



Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 06:29 PM EDT

PDB ID : 7LOK
EMDB ID : EMD-23465
Title : Structure of CD4 mimetic M48U1 in complex with BG505 SOSIP.664 HIV-1 Env trimer and 17b Fab
Authors : Jette, C.A.; Bjorkman, P.J.
Deposited on : 2021-02-10
Resolution : 3.90 Å (reported)
Based on initial models : 4JZZ, 2NXY, 6U0L

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

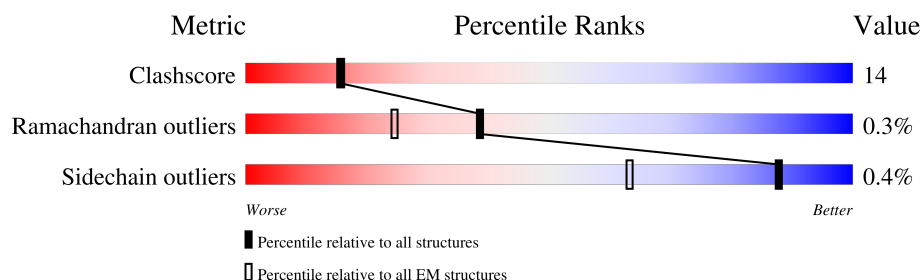
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



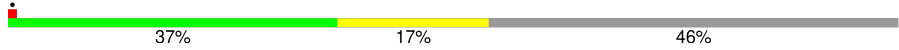

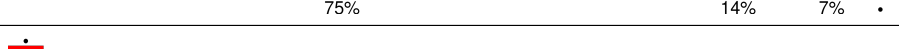
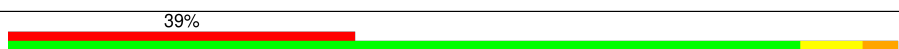

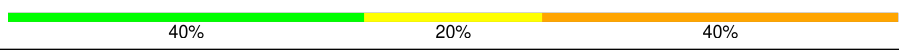


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	
1	C	479	
1	E	479	
2	B	153	
2	D	153	
2	F	153	
3	J	214	
3	L	214	

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Mol	Chain	Length	Quality of chain
4	K	239	
4	M	239	
5	G	28	
5	H	28	
5	I	28	
6	N	6	
7	O	5	
8	P	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	U2X	I	23	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14498 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 Envelope glycoprotein BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	358	Total	C	N	O	S	0	0
			2802	1769	487	522	24		
1	A	363	Total	C	N	O	S	0	0
			2832	1786	499	523	24		
1	E	353	Total	C	N	O		0	0
			1751	1041	355	355			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	509	ARG	GLU	engineered mutation	UNP Q2N0S6
C	510	ARG	LYS	engineered mutation	UNP Q2N0S6
C	511	ARG	-	insertion	UNP Q2N0S6
C	512	ARG	-	insertion	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	GLU	engineered mutation	UNP Q2N0S6
A	510	ARG	LYS	engineered mutation	UNP Q2N0S6
A	511	ARG	-	insertion	UNP Q2N0S6
A	512	ARG	-	insertion	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	GLU	engineered mutation	UNP Q2N0S6
E	510	ARG	LYS	engineered mutation	UNP Q2N0S6
E	511	ARG	-	insertion	UNP Q2N0S6
E	512	ARG	-	insertion	UNP Q2N0S6

- Molecule 2 is a protein called Envelope Glycoprotein BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			991	631	173	181	6		
2	B	123	Total	C	N	O	S	0	0
			986	624	173	183	6		
2	F	128	Total	C	N	O		0	0
			631	375	128	128			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6
D	605	CYS	THR	engineered mutation	UNP Q2N0S6
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called 17b Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			810	507	140	160	3		
3	L	109	Total	C	N	O	S	0	0
			835	523	144	165	3		

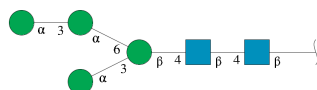
- Molecule 4 is a protein called 17b Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	129	Total	C	N	O	S	1	0
			999	628	171	197	3		
4	M	129	Total	C	N	O	S	1	0
			999	628	171	197	3		

- Molecule 5 is a protein called M48U1.

