Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 10:59 AM JST

PDB ID	:	6J8E
EMDB ID	:	EMD-9780
Title	:	Human Nav1.2-beta2-KIIIA ternary complex
Authors	:	Pan, X.; Li, Z.; Huang, X.; Huang, G.; Yan, N.
Deposited on	:	2019-01-18
Resolution	:	3.00 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:

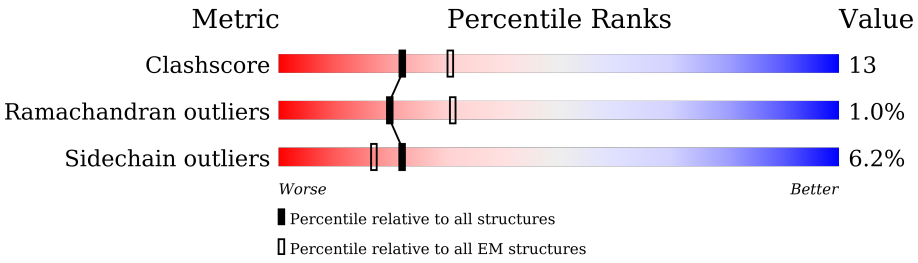
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

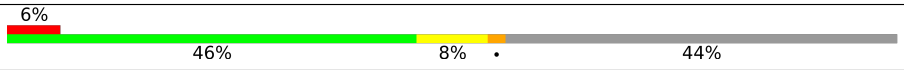
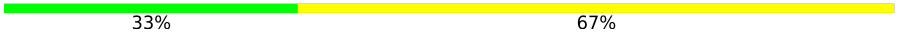
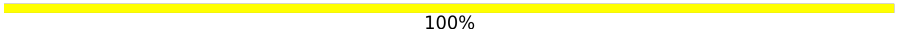
The reported resolution of this entry is 3.00 Å.

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	C	122	
2	A	2048	
3	D	16	
4	B	3	
5	E	2	
5	F	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10482 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 subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	122	Total	C	N	O	S	4	0
			1004	628	178	188	10		

- Molecule 2 is a protein called Sodium channel protein type 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1139	Total	C	N	O	S	0	0
			9193	6104	1430	1581	78		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q99250
A	-41	ALA	-	expression tag	UNP Q99250
A	-40	SER	-	expression tag	UNP Q99250
A	-39	TRP	-	expression tag	UNP Q99250
A	-38	SER	-	expression tag	UNP Q99250
A	-37	HIS	-	expression tag	UNP Q99250
A	-36	PRO	-	expression tag	UNP Q99250
A	-35	GLN	-	expression tag	UNP Q99250
A	-34	PHE	-	expression tag	UNP Q99250
A	-33	GLU	-	expression tag	UNP Q99250
A	-32	LYS	-	expression tag	UNP Q99250
A	-31	GLY	-	expression tag	UNP Q99250
A	-30	GLY	-	expression tag	UNP Q99250
A	-29	GLY	-	expression tag	UNP Q99250
A	-28	ALA	-	expression tag	UNP Q99250
A	-27	ARG	-	expression tag	UNP Q99250
A	-26	GLY	-	expression tag	UNP Q99250
A	-25	GLY	-	expression tag	UNP Q99250
A	-24	SER	-	expression tag	UNP Q99250
A	-23	GLY	-	expression tag	UNP Q99250
A	-22	GLY	-	expression tag	UNP Q99250

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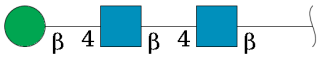
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	GLY	-	expression tag	UNP Q99250
A	-20	SER	-	expression tag	UNP Q99250
A	-19	TRP	-	expression tag	UNP Q99250
A	-18	SER	-	expression tag	UNP Q99250
A	-17	HIS	-	expression tag	UNP Q99250
A	-16	PRO	-	expression tag	UNP Q99250
A	-15	GLN	-	expression tag	UNP Q99250
A	-14	PHE	-	expression tag	UNP Q99250
A	-13	GLU	-	expression tag	UNP Q99250
A	-12	LYS	-	expression tag	UNP Q99250
A	-11	GLY	-	expression tag	UNP Q99250
A	-10	PHE	-	expression tag	UNP Q99250
A	-9	ASP	-	expression tag	UNP Q99250
A	-8	TYR	-	expression tag	UNP Q99250
A	-7	LYS	-	expression tag	UNP Q99250
A	-6	ASP	-	expression tag	UNP Q99250
A	-5	ASP	-	expression tag	UNP Q99250
A	-4	ASP	-	expression tag	UNP Q99250
A	-3	ASP	-	expression tag	UNP Q99250
A	-2	LYS	-	expression tag	UNP Q99250
A	-1	GLY	-	expression tag	UNP Q99250
A	0	THR	-	expression tag	UNP Q99250

- Molecule 3 is a protein called Mu-conotoxin KIIIA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	16	Total	C	N	O	S	1	0
			136	76	31	23	6		

- Molecule 4 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.

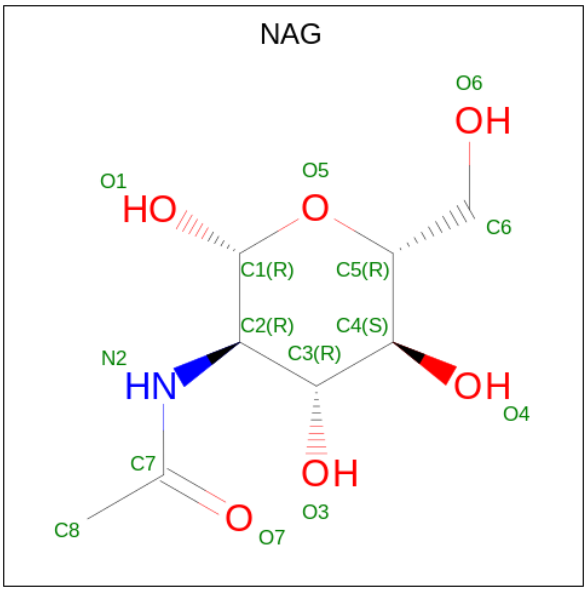


Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

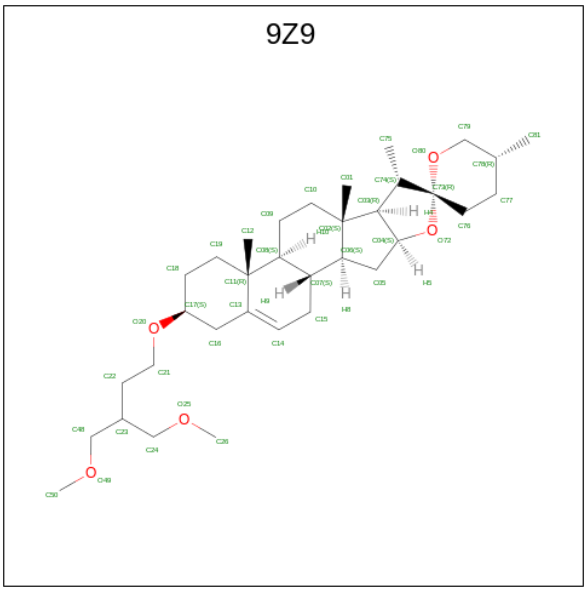
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 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	
7	A	1	39	34	5	0

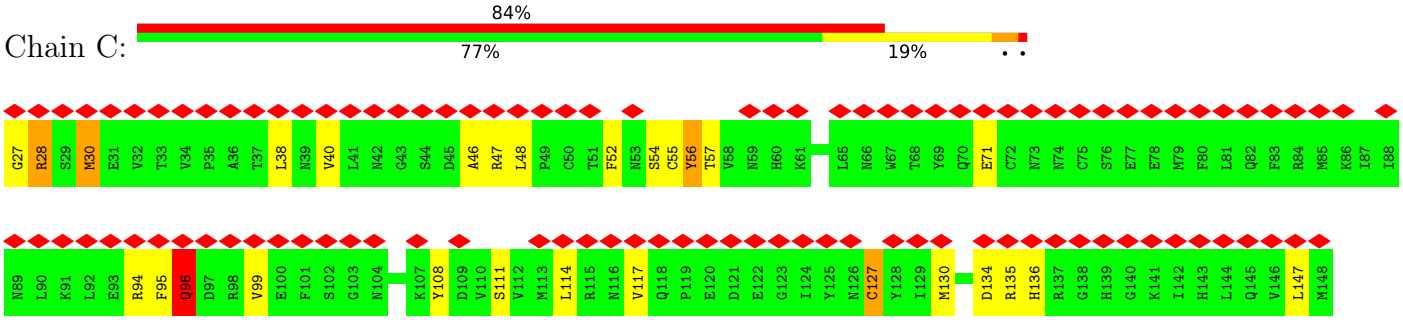
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
8	A	1	1	1	0

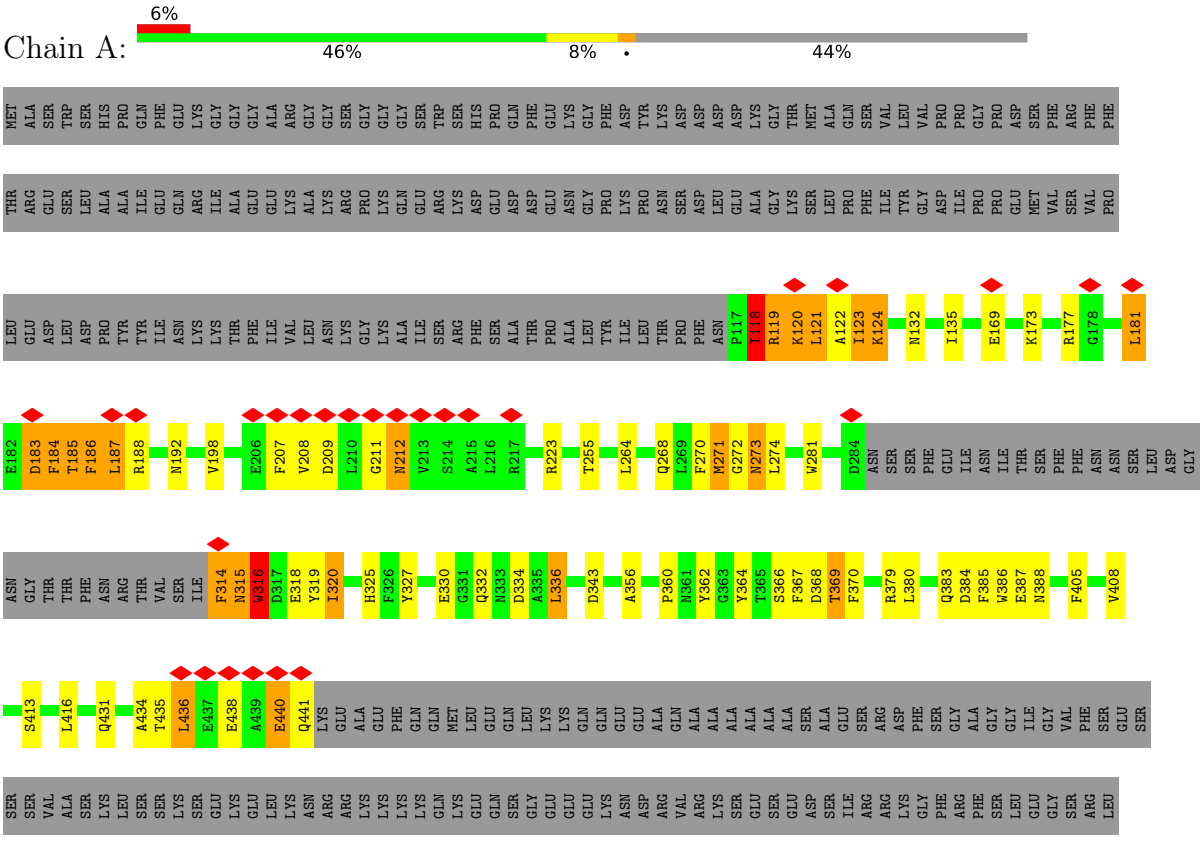
3 Residue-property plots (i)

