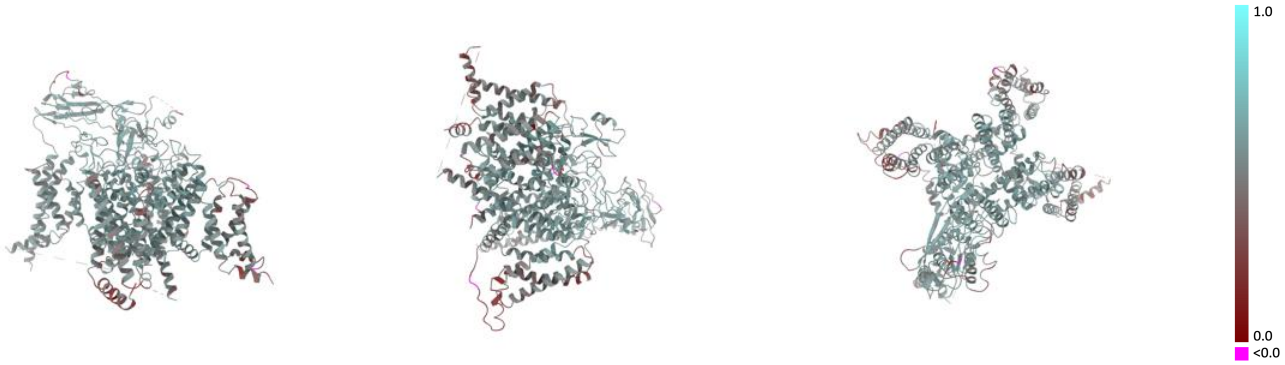
Y



Z

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

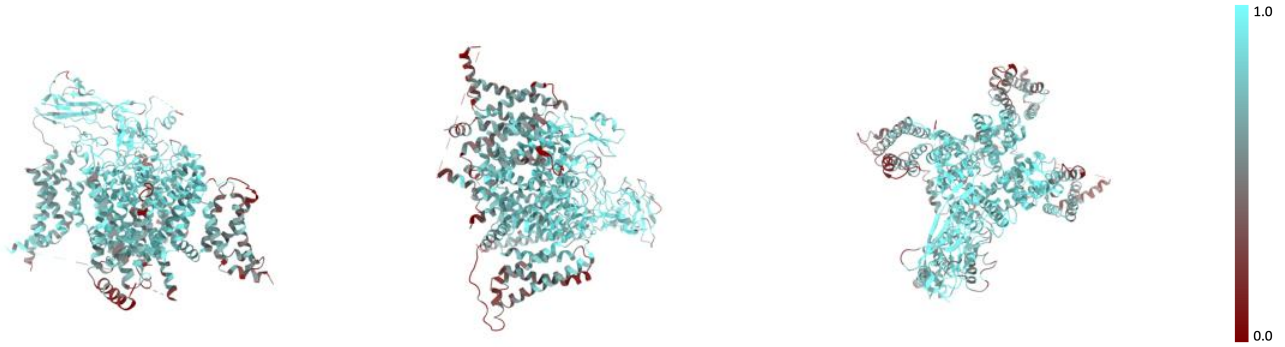
9.2 Q-score mapped to coordinate model (i)



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.

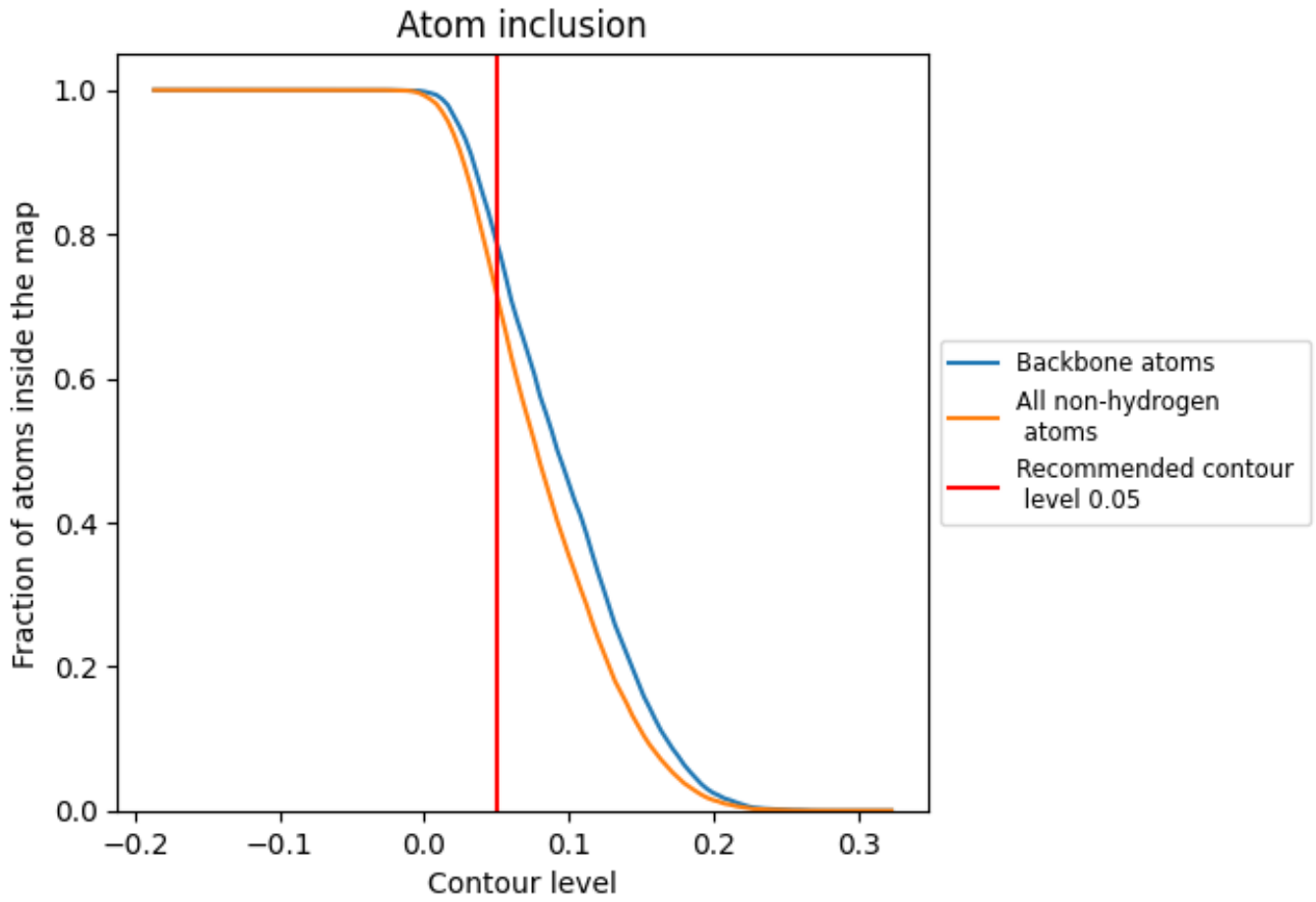
9.3 Atom inclusion mapped to coordinate model (i)



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, 79% of all backbone atoms, 72% 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	0.7171	0.5260
A	0.7111	0.5270
B	0.7560	0.5230
C	0.8718	0.5550
D	0.6071	0.4780
E	0.6429	0.4890