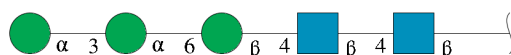
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	28	Total	C	N	O	S	0	1
			209	133	38	32	6		
5	H	28	Total	C	N	O	S	0	1
			209	133	38	32	6		
5	I	28	Total	C	N	O		0	1
			149	94	27	28			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
6	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-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
7	O	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
8	P	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

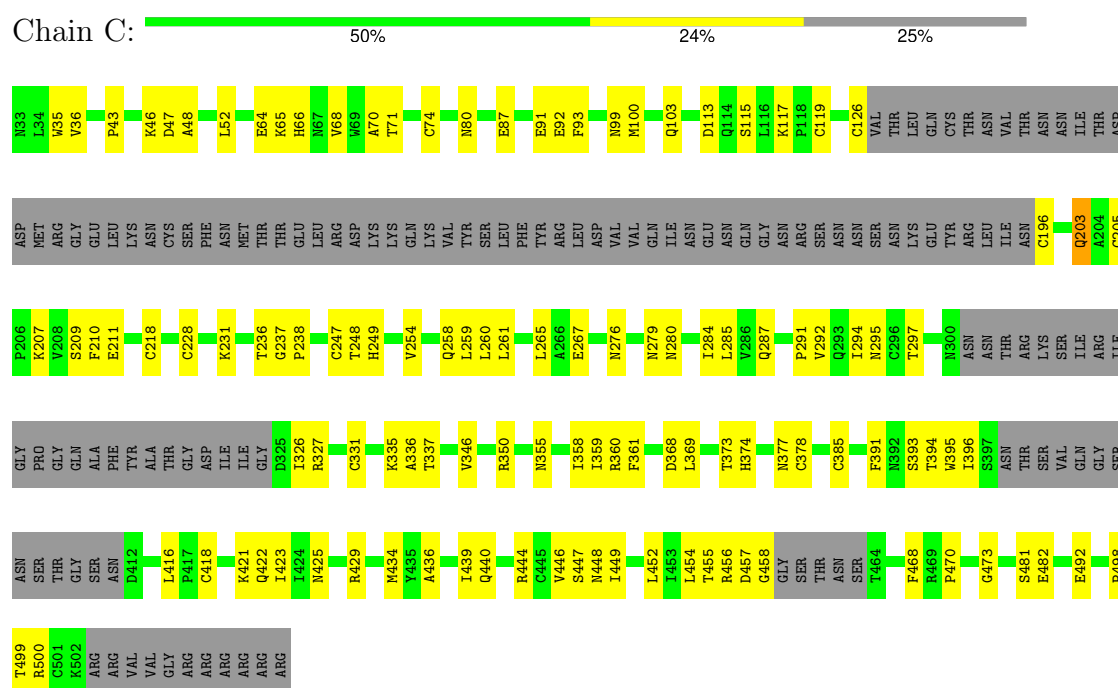


Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	

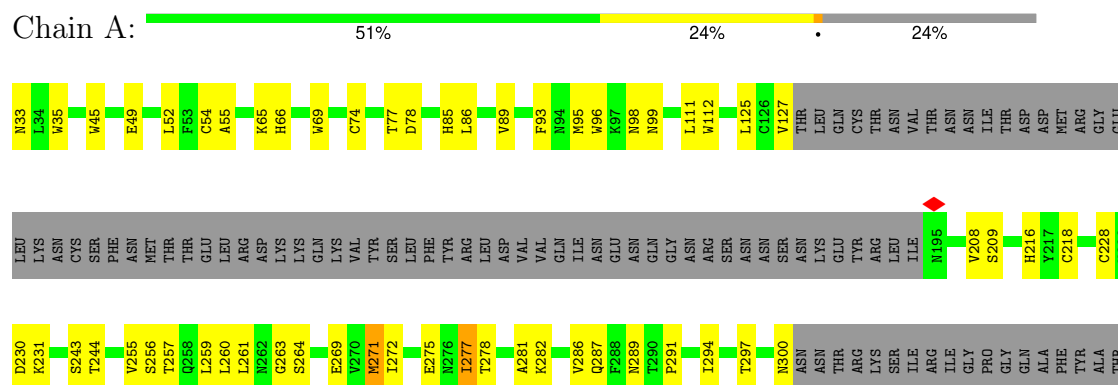
3 Residue-property plots

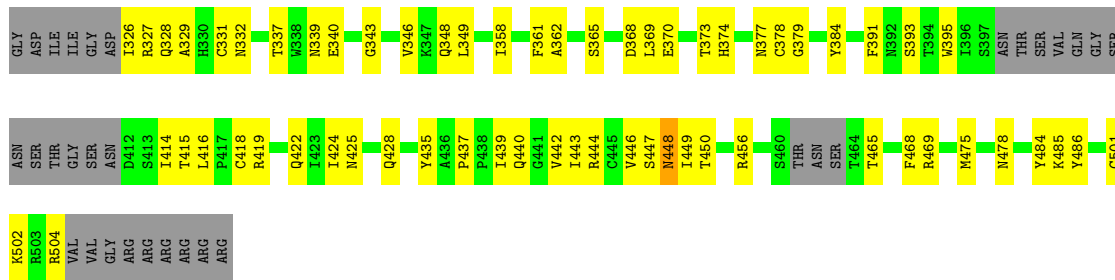
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Envelope glycoprotein BG505 SOSIP.664 gp120