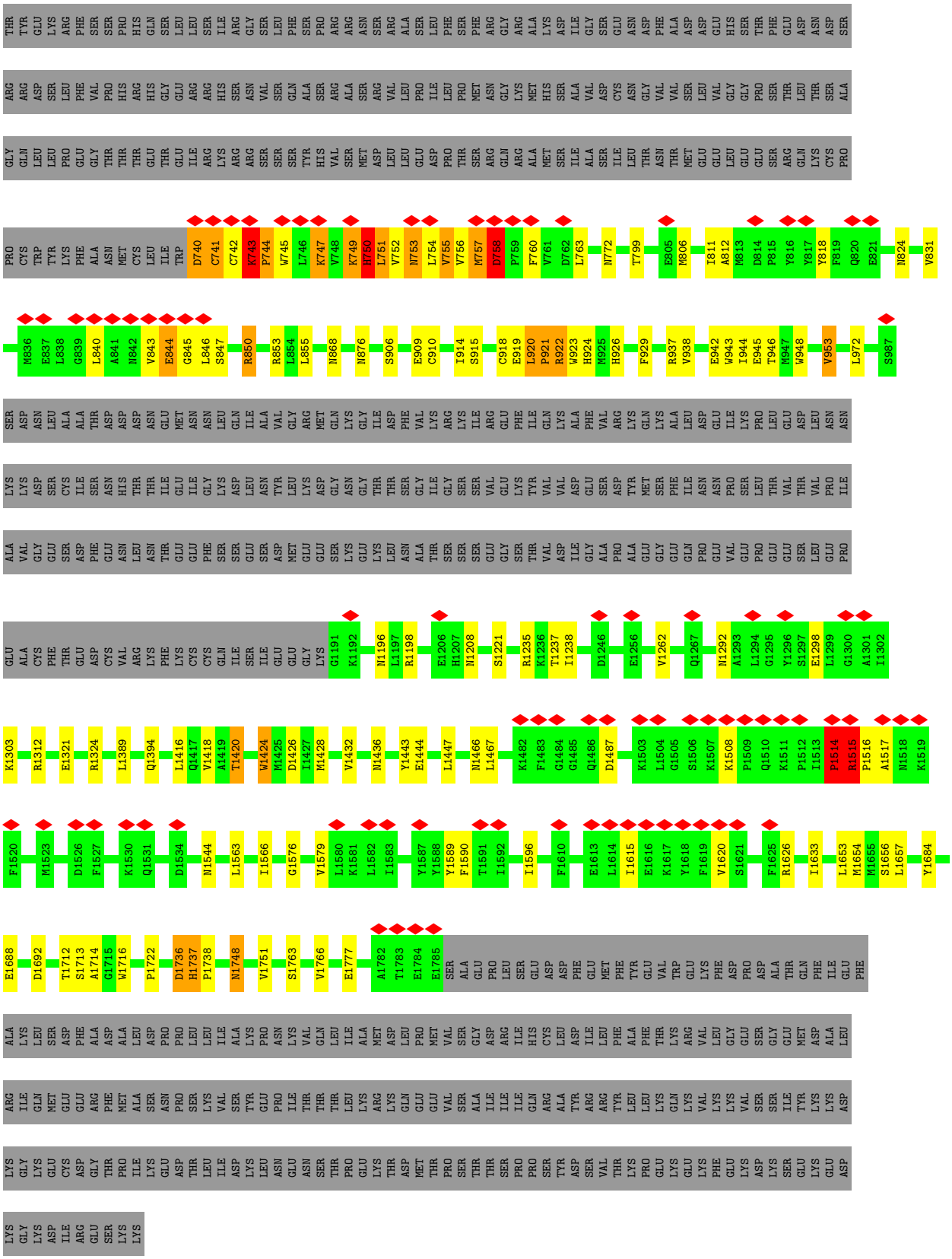
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Sodium channel subunit beta-2



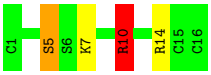
• Molecule 2: Sodium channel protein type 2 subunit alpha





• Molecule 3: Mu-conotoxin KIIIA

Chain D:

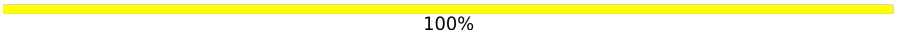


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200275	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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	0.287	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	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, 9Z9, NA, NAG

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	C	0.51	1/1038 (0.1%)	0.79	5/1402 (0.4%)
2	A	0.39	1/9423 (0.0%)	0.70	13/12774 (0.1%)
3	D	0.60	0/138	1.53	7/182 (3.8%)
All	All	0.40	2/10599 (0.0%)	0.73	25/14358 (0.2%)

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
2	A	0	5
3	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	CYS	CB-SG	11.33	2.01	1.82
2	A	921	PRO	N-CD	5.11	1.55	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	96	GLN	O-C-N	12.49	142.68	122.70
2	A	743	LYS	C-N-CD	-11.80	94.64	120.60
2	A	212	ASN	N-CA-CB	11.63	131.53	110.60
1	C	96	GLN	CA-C-N	-9.66	95.95	117.20
3	D	5	SER	CB-CA-C	-9.09	92.82	110.10
2	A	211	GLY	N-CA-C	8.61	134.63	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	10[A]	ARG	CA-C-O	7.96	136.81	120.10
3	D	10[B]	ARG	CA-C-O	7.96	136.81	120.10
1	C	127	CYS	CA-CB-SG	7.86	128.15	114.00
1	C	96	GLN	C-N-CA	-7.35	103.33	121.70
3	D	10[A]	ARG	CA-C-N	-6.65	102.57	117.20
3	D	10[B]	ARG	CA-C-N	-6.65	102.57	117.20
1	C	30	MET	C-N-CA	6.52	138.00	121.70
2	A	1736	ASP	CB-CG-OD1	6.43	124.09	118.30
2	A	343	ASP	CB-CG-OD1	6.36	124.02	118.30
2	A	336	LEU	CA-CB-CG	5.91	128.88	115.30
2	A	360	PRO	C-N-CA	5.85	136.32	121.70
2	A	1514	PRO	C-N-CA	5.68	135.90	121.70
2	A	920	LEU	C-N-CD	5.60	140.15	128.40
2	A	972	LEU	CA-CB-CG	5.59	128.15	115.30
2	A	1653	LEU	CB-CG-CD2	-5.27	102.05	111.00
2	A	1487	ASP	CB-CG-OD1	5.22	123.00	118.30
2	A	1467	LEU	CA-CB-CG	5.12	127.07	115.30
3	D	10[A]	ARG	N-CA-C	5.02	124.56	111.00
3	D	10[B]	ARG	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1514	PRO	Peptide
2	A	1515	ARG	Peptide
2	A	1516	PRO	Peptide
2	A	281	TRP	Peptide
2	A	334	ASP	Peptide
3	D	10[B]	ARG	Mainchain

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	C	1004	0	971	27	0
2	A	9193	0	9328	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	136	0	119	2	0
4	B	39	0	34	0	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
6	A	14	0	13	0	0
7	A	39	0	0	0	0
8	A	1	0	0	0	0
All	All	10482	0	10515	269	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 13.