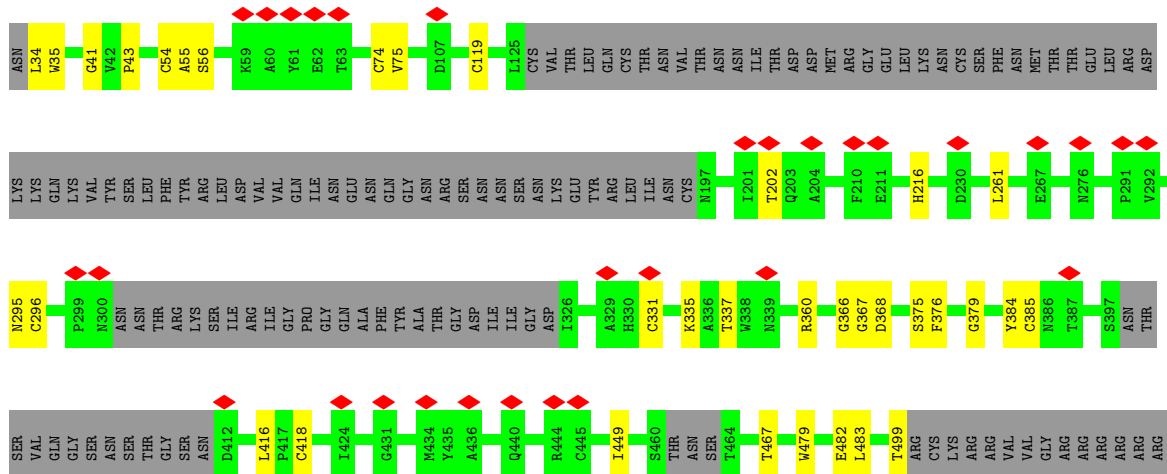


- Molecule 1: Envelope glycoprotein BG505 SOSIP.664 gp120

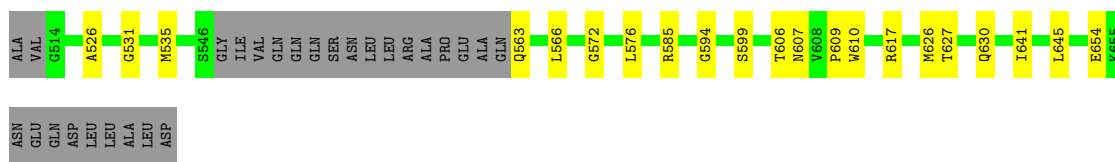




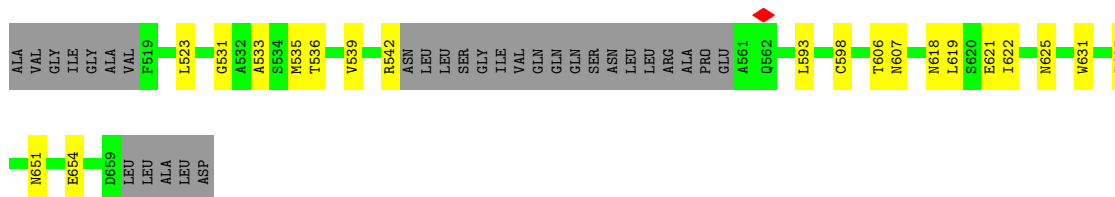
- Molecule 1: Envelope glycoprotein BG505 SOSIP.664 gp120



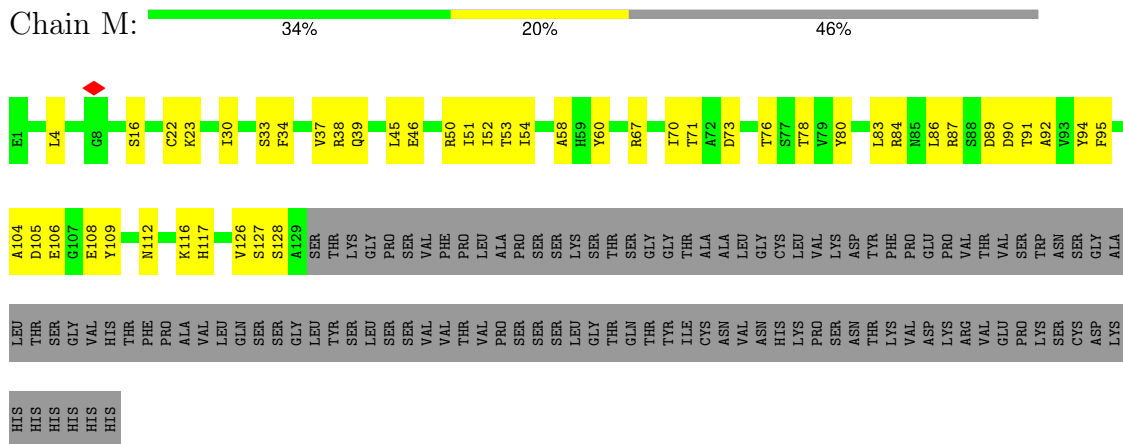
- Molecule 2: Envelope Glycoprotein BG505 SOSIP.664 gp41



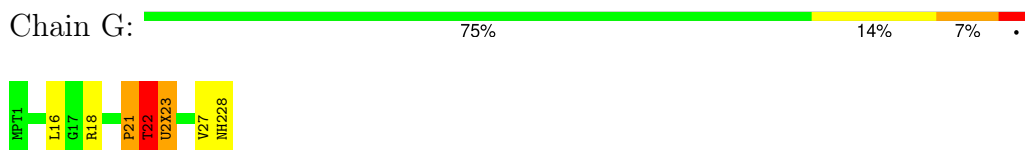
- Molecule 2: Envelope Glycoprotein BG505 SOSIP.664 gp41