All (269) 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:C:127:CYS:CB	1:C:127:CYS:SG	2.01	1.48
2:A:743:LYS:HG2	2:A:744:PRO:CD	1.45	1.43
2:A:743:LYS:CG	2:A:744:PRO:HD3	1.55	1.35
2:A:121:LEU:HD13	2:A:122:ALA:N	1.47	1.25
2:A:752:VAL:HG21	2:A:811:ILE:CG2	1.70	1.20
2:A:1736:ASP:O	2:A:1738:PRO:HD3	1.37	1.18
2:A:184:PHE:CB	2:A:187:LEU:HD23	1.74	1.17
2:A:752:VAL:HG21	2:A:811:ILE:HG21	1.20	1.14
2:A:743:LYS:CG	2:A:744:PRO:CD	2.19	1.11
2:A:752:VAL:HG11	2:A:811:ILE:HB	1.34	1.09
2:A:119:ARG:H	2:A:119:ARG:HD3	1.12	1.09
2:A:431:GLN:O	2:A:435:THR:HG23	1.53	1.09
2:A:383:GLN:HE21	2:A:413:SER:HB3	1.18	1.08
2:A:177:ARG:HB2	2:A:185:THR:HB	1.12	1.07
2:A:314:PHE:HB3	2:A:318:GLU:CB	1.88	1.04
2:A:184:PHE:CD2	2:A:187:LEU:HB2	1.94	1.03
2:A:743:LYS:CB	2:A:744:PRO:HD2	1.89	1.02
2:A:177:ARG:CB	2:A:185:THR:HB	1.89	1.01
2:A:753:ASN:HA	2:A:812:ALA:HB1	1.43	0.99
2:A:743:LYS:CB	2:A:744:PRO:CD	2.39	0.99
2:A:743:LYS:HB3	2:A:744:PRO:HD2	1.43	0.97
2:A:314:PHE:HB3	2:A:318:GLU:HB3	1.48	0.94
2:A:320:ILE:HD13	2:A:356:ALA:CB	1.96	0.94
2:A:922:ARG:HH21	2:A:922:ARG:HG3	1.35	0.92
2:A:184:PHE:HB2	2:A:187:LEU:HD23	1.50	0.90
2:A:184:PHE:HB3	2:A:187:LEU:HD23	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:752:VAL:HG11	2:A:811:ILE:CB	2.05	0.87
2:A:1712:THR:O	2:A:1713:SER:OG	1.93	0.86
2:A:184:PHE:HD2	2:A:187:LEU:HB2	1.38	0.84
2:A:383:GLN:HE21	2:A:413:SER:CB	1.88	0.84
2:A:383:GLN:NE2	2:A:413:SER:HB3	1.93	0.84
1:C:95:PHE:O	1:C:96:GLN:HB2	1.78	0.83
2:A:752:VAL:CG2	2:A:811:ILE:HG21	2.05	0.83
2:A:121:LEU:HD13	2:A:122:ALA:H	1.40	0.83
2:A:753:ASN:CA	2:A:812:ALA:HB1	2.08	0.82
2:A:186:PHE:O	2:A:186:PHE:CD1	2.33	0.82
2:A:1447:LEU:O	2:A:1447:LEU:HD23	1.80	0.81
2:A:752:VAL:HG21	2:A:811:ILE:HG22	1.63	0.81
2:A:1737:HIS:CD2	2:A:1737:HIS:H	1.95	0.81
2:A:184:PHE:HB2	2:A:187:LEU:CD2	2.10	0.81
2:A:743:LYS:CG	2:A:744:PRO:HD2	2.04	0.81
2:A:118:ILE:HB	2:A:119:ARG:HD3	1.64	0.80
2:A:184:PHE:CB	2:A:187:LEU:CD2	2.59	0.80
2:A:119:ARG:O	2:A:123:ILE:HG22	1.81	0.79
2:A:436:LEU:CD1	2:A:440:GLU:OE1	2.30	0.79
2:A:752:VAL:CG2	2:A:811:ILE:CG2	2.58	0.78
2:A:270:PHE:O	2:A:367:PHE:HB2	1.83	0.77
2:A:121:LEU:CD1	2:A:122:ALA:N	2.39	0.77
2:A:121:LEU:C	2:A:121:LEU:HD22	2.06	0.77
2:A:119:ARG:HD3	2:A:119:ARG:N	1.96	0.76
2:A:757:MET:O	2:A:757:MET:HG2	1.85	0.75
2:A:747:LYS:O	2:A:747:LYS:HD3	1.85	0.75
2:A:121:LEU:HD13	2:A:122:ALA:CA	2.17	0.75
2:A:1688:GLU:HB2	2:A:1722:PRO:HB3	1.69	0.75
2:A:124:LYS:HB2	2:A:124:LYS:NZ	2.01	0.74
2:A:441:GLN:HA	2:A:441:GLN:NE2	2.03	0.74
2:A:752:VAL:HB	2:A:812:ALA:HB2	1.68	0.74
2:A:173:LYS:CD	2:A:186:PHE:HD2	2.01	0.73
2:A:327:TYR:CD2	2:A:336:LEU:HD12	2.24	0.73
1:C:56:TYR:CD2	1:C:134:ASP:HB2	2.23	0.72
2:A:920:LEU:HD22	2:A:924:HIS:CG	2.25	0.72
2:A:320:ILE:HD13	2:A:356:ALA:HB3	1.72	0.71
2:A:124:LYS:HB2	2:A:124:LYS:HZ3	1.56	0.71
1:C:99:VAL:HG22	1:C:114:LEU:HD13	1.72	0.71
2:A:119:ARG:H	2:A:119:ARG:CD	1.97	0.71
1:C:28:ARG:O	1:C:136:HIS:CD2	2.44	0.71
1:C:95:PHE:O	1:C:96:GLN:CB	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:441:GLN:HA	2:A:441:GLN:HE21	1.55	0.70
2:A:314:PHE:CB	2:A:318:GLU:HB3	2.20	0.70
2:A:366:SER:HB2	2:A:368:ASP:OD1	1.91	0.70
2:A:743:LYS:HG2	2:A:744:PRO:HD3	0.74	0.70
2:A:752:VAL:HG11	2:A:811:ILE:CG2	2.21	0.69
2:A:921:PRO:HD2	2:A:924:HIS:HB3	1.74	0.69
2:A:186:PHE:CD1	2:A:186:PHE:C	2.63	0.68
2:A:121:LEU:HD22	2:A:121:LEU:O	1.94	0.68
2:A:754:LEU:HD23	2:A:754:LEU:O	1.93	0.68
2:A:177:ARG:HG3	2:A:185:THR:OG1	1.94	0.68
2:A:173:LYS:HD3	2:A:186:PHE:HD2	1.58	0.68
2:A:186:PHE:C	2:A:186:PHE:HD1	1.95	0.68
2:A:315:ASN:N	2:A:315:ASN:HD22	1.93	0.67
2:A:327:TYR:HD2	2:A:336:LEU:HD12	1.58	0.67
2:A:929:PHE:CE2	2:A:1447:LEU:HD21	2.31	0.66
2:A:184:PHE:CG	2:A:187:LEU:HD23	2.31	0.66
2:A:173:LYS:CD	2:A:186:PHE:CD2	2.80	0.65
2:A:753:ASN:HA	2:A:812:ALA:CB	2.22	0.65
2:A:922:ARG:HH21	2:A:922:ARG:CG	2.10	0.65
2:A:320:ILE:HD13	2:A:356:ALA:HB2	1.79	0.64
2:A:314:PHE:HB3	2:A:318:GLU:HB2	1.79	0.64
2:A:749:LYS:HE3	2:A:811:ILE:O	1.98	0.63
2:A:1684:TYR:CD1	2:A:1737:HIS:HE1	2.16	0.63
1:C:135:ARG:NE	2:A:918:CYS:O	2.31	0.63
2:A:844:GLU:HG3	2:A:844:GLU:O	1.98	0.63
2:A:186:PHE:CD2	2:A:192:ASN:ND2	2.67	0.63
2:A:185:THR:OG1	2:A:186:PHE:N	2.32	0.63
2:A:743:LYS:HB2	2:A:743:LYS:NZ	2.14	0.62
2:A:752:VAL:O	2:A:755:VAL:HG12	1.98	0.62
2:A:1447:LEU:HD23	2:A:1447:LEU:C	2.20	0.62
2:A:120:LYS:O	2:A:123:ILE:CG2	2.47	0.62
2:A:749:LYS:HG3	2:A:750:HIS:N	2.13	0.62
2:A:914:ILE:O	2:A:915:SER:HB3	1.99	0.62
2:A:1684:TYR:CD1	2:A:1737:HIS:CE1	2.88	0.62
2:A:119:ARG:O	2:A:123:ILE:CG2	2.48	0.62
2:A:436:LEU:HD11	2:A:440:GLU:OE1	1.98	0.62
2:A:740:ASP:OD1	2:A:740:ASP:N	2.31	0.62
2:A:943:TRP:CZ3	2:A:944:ILE:HD13	2.35	0.62
1:C:56:TYR:CE2	1:C:134:ASP:CB	2.82	0.61
2:A:121:LEU:HD13	2:A:122:ALA:CB	2.29	0.61
2:A:270:PHE:O	2:A:367:PHE:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:314:PHE:CB	2:A:318:GLU:CB	2.74	0.61
1:C:27:GLY:O	1:C:136:HIS:CE1	2.54	0.61
1:C:99:VAL:HG22	1:C:114:LEU:CD1	2.31	0.61
2:A:184:PHE:CD2	2:A:187:LEU:CB	2.80	0.61
2:A:436:LEU:HD12	2:A:440:GLU:OE1	2.01	0.60
2:A:1432:VAL:HG13	2:A:1447:LEU:HA	1.83	0.60
2:A:922:ARG:HG3	2:A:922:ARG:NH2	2.14	0.60
2:A:924:HIS:HD2	2:A:926:HIS:H	1.48	0.60
2:A:316:TRP:HA	2:A:316:TRP:CE3	2.36	0.60
2:A:758:ASP:N	2:A:758:ASP:OD1	2.35	0.60
1:C:27:GLY:HA3	2:A:909:GLU:HB3	1.84	0.60
2:A:314:PHE:CB	2:A:318:GLU:HG2	2.32	0.59
2:A:756:VAL:HG23	2:A:756:VAL:O	2.00	0.59
2:A:173:LYS:HD2	2:A:186:PHE:CD2	2.37	0.59
2:A:1748:ASN:HB3	2:A:1751:VAL:HG22	1.84	0.59
2:A:314:PHE:HB2	2:A:318:GLU:HG2	1.84	0.59
2:A:380:LEU:HD23	2:A:386:TRP:HB2	1.85	0.59
2:A:1654:MET:HA	2:A:1657:LEU:HD23	1.85	0.59
2:A:198:VAL:HG21	2:A:223:ARG:HB3	1.84	0.59
1:C:56:TYR:CE2	1:C:134:ASP:HB2	2.38	0.58
2:A:320:ILE:HG23	2:A:320:ILE:O	2.03	0.58
2:A:749:LYS:HE2	2:A:812:ALA:HA	1.86	0.58
2:A:362:TYR:HB2	2:A:364:TYR:CD2	2.39	0.58
2:A:121:LEU:CD1	2:A:122:ALA:HB2	2.34	0.57
2:A:752:VAL:CG2	2:A:811:ILE:HG22	2.30	0.57
2:A:384:ASP:OD2	2:A:944:ILE:HB	2.05	0.56
2:A:431:GLN:O	2:A:435:THR:CG2	2.43	0.56
2:A:749:LYS:O	2:A:752:VAL:N	2.38	0.56
2:A:362:TYR:CD2	2:A:948:TRP:HB3	2.41	0.56
2:A:184:PHE:CD1	2:A:184:PHE:N	2.73	0.56
2:A:186:PHE:CD2	2:A:192:ASN:CG	2.79	0.56
2:A:1416:LEU:O	2:A:1420:THR:OG1	2.24	0.56
2:A:387:GLU:HG2	2:A:1714:ALA:HB1	1.88	0.55
2:A:753:ASN:CA	2:A:812:ALA:CB	2.84	0.55
2:A:362:TYR:HD2	2:A:948:TRP:HB3	1.71	0.55
1:C:135:ARG:HE	2:A:918:CYS:CB	2.19	0.55
2:A:314:PHE:CD1	2:A:314:PHE:N	2.73	0.55
2:A:920:LEU:HD22	2:A:924:HIS:CD2	2.43	0.54
2:A:1418:VAL:HA	2:A:1424:TRP:HB3	1.88	0.54
2:A:120:LYS:O	2:A:123:ILE:HG23	2.06	0.54
2:A:753:ASN:N	2:A:812:ALA:CB	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:772:ASN:HD21	2:A:853:ARG:HH21	1.53	0.54
2:A:1432:VAL:HG12	2:A:1444:GLU:HA	1.89	0.54
2:A:121:LEU:HD13	2:A:121:LEU:C	2.23	0.53
2:A:380:LEU:O	2:A:413:SER:OG	2.26	0.53
2:A:937:ARG:NH2	2:A:946:THR:HG23	2.23	0.53
2:A:749:LYS:O	2:A:750:HIS:C	2.46	0.53
2:A:264:LEU:O	2:A:268:GLN:NE2	2.41	0.53
2:A:929:PHE:CE2	2:A:1447:LEU:CD2	2.91	0.53
2:A:753:ASN:N	2:A:812:ALA:HB2	2.24	0.53
2:A:1737:HIS:H	2:A:1737:HIS:HD2	1.52	0.53
1:C:135:ARG:HE	2:A:918:CYS:HB3	1.74	0.53
2:A:747:LYS:HD3	2:A:747:LYS:C	2.28	0.53
2:A:135:ILE:HD12	2:A:169:GLU:HG3	1.91	0.52
2:A:1221:SER:HG	2:A:1312:ARG:HH11	1.57	0.52
1:C:56:TYR:CE2	1:C:134:ASP:HA	2.43	0.52
2:A:314:PHE:HB3	2:A:318:GLU:CG	2.40	0.52
2:A:749:LYS:CE	2:A:812:ALA:HA	2.39	0.52
2:A:942:GLU:OE2	2:A:1424:TRP:NE1	2.43	0.52
2:A:1424:TRP:HB2	2:A:1428:MET:HE3	1.92	0.51
1:C:47:ARG:NH2	1:C:111[B]:SER:OG	2.43	0.51
2:A:368:ASP:O	2:A:369:THR:CB	2.57	0.51
2:A:743:LYS:CB	2:A:743:LYS:NZ	2.73	0.51
2:A:910:CYS:HB2	2:A:953:VAL:HG22	1.93	0.51
2:A:186:PHE:CE2	2:A:192:ASN:ND2	2.79	0.51
2:A:937:ARG:HH21	2:A:946:THR:HG23	1.76	0.51
2:A:173:LYS:HD2	2:A:186:PHE:CE2	2.45	0.51
1:C:56:TYR:HE2	1:C:134:ASP:CG	2.14	0.51
2:A:255:THR:HG22	2:A:416:LEU:HD22	1.93	0.50
2:A:1684:TYR:CG	2:A:1737:HIS:HE1	2.28	0.50
2:A:177:ARG:HG3	2:A:185:THR:CB	2.42	0.50
2:A:744:PRO:HA	2:A:747:LYS:HB3	1.94	0.50
2:A:1712:THR:C	2:A:1713:SER:HG	2.05	0.50
2:A:384:ASP:O	2:A:385:PHE:HB3	2.12	0.49
2:A:1443:TYR:CD1	2:A:1443:TYR:C	2.86	0.49
1:C:56:TYR:CE2	1:C:134:ASP:CA	2.96	0.49
2:A:315:ASN:N	2:A:315:ASN:ND2	2.60	0.49
2:A:318:GLU:O	2:A:318:GLU:HG3	2.12	0.49
2:A:434:ALA:O	2:A:438:GLU:CG	2.60	0.49
2:A:1426:ASP:OD1	3:D:10[B]:ARG:NH1	2.45	0.49
2:A:271:MET:HB2	2:A:1626:ARG:NH2	2.28	0.48
2:A:1198:ARG:NE	2:A:1262:VAL:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:177:ARG:CG	2:A:185:THR:HB	2.40	0.48
2:A:1443:TYR:CD1	2:A:1444:GLU:HB2	2.49	0.48
2:A:272:GLY:O	2:A:274:LEU:N	2.46	0.48
2:A:752:VAL:CB	2:A:811:ILE:HG22	2.44	0.48
2:A:906:SER:HA	2:A:909:GLU:HG2	1.96	0.48
2:A:752:VAL:CB	2:A:812:ALA:HB2	2.42	0.47
2:A:752:VAL:C	2:A:812:ALA:HB2	2.35	0.47
1:C:56:TYR:HE2	1:C:134:ASP:CB	2.25	0.47
2:A:847:SER:O	2:A:850:ARG:HG3	2.14	0.47
2:A:119:ARG:HG3	2:A:119:ARG:HH11	1.78	0.47
2:A:121:LEU:HD13	2:A:122:ALA:HB2	1.93	0.47
2:A:177:ARG:CB	2:A:185:THR:CB	2.77	0.47
2:A:327:TYR:CE2	2:A:336:LEU:HD12	2.49	0.47
2:A:755:VAL:HG13	2:A:756:VAL:HG13	1.97	0.47
2:A:1713:SER:O	2:A:1716:TRP:HD1	1.97	0.47
1:C:52:PHE:O	1:C:108:TYR:HB3	2.15	0.46
2:A:184:PHE:HB2	2:A:187:LEU:HD22	1.97	0.46
1:C:56:TYR:HD2	1:C:134:ASP:HB2	1.76	0.46
2:A:441:GLN:HE21	2:A:441:GLN:CA	2.20	0.46
2:A:750:HIS:C	2:A:750:HIS:CD2	2.88	0.46
2:A:1298:GLU:HG2	2:A:1303:LYS:HD3	1.97	0.46
2:A:844:GLU:HA	2:A:845:GLY:HA2	1.52	0.46
2:A:921:PRO:HG2	2:A:923:TRP:O	2.17	0.45
2:A:1563:LEU:HA	2:A:1566:ILE:HG22	1.98	0.45
2:A:1692:ASP:N	2:A:1692:ASP:OD1	2.49	0.45
2:A:741:CYS:SG	2:A:742:CYS:N	2.89	0.45
1:C:52:PHE:CZ	1:C:108:TYR:HA	2.52	0.45
2:A:818:TYR:CZ	2:A:824:ASN:HB3	2.52	0.44
2:A:929:PHE:HE2	2:A:1447:LEU:HD21	1.78	0.44
2:A:943:TRP:CZ3	2:A:944:ILE:CD1	3.00	0.44
2:A:320:ILE:CD1	2:A:356:ALA:HB3	2.45	0.44
1:C:95:PHE:O	1:C:96:GLN:HG3	2.18	0.43
2:A:1389:LEU:HD22	2:A:1394:GLN:HG3	2.00	0.43
1:C:94:ARG:HG3	1:C:95:PHE:N	2.33	0.43
2:A:181:LEU:C	2:A:181:LEU:HD22	2.39	0.43
2:A:922:ARG:CG	2:A:922:ARG:NH2	2.73	0.43
2:A:124:LYS:NZ	2:A:124:LYS:CB	2.73	0.43
2:A:1656:SER:HB3	2:A:1777:GLU:HG3	2.00	0.43
2:A:268:GLN:HE21	2:A:1633:ILE:HD11	1.84	0.43
2:A:1237:THR:HG23	2:A:1238:ILE:HG13	2.01	0.43
2:A:806:MET:HG2	2:A:831:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:177:ARG:CG	2:A:185:THR:CB	2.97	0.43
2:A:121:LEU:CD1	2:A:122:ALA:H	2.21	0.42
2:A:436:LEU:HD12	2:A:436:LEU:O	2.19	0.42
2:A:272:GLY:O	2:A:273:ASN:C	2.54	0.42
2:A:938:VAL:HG13	2:A:943:TRP:HB3	2.00	0.42
2:A:405:PHE:HA	2:A:408:VAL:HG12	2.01	0.42
2:A:752:VAL:CG1	2:A:811:ILE:CG2	2.95	0.42
2:A:1447:LEU:C	2:A:1447:LEU:CD2	2.85	0.42
2:A:1615:ILE:HG23	2:A:1620:VAL:HG23	2.00	0.42
2:A:184:PHE:HB3	2:A:187:LEU:CD2	2.34	0.42
2:A:274:LEU:HD12	2:A:366:SER:HA	2.01	0.42
2:A:1235:ARG:HD3	2:A:1238:ILE:HD12	2.01	0.42
2:A:1424:TRP:CE3	2:A:1428:MET:HE3	2.55	0.42
2:A:799:THR:OG1	2:A:853:ARG:NH1	2.53	0.42
2:A:945:GLU:OE1	3:D:7:LYS:NZ	2.50	0.42
2:A:314:PHE:CB	2:A:318:GLU:CG	2.94	0.41
2:A:929:PHE:CD2	2:A:1447:LEU:HD21	2.55	0.41
2:A:1321:GLU:HG2	2:A:1324:ARG:HH12	1.86	0.41
2:A:319:TYR:CE1	2:A:325:HIS:CE1	3.07	0.41
2:A:843:VAL:HB	2:A:846:LEU:CB	2.50	0.41
2:A:749:LYS:O	2:A:751:LEU:N	2.54	0.41
2:A:184:PHE:HB2	2:A:185:THR:H	1.60	0.41
2:A:1763:SER:HA	2:A:1766:VAL:HG12	2.02	0.41
1:C:40:VAL:HG11	1:C:46:ALA:HB2	2.02	0.41
2:A:924:HIS:CD2	2:A:926:HIS:H	2.34	0.41
2:A:1576:GLY:HA2	2:A:1579:VAL:HG12	2.03	0.41
2:A:187:LEU:HD13	2:A:187:LEU:HA	1.88	0.41
2:A:1590:PHE:HD1	2:A:1596:ILE:HG12	1.86	0.41
2:A:272:GLY:C	2:A:274:LEU:N	2.72	0.41
2:A:760:PHE:HB2	2:A:763:LEU:HB3	2.03	0.41
2:A:1514:PRO:HB2	2:A:1515:ARG:H	1.73	0.41
2:A:1737:HIS:CD2	2:A:1737:HIS:N	2.73	0.41
2:A:1432:VAL:CG1	2:A:1444:GLU:HG2	2.51	0.40
1:C:38:LEU:HD23	1:C:48:LEU:HD22	2.03	0.40
2:A:183:ASP:HB2	2:A:184:PHE:H	1.57	0.40
2:A:929:PHE:HE2	2:A:1447:LEU:CD2	2.33	0.40
2:A:1515:ARG:HG3	2:A:1517:ALA:HA	2.04	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	C	124/122 (102%)	117 (94%)	6 (5%)	1 (1%)	19	57
2	A	1131/2048 (55%)	1042 (92%)	77 (7%)	12 (1%)	14	50
3	D	15/16 (94%)	15 (100%)	0	0	100	100
All	All	1270/2186 (58%)	1174 (92%)	83 (6%)	13 (1%)	20	53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	GLN
2	A	369	THR
2	A	1514	PRO
2	A	208	VAL
2	A	212	ASN
2	A	370	PHE
2	A	758	ASP
2	A	118	ILE
2	A	273	ASN
2	A	1515	ARG
2	A	750	HIS
2	A	316	TRP
2	A	1589	TYR