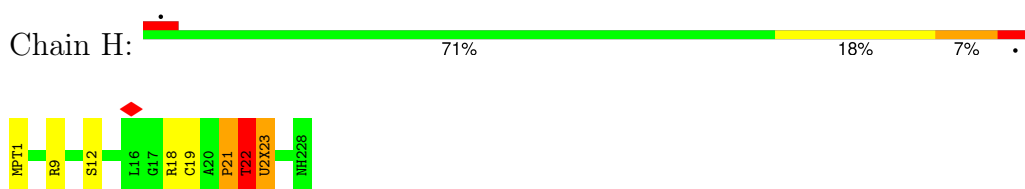
- Molecule 2: Envelope Glycoprotein BG505 SOSIP.664 gp41



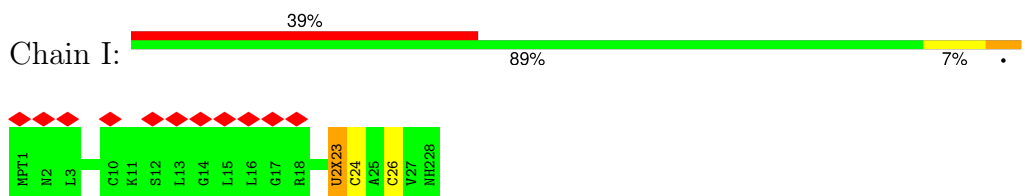
- Molecule 5: M48U1



- Molecule 5: M48U1



- Molecule 5: M48U1

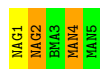


- Molecule 6: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  25% 75%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263981	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	282.624, 282.624, 282.624	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.104, 1.104, 1.104	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, MPT, NH2, NAG, U2X, BMA, DPR

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	0.41	0/2896	0.53	0/3937
1	C	0.36	0/2866	0.50	0/3897
1	E	0.33	0/1747	0.58	0/2425
2	B	0.31	0/1005	0.43	0/1361
2	D	0.32	0/1010	0.43	0/1370
2	F	0.24	0/629	0.41	0/872
3	J	0.31	0/830	0.54	1/1130 (0.1%)
3	L	0.31	0/855	0.50	0/1163
4	K	0.28	0/1026	0.46	0/1392
4	M	0.30	0/1026	0.47	0/1392
5	G	0.36	0/176	0.65	1/231 (0.4%)
5	H	0.33	0/176	0.70	1/231 (0.4%)
5	I	0.31	0/115	0.57	0/155
All	All	0.34	0/14357	0.51	3/19556 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	22	THR	N-CA-C	-6.87	92.45	111.00
5	H	22	THR	N-CA-C	-6.80	92.65	111.00
3	J	38	GLN	C-N-CA	-5.12	108.89	121.70

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	2832	0	2767	103	0
1	C	2802	0	2741	88	0
1	E	1751	0	771	48	0
2	B	986	0	963	13	0
2	D	991	0	977	17	0
2	F	631	0	287	9	0
3	J	810	0	774	31	0
3	L	835	0	805	22	0
4	K	999	0	962	27	0
4	M	999	0	962	31	0
5	G	209	0	214	7	0
5	H	209	0	214	8	0
5	I	149	0	85	25	0
6	N	72	0	61	3	0
7	O	61	0	52	8	0
8	P	50	0	43	3	0
9	A	84	0	78	5	0
9	C	14	0	13	1	0
9	E	14	0	13	1	0
All	All	14498	0	12782	391	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 14.