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	C	117/114 (103%)	108 (92%)	9 (8%)	13 42
2	A	1014/1817 (56%)	954 (94%)	60 (6%)	19 54
3	D	17/16 (106%)	15 (88%)	2 (12%)	5 22
All	All	1148/1947 (59%)	1077 (94%)	71 (6%)	22 52

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	28	ARG
1	C	30	MET
1	C	54	SER
1	C	55	CYS
1	C	56	TYR
1	C	57	THR
1	C	71	GLU
1	C	130	MET
1	C	147	LEU
2	A	118	ILE
2	A	119	ARG
2	A	120	LYS
2	A	121	LEU
2	A	123	ILE
2	A	124	LYS
2	A	132	ASN
2	A	181	LEU
2	A	183	ASP
2	A	184	PHE
2	A	185	THR
2	A	186	PHE
2	A	187	LEU
2	A	188	ARG
2	A	207	PHE
2	A	209	ASP
2	A	271	MET
2	A	314	PHE
2	A	315	ASN
2	A	316	TRP
2	A	320	ILE
2	A	330	GLU
2	A	332	GLN
2	A	379	ARG
2	A	388	ASN

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Mol	Chain	Res	Type
2	A	436	LEU
2	A	440	GLU
2	A	740	ASP
2	A	741	CYS
2	A	743	LYS
2	A	744	PRO
2	A	745	TRP
2	A	747	LYS
2	A	749	LYS
2	A	750	HIS
2	A	751	LEU
2	A	753	ASN
2	A	755	VAL
2	A	757	MET
2	A	758	ASP
2	A	840	LEU
2	A	844	GLU
2	A	850	ARG
2	A	855	LEU
2	A	868	ASN
2	A	876	ASN
2	A	919	GLU
2	A	922	ARG
2	A	953	VAL
2	A	1196	ASN
2	A	1208	ASN
2	A	1292	ASN
2	A	1420	THR
2	A	1424	TRP
2	A	1436	ASN
2	A	1466	ASN
2	A	1508	LYS
2	A	1544	ASN
2	A	1737	HIS
2	A	1748	ASN
3	D	5	SER
3	D	14	ARG

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

Mol	Chain	Res	Type
1	C	70	GLN

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Mol	Chain	Res	Type
1	C	118	GLN
1	C	136	HIS
2	A	132	ASN
2	A	268	GLN
2	A	315	ASN
2	A	361	ASN
2	A	383	GLN
2	A	388	ASN
2	A	418	ASN
2	A	441	GLN
2	A	750	HIS
2	A	772	ASN
2	A	780	HIS
2	A	868	ASN
2	A	876	ASN
2	A	924	HIS
2	A	1196	ASN
2	A	1208	ASN
2	A	1292	ASN
2	A	1436	ASN
2	A	1475	ASN
2	A	1737	HIS
2	A	1748	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	$\#\|Z\| > 2$
4	NAG	B	1	2,4	14,14,15	0.53	0	17,19,21	0.73	0
4	NAG	B	2	4	14,14,15	0.53	0	17,19,21	1.31	2 (11%)
4	BMA	B	3	4	11,11,12	1.28	2 (18%)	15,15,17	1.98	5 (33%)
5	NAG	E	1	2,5	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
5	NAG	E	2	5	14,14,15	0.70	1 (7%)	17,19,21	0.79	1 (5%)
5	NAG	F	1	2,5	14,14,15	0.56	0	17,19,21	1.18	1 (5%)
5	NAG	F	2	5	14,14,15	0.36	0	17,19,21	0.43	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	B	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	C1-C2	2.40	1.55	1.52
4	B	3	BMA	O5-C5	2.36	1.48	1.43
4	B	3	BMA	C1-C2	2.16	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	3	BMA	C1-O5-C5	5.01	118.98	112.19
5	F	1	NAG	C1-O5-C5	3.77	117.30	112.19
4	B	2	NAG	C1-O5-C5	3.37	116.76	112.19
4	B	3	BMA	O2-C2-C3	-3.26	103.60	110.14
4	B	3	BMA	C1-C2-C3	2.84	113.16	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C1-O5-C5	2.71	115.86	112.19
4	B	3	BMA	C2-C3-C4	2.67	115.51	110.89
4	B	2	NAG	O4-C4-C3	2.53	116.21	110.35
4	B	3	BMA	O5-C1-C2	2.24	114.23	110.77
5	E	1	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

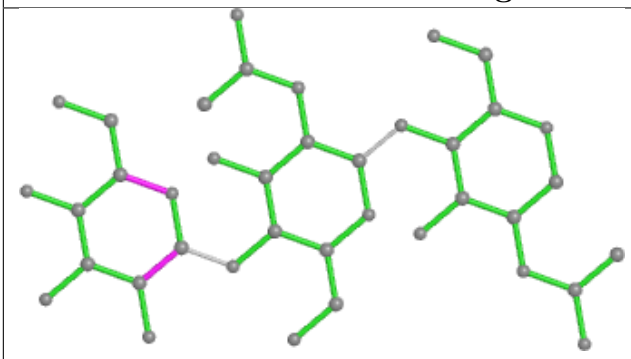
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

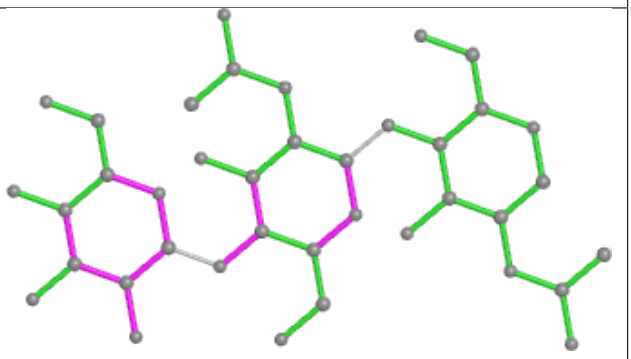
No monomer is involved in short contacts.