All (391) 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)
2:F:522:PHE:CB	1:E:41:GLY:O	1.68	1.40
1:E:367:GLY:HA2	5:I:26:CYS:CB	1.53	1.39
2:F:523:LEU:CB	1:E:43:PRO:O	1.72	1.36
1:A:263:GLY:HA3	1:A:450:THR:OG1	1.30	1.27
1:E:367:GLY:CA	5:I:26:CYS:CB	2.19	1.20
1:E:376:PHE:HA	5:I:23:U2X:C6	1.76	1.16
1:A:365:SER:HG	5:G:28:NH2:N	1.51	1.05
1:E:367:GLY:HA3	5:I:26:CYS:H	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:CA	1:A:450:THR:OG1	2.06	1.03
1:A:485:LYS:O	1:A:486:TYR:CD2	2.19	0.94
1:C:218:CYS:HA	1:C:247:CYS:HB3	1.47	0.93
1:A:331:CYS:HB2	1:A:416:LEU:HB2	1.52	0.91
1:E:376:PHE:CA	5:I:23:U2X:C6	2.49	0.90
1:A:263:GLY:O	1:A:450:THR:HG21	1.71	0.89
1:C:261:LEU:HD11	1:C:374:HIS:NE2	1.88	0.89
1:C:211:GLU:OE1	1:C:211:GLU:N	2.08	0.86
1:E:367:GLY:HA3	5:I:26:CYS:N	1.90	0.85
1:E:366:GLY:O	5:I:26:CYS:CB	2.25	0.84
1:E:376:PHE:HA	5:I:23:U2X:H62	1.56	0.84
1:A:96:TRP:CG	1:A:275:GLU:OE1	2.30	0.84
1:E:376:PHE:HA	5:I:23:U2X:C1	2.11	0.80
2:F:519:PHE:O	1:E:43:PRO:CB	2.30	0.79
2:F:522:PHE:CA	1:E:41:GLY:O	2.31	0.78
1:E:376:PHE:HA	5:I:23:U2X:H61	1.66	0.77
1:A:378:CYS:HA	7:O:2:NAG:H81	1.67	0.76
1:E:366:GLY:O	5:I:26:CYS:O	2.04	0.76
1:A:277:ILE:HG23	1:A:278:THR:HG23	1.65	0.76
1:A:393:SER:OG	1:A:395:TRP:NE1	2.18	0.76
1:E:376:PHE:N	5:I:23:U2X:H61	2.01	0.76
1:E:376:PHE:CA	5:I:23:U2X:H61	2.15	0.75
5:H:1:MPT:CB	5:H:19:CYS:HG	1.98	0.75
1:C:294:ILE:HG22	1:C:447:SER:O	1.87	0.74
1:E:376:PHE:CA	5:I:23:U2X:H62	2.14	0.74
7:O:2:NAG:O7	7:O:2:NAG:O3	2.05	0.73
4:K:67:ARG:HH21	4:K:83:LEU:HD21	1.55	0.71
4:K:91:THR:HG23	4:K:125:THR:HA	1.71	0.71
1:E:295:ASN:HB3	9:E:601:NAG:C7	2.21	0.70
1:A:475:MET:SD	1:A:478:ASN:ND2	2.65	0.70
1:C:259:LEU:HB2	1:C:374:HIS:HD2	1.57	0.69
3:J:54:ARG:NH1	3:J:63:SER:HG	1.91	0.69
3:J:19:ALA:HB3	3:J:75:ILE:HB	1.74	0.68
5:H:1:MPT:HG	5:H:19:CYS:HG	0.98	0.68
1:A:379:GLY:H	7:O:2:NAG:H81	1.58	0.68
4:M:108:GLU:OE1	4:M:109:TYR:N	2.26	0.68
1:A:327:ARG:O	1:A:419:ARG:NH2	2.26	0.68
1:A:263:GLY:HA3	1:A:450:THR:HG1	1.58	0.67
1:C:236:THR:HG22	1:C:237:GLY:H	1.60	0.66
3:J:8:PRO:HG3	3:J:11:LEU:HD13	1.77	0.66
1:E:376:PHE:HA	5:I:23:U2X:H11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:120:GLN:NE2	4:K:121:GLY:O	2.29	0.66
1:C:331:CYS:HB3	1:C:416:LEU:HB2	1.78	0.66
4:K:31:ARG:NH2	4:K:105:ASP:OD2	2.29	0.66
1:A:294:ILE:HD12	1:A:449:ILE:HD11	1.78	0.66
4:M:38:ARG:NE	4:M:46:GLU:OE1	2.29	0.66
3:J:54:ARG:NH1	3:J:63:SER:OG	2.30	0.65
1:E:367:GLY:N	5:I:26:CYS:CB	2.60	0.65
3:J:37:GLN:HB2	3:J:47:LEU:HD11	1.78	0.65
1:A:291:PRO:HB2	1:A:448:ASN:HB3	1.79	0.64
3:L:38:GLN:NE2	3:L:39:LYS:O	2.30	0.64
1:C:350:ARG:HD3	1:C:355:ASN:HA	1.78	0.64
8:P:1:NAG:H82	8:P:1:NAG:O3	1.97	0.64
1:E:366:GLY:O	5:I:26:CYS:C	2.36	0.64
2:D:617:ARG:NH1	2:D:626:MET:SD	2.71	0.64
1:E:375:SER:O	5:I:23:U2X:H22	1.97	0.63
1:C:373:THR:OG1	1:C:385:CYS:O	2.16	0.63
1:C:499:THR:HG22	1:C:500:ARG:H	1.63	0.63
2:F:568:LEU:O	2:F:572:GLY:N	2.29	0.62
1:E:479:TRP:O	1:E:482:GLU:N	2.29	0.62
1:A:365:SER:OG	5:G:28:NH2:N	2.29	0.62
1:A:230:ASP:OD1	1:A:231:LYS:N	2.32	0.62
1:A:260:LEU:O	1:A:261:LEU:HD12	1.99	0.62
1:A:328:GLN:HB3	1:A:419:ARG:HH21	1.65	0.62
4:K:6:GLU:HB2	4:K:120:GLN:HE22	1.65	0.62
2:D:627:THR:H	2:D:630:GLN:HE21	1.47	0.62
1:A:393:SER:HG	1:A:395:TRP:HE1	1.48	0.62
1:A:373:THR:HG22	1:A:374:HIS:H	1.63	0.61
1:E:366:GLY:C	5:I:26:CYS:CB	2.67	0.61
3:L:29:VAL:O	3:L:29:VAL:HG12	2.00	0.61
3:J:35:TRP:HD1	3:J:48:ILE:HB	1.64	0.60
4:K:116:LYS:HG3	4:K:117:HIS:CD2	2.36	0.60
3:J:15:PRO:HA	3:J:78:LEU:HD22	1.83	0.60
7:O:4:MAN:O6	7:O:4:MAN:O4	2.18	0.59
1:A:456:ARG:HG2	1:A:468:PHE:HE1	1.68	0.59
1:A:89:VAL:O	1:A:89:VAL:HG13	2.03	0.59
1:C:346:VAL:HG23	1:C:359:ILE:HD11	1.83	0.59
4:M:16:SER:O	4:M:86:LEU:HG	2.03	0.59
1:A:485:LYS:O	1:A:485:LYS:HG3	2.02	0.59
1:C:423:ILE:HG22	1:C:434:MET:HB2	1.85	0.59
9:A:605:NAG:C3	9:A:605:NAG:H83	2.33	0.59
4:M:60:TYR:OH	4:M:70:ILE:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:O	1:A:418:CYS:N	2.36	0.58
1:E:56:SER:N	1:E:75:VAL:O	2.36	0.58
1:A:45:TRP:HE1	2:B:523:LEU:HD13	1.66	0.58
1:A:209:SER:HB3	7:O:4:MAN:H61	1.84	0.58
1:A:362:ALA:HB3	1:A:469:ARG:HG2	1.85	0.58