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

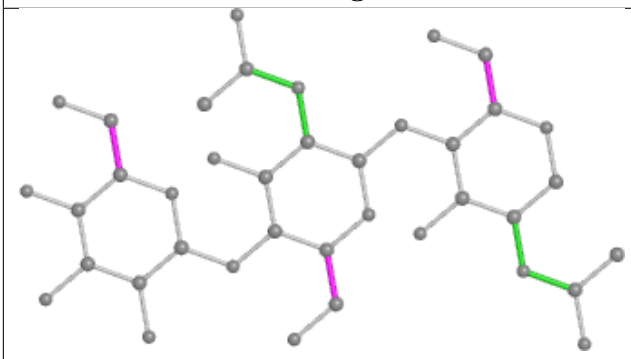
Oligosaccharide Chain B



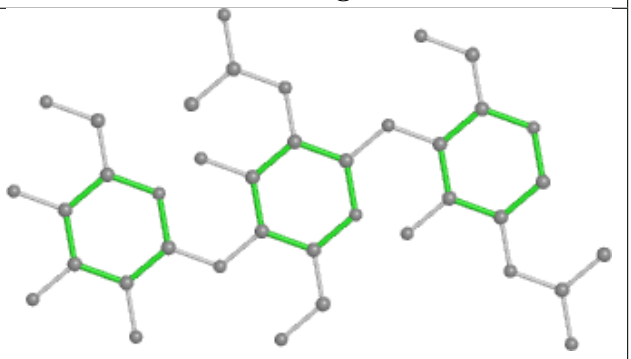
Bond lengths



Bond angles

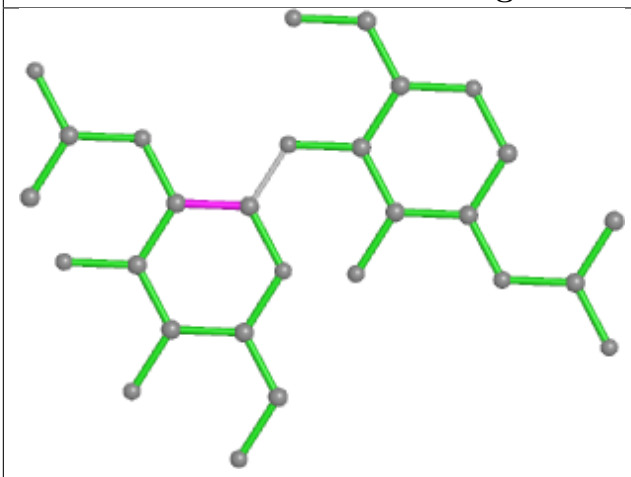


Torsions

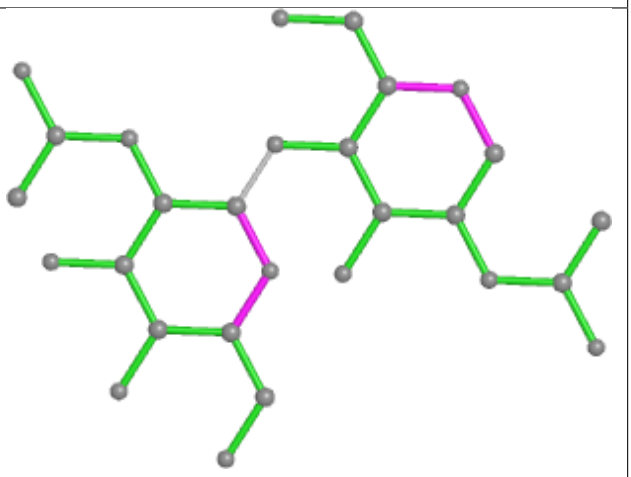


Rings

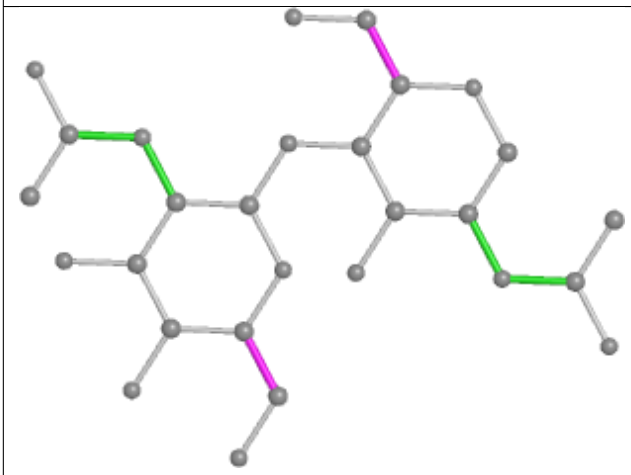
Oligosaccharide Chain E



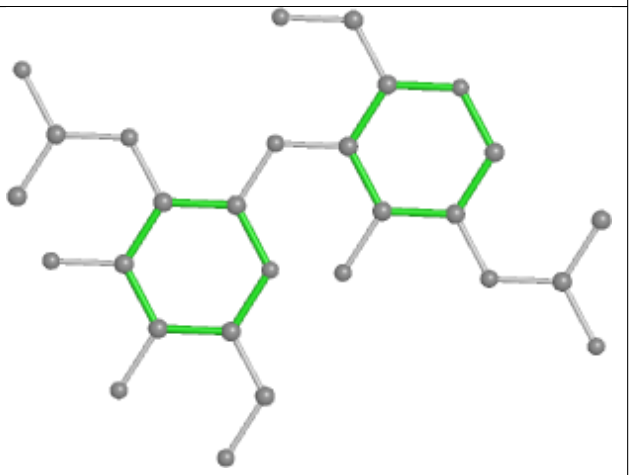
Bond lengths



Bond angles

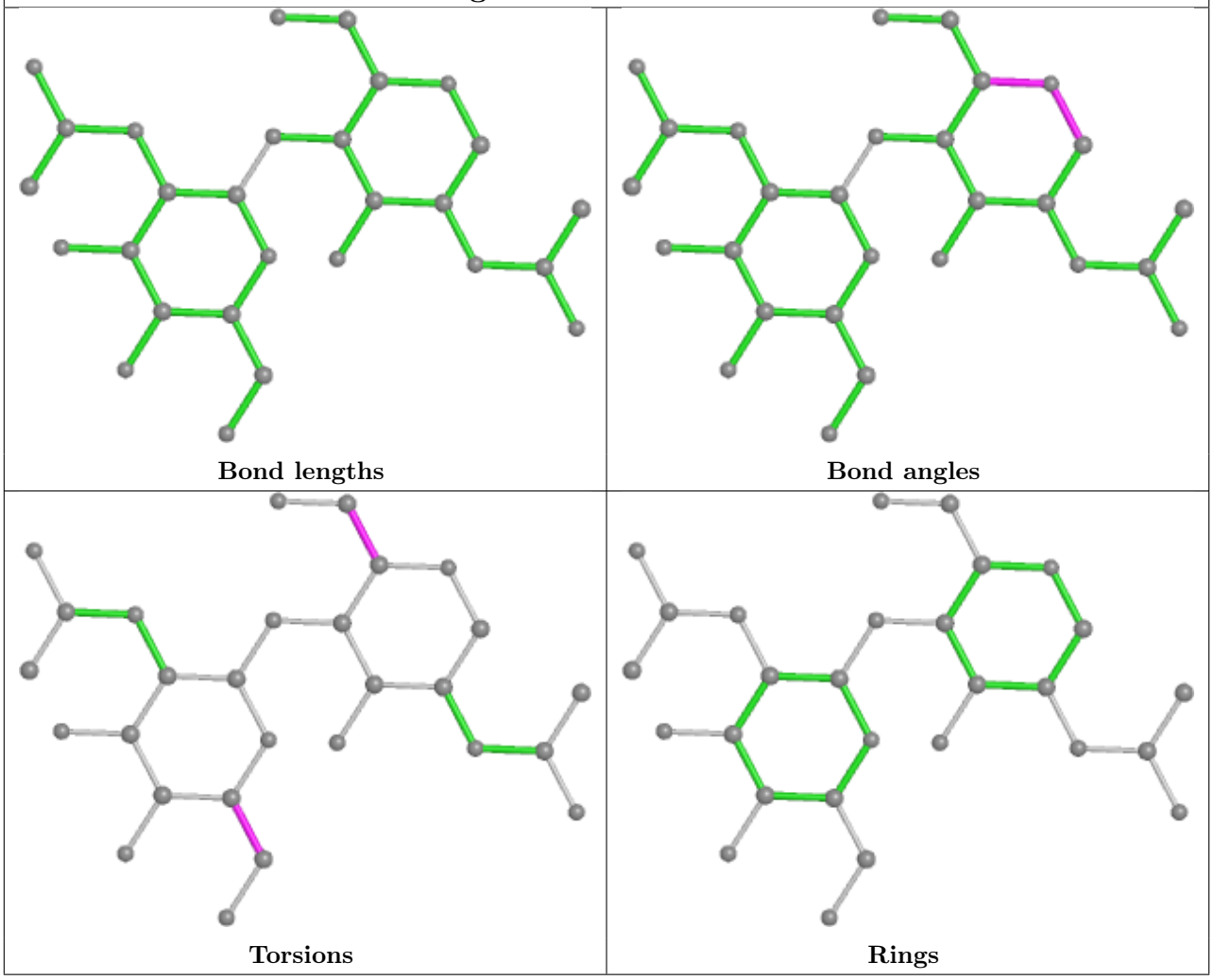


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	NAG	A	2106	2	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
7	9Z9	A	2109	-	44,44,44	0.63	2 (4%)	66,68,68	1.04	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	2106	2	-	2/6/23/26	0/1/1/1
7	9Z9	A	2109	-	-	8/12/100/100	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2109	9Z9	O80-C79	-2.05	1.40	1.43
7	A	2109	9Z9	O72-C04	-2.01	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2109	9Z9	O80-C73-C76	4.59	115.04	110.77
7	A	2109	9Z9	C77-C78-C79	3.10	112.87	108.56
6	A	2106	NAG	C1-O5-C5	2.97	116.22	112.19
7	A	2109	9Z9	C79-O80-C73	2.39	118.24	113.72
7	A	2109	9Z9	O80-C73-O72	-2.03	104.12	109.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2109	9Z9	C22-C21-O20-C17
7	A	2109	9Z9	C48-C23-C24-O25
7	A	2109	9Z9	C24-C23-C48-O49
6	A	2106	NAG	O5-C5-C6-O6
7	A	2109	9Z9	C21-C22-C23-C24
7	A	2109	9Z9	O20-C21-C22-C23
7	A	2109	9Z9	C22-C23-C24-O25
7	A	2109	9Z9	C22-C23-C48-O49
7	A	2109	9Z9	C23-C24-O25-C26
6	A	2106	NAG	C4-C5-C6-O6

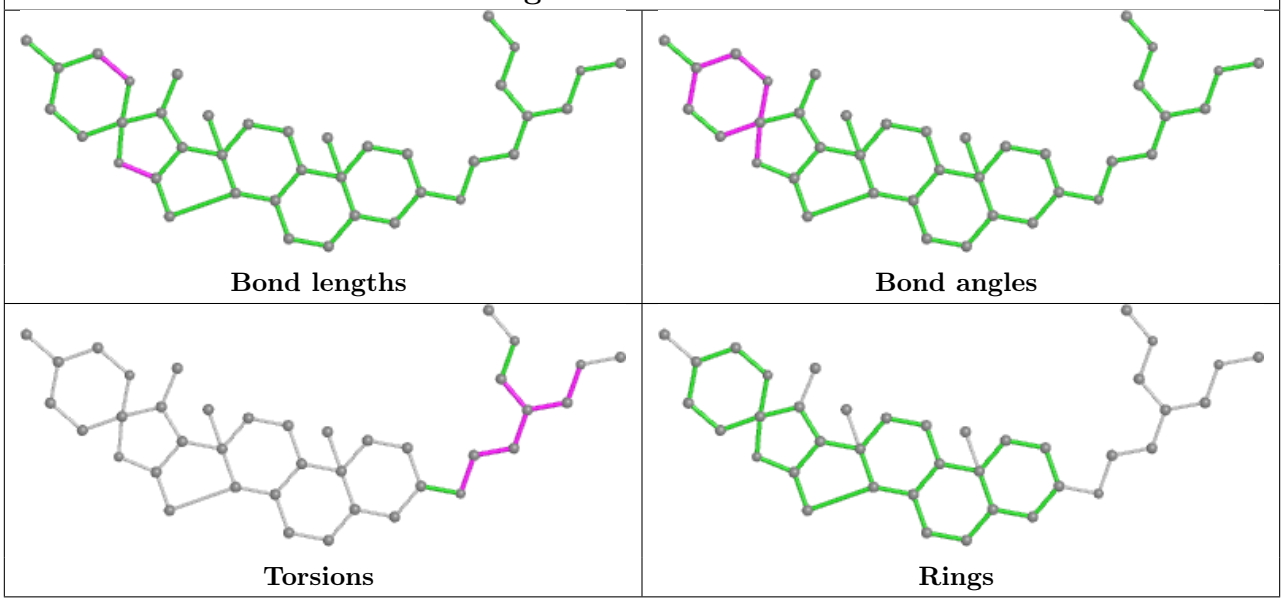
There are no ring outliers.

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 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 9Z9 A 2109



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.

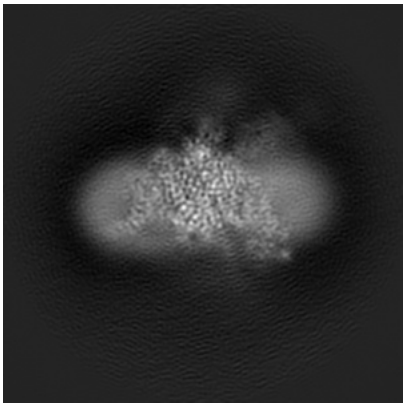
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9780. These allow visual inspection of the internal detail of the map and identification of artifacts.

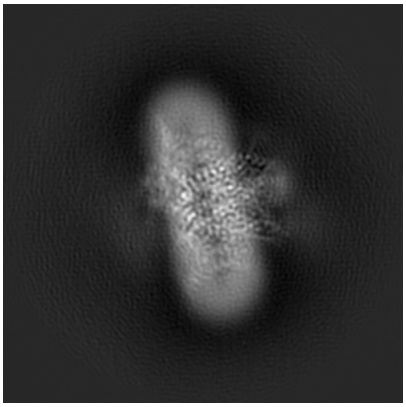
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

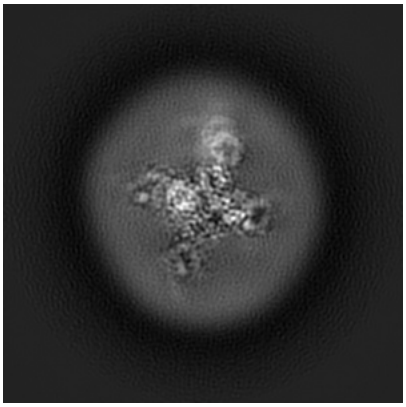
6.1.1 Primary map



X



Y

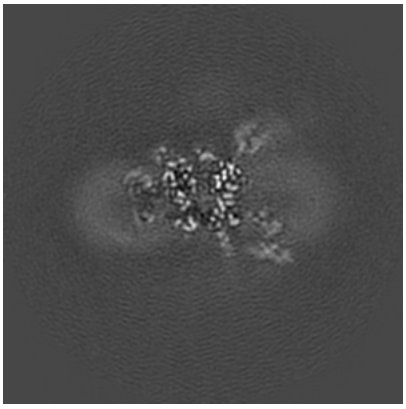


Z

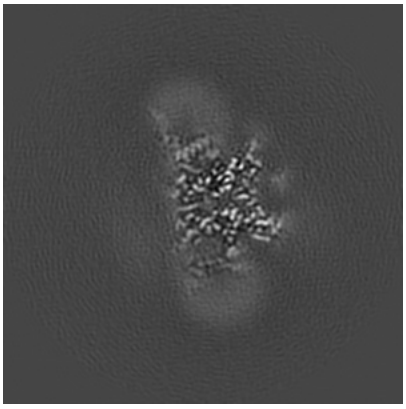
The images above show the map projected in three orthogonal directions.

6.2 Central slices

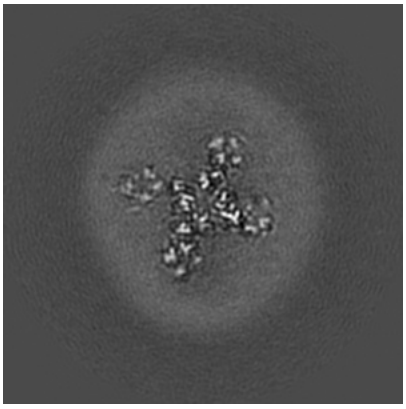
6.2.1 Primary map



X Index: 120



Y Index: 120

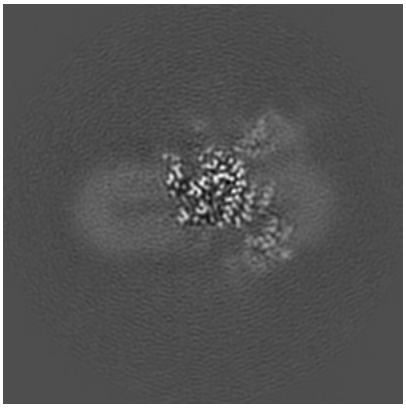


Z Index: 120

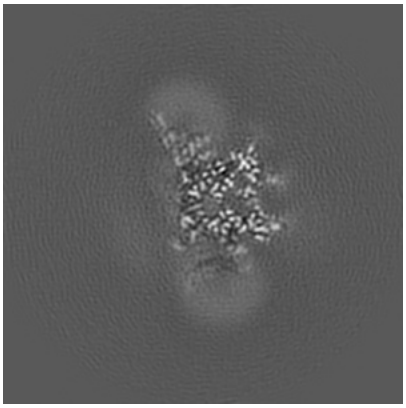
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

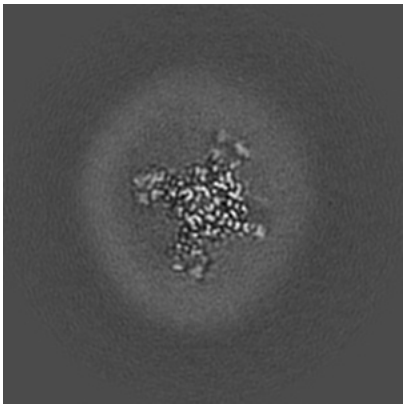
6.3.1 Primary map



X Index: 129



Y Index: 118



Z Index: 130

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.

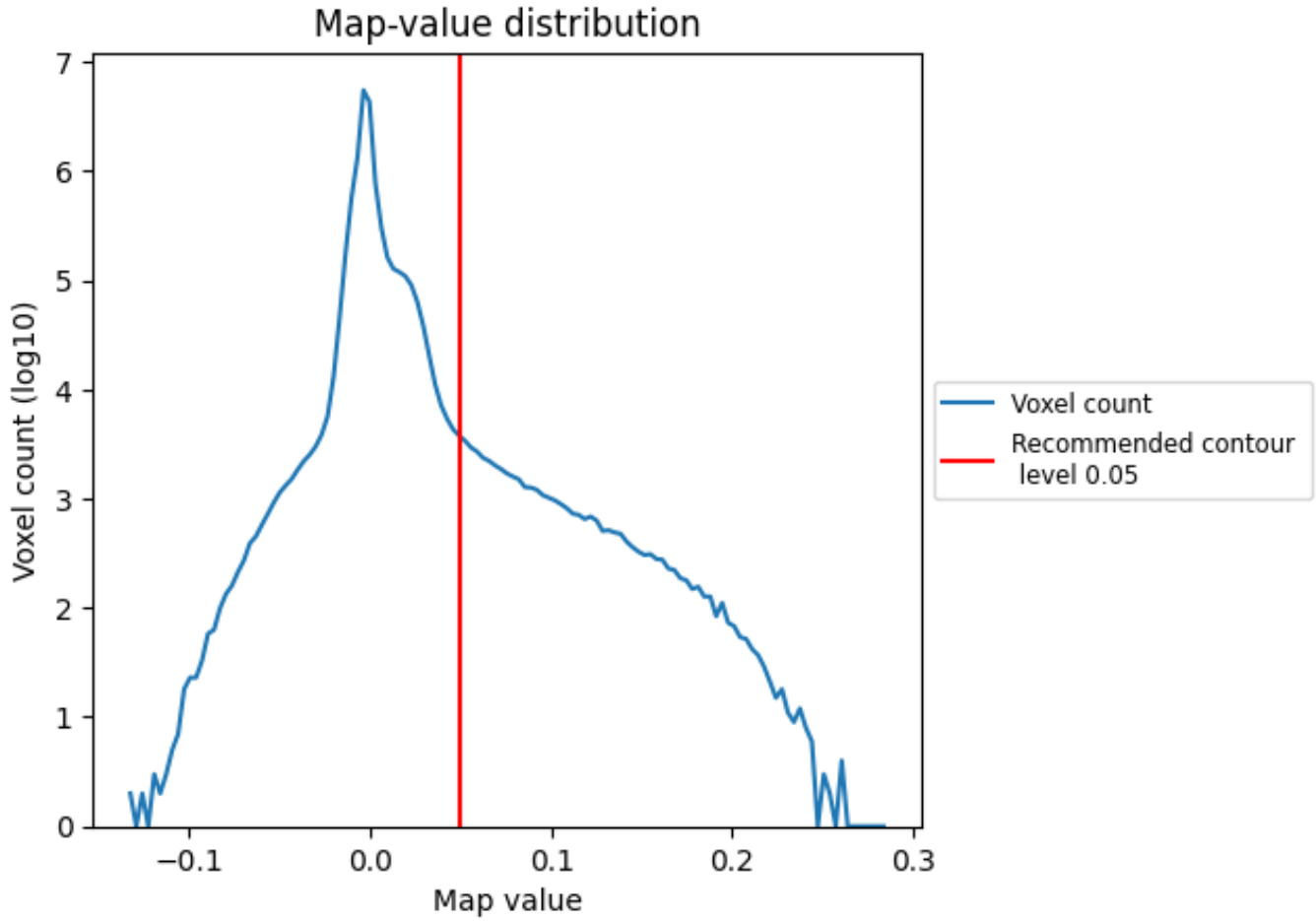
6.5 Mask visualisation (i)

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

7 Map analysis

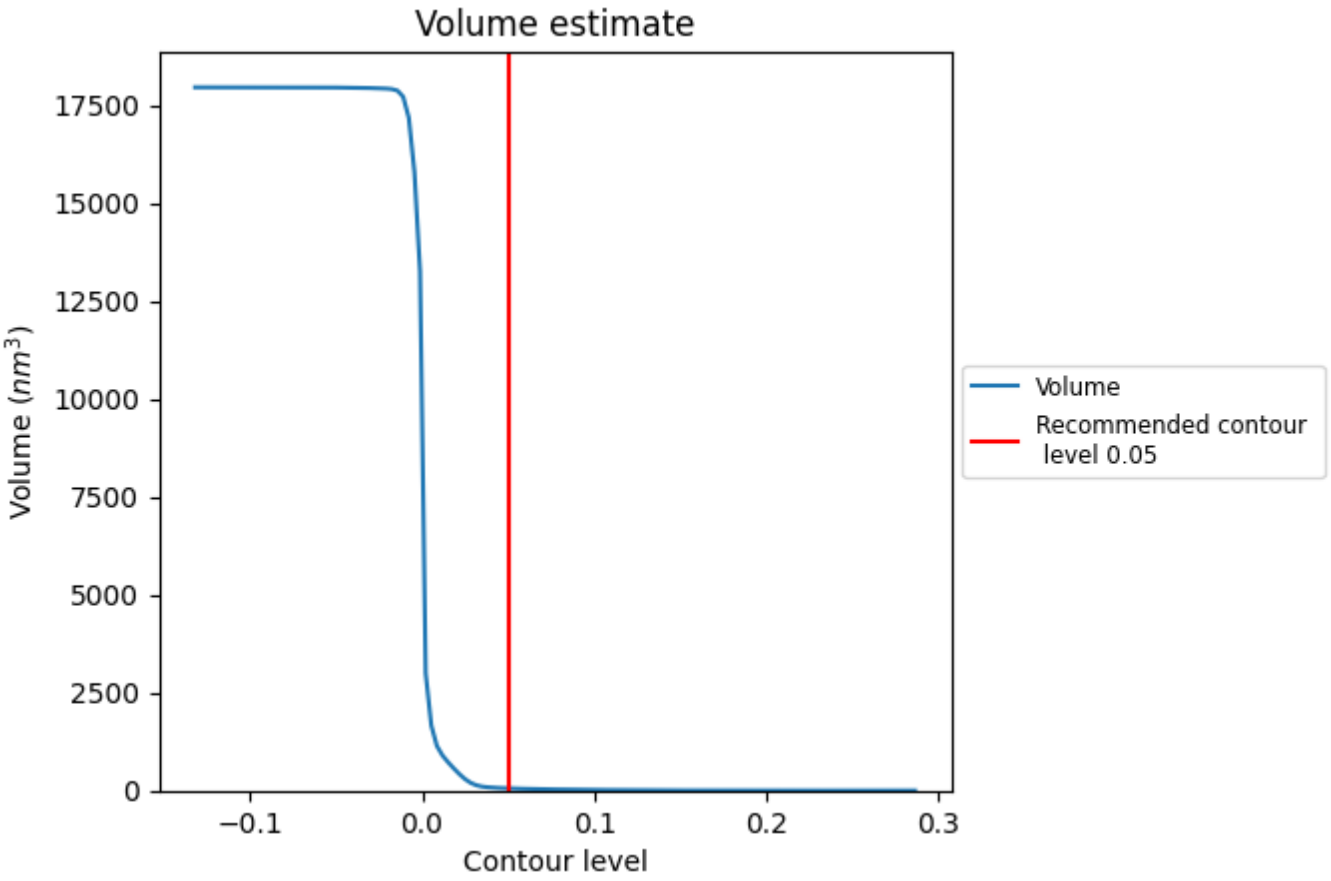
This section contains the results of statistical analysis of the map.

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.

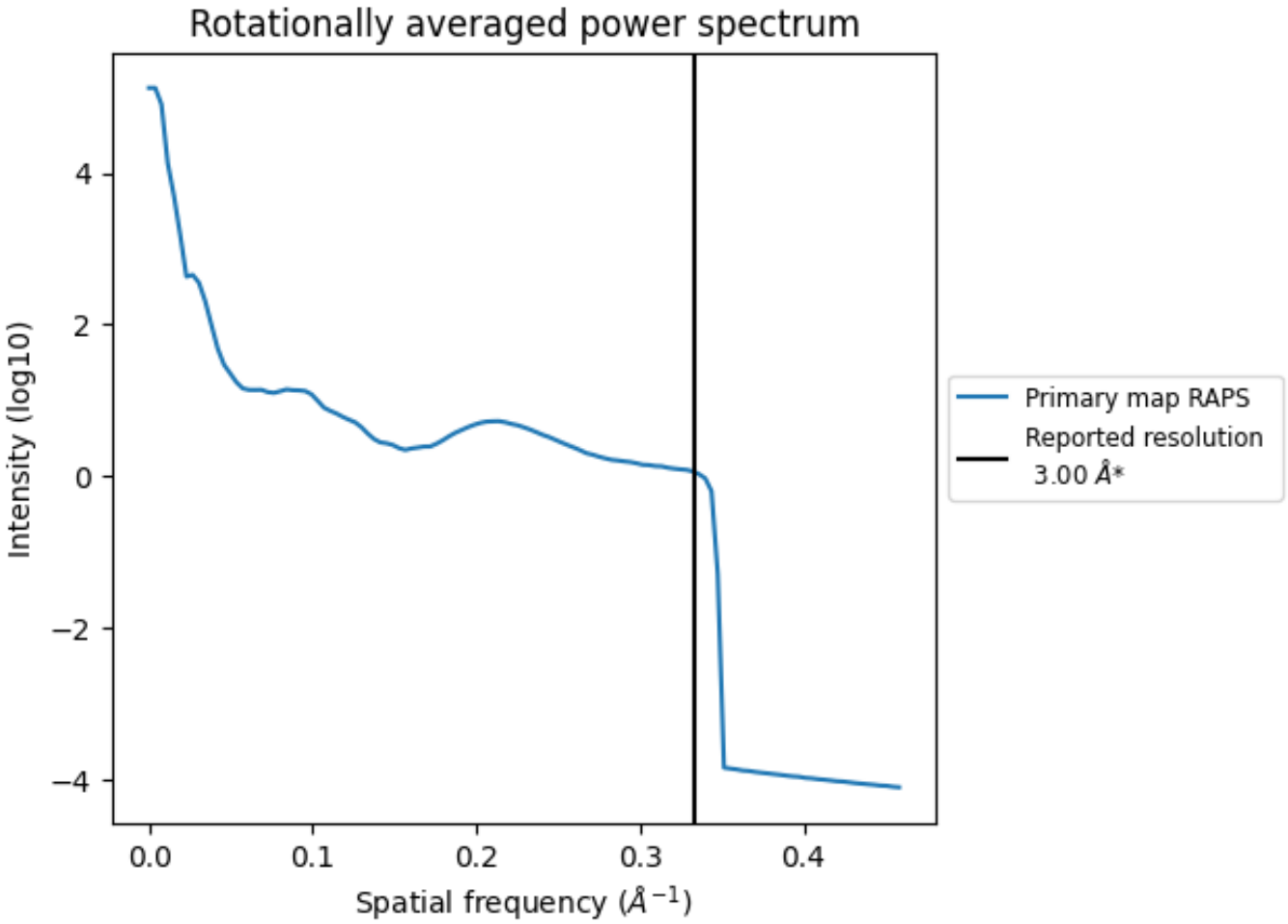
7.2 Volume estimate



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 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 0.333 $Å^{-1}$

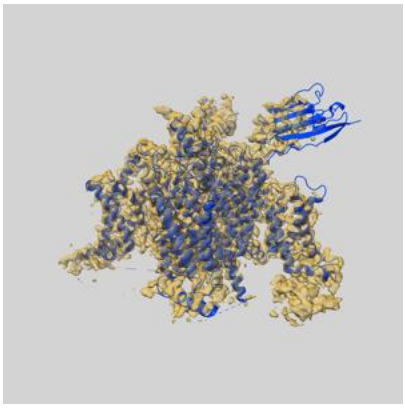
8 Fourier-Shell correlation (i)

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

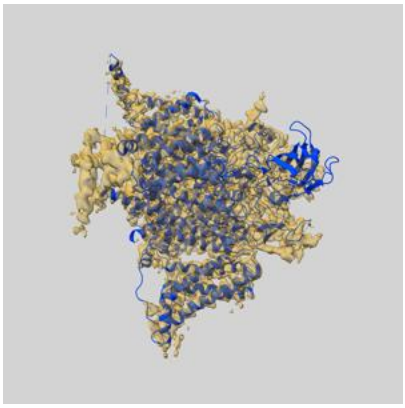
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9780 and PDB model 6J8E. Per-residue inclusion information can be found in section 3 on page 7.

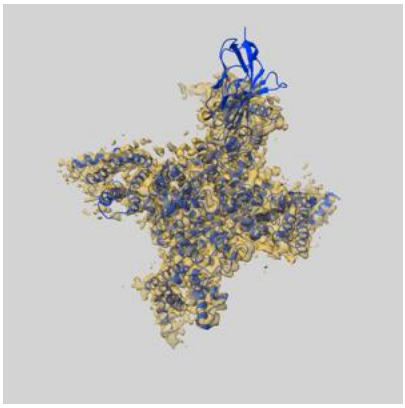
9.1 Map-model overlay



X



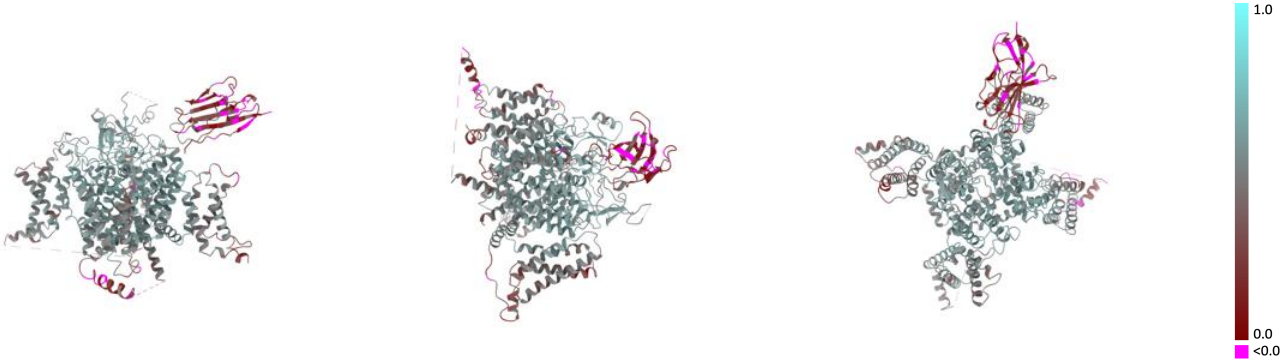
Y



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.

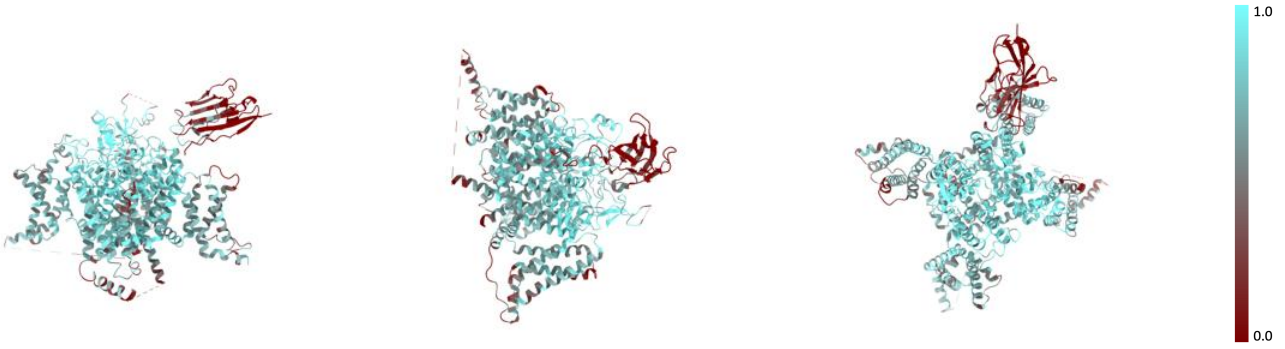
9.2 Q-score mapped to coordinate model (i)



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.

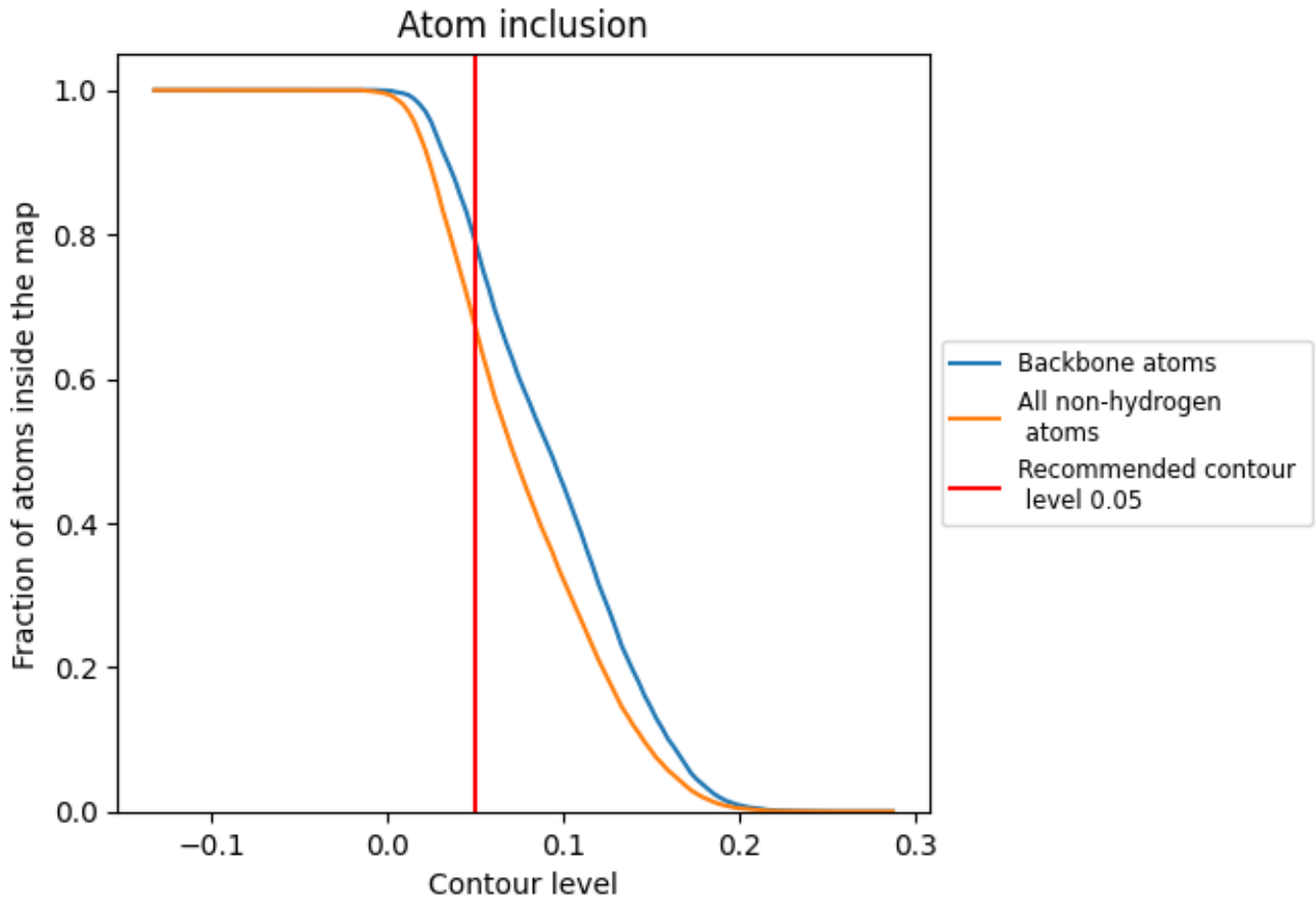
9.3 Atom inclusion mapped to coordinate model (i)



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, 67% 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	0.6710	0.4770
A	0.7213	0.5090
B	0.8462	0.5270
C	0.1629	0.1620
D	0.8667	0.5920
E	0.7143	0.4810
F	0.7857	0.4430