1:E:375:SER:C	5:I:23:U2X:H61	2.23	0.58
1:C:35:TRP:HD1	2:D:609:PRO:HA	1.67	0.58
1:C:284:ILE:HD11	1:C:454:LEU:HD12	1.84	0.58
5:H:21:DPR:HA	5:H:23:U2X:HB3	1.86	0.58
1:C:35:TRP:CD1	2:D:609:PRO:HA	2.39	0.58
1:C:456:ARG:HG3	1:C:468:PHE:HE1	1.69	0.58
6:N:2:NAG:O3	6:N:2:NAG:H82	2.03	0.58
1:A:361:PHE:O	1:A:391:PHE:O	2.22	0.58
3:L:90:GLN:NE2	3:L:99:THR:OG1	2.34	0.57
3:L:39:LYS:HB2	3:L:42:GLN:HB2	1.85	0.57
1:A:243:SER:OG	1:A:244:THR:N	2.37	0.57
1:C:327:ARG:HH21	1:C:422:GLN:HE22	1.51	0.57
1:A:329:ALA:N	1:A:418:CYS:O	2.37	0.56
1:A:504:ARG:O	1:A:504:ARG:NH1	2.32	0.56
1:C:113:ASP:OD2	1:C:429:ARG:NH2	2.36	0.56
9:A:605:NAG:H83	9:A:605:NAG:O3	2.05	0.56
1:C:259:LEU:HB2	1:C:374:HIS:CD2	2.40	0.56
4:K:38:ARG:NE	4:K:46:GLU:OE1	2.31	0.56
1:A:263:GLY:O	1:A:450:THR:CG2	2.50	0.56
1:A:49:GLU:OE1	1:A:99:ASN:ND2	2.39	0.56
1:A:297:THR:OG1	1:A:443:ILE:O	2.11	0.56
1:A:361:PHE:HB3	1:A:391:PHE:HB3	1.86	0.56
3:L:20:THR:HA	3:L:74:THR:HA	1.88	0.56
1:C:209:SER:HA	6:N:4:MAN:H62	1.87	0.56
3:J:6:GLN:OE1	3:J:103:GLY:N	2.28	0.56
4:M:60:TYR:HE2	4:M:70:ILE:HG13	1.70	0.56
1:A:485:LYS:C	1:A:486:TYR:CD2	2.79	0.56
1:E:368:ASP:CB	5:I:24:CYS:O	2.54	0.56
1:C:70:ALA:O	1:C:74:CYS:HB2	2.06	0.55
1:C:294:ILE:CG2	1:C:447:SER:O	2.55	0.55
3:L:21:LEU:N	3:L:73:LEU:O	2.35	0.55
1:C:368:ASP:OD2	1:C:425:ASN:ND2	2.40	0.55
4:K:3:GLN:N	4:K:25:SER:O	2.37	0.55
1:C:231:LYS:NZ	1:C:267:GLU:OE2	2.33	0.55
1:C:331:CYS:HB2	1:C:418:CYS:SG	2.47	0.55
1:A:281:ALA:HA	5:G:18:ARG:HH12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:OE2	1:A:384:TYR:OH	2.22	0.54
1:A:424:ILE:HD11	1:A:435:TYR:HE2	1.72	0.54
1:C:482:GLU:OE2	1:C:482:GLU:N	2.40	0.54
1:E:367:GLY:CA	5:I:26:CYS:N	2.65	0.54
1:A:98:ASN:OD1	1:A:99:ASN:N	2.41	0.54
1:E:416:LEU:O	1:E:418:CYS:N	2.41	0.54
1:C:374:HIS:O	1:C:374:HIS:ND1	2.41	0.54
1:C:43:PRO:HB2	2:D:526:ALA:HB2	1.90	0.54
4:M:23:LYS:HD2	4:M:78:THR:HG22	1.89	0.54
1:C:210:PHE:C	1:C:211:GLU:OE1	2.45	0.53
1:A:291:PRO:HB2	1:A:448:ASN:CB	2.38	0.53
1:E:385:CYS:HA	1:E:418:CYS:HA	1.88	0.53
1:C:93:PHE:CE2	1:C:228:CYS:HB2	2.43	0.53
2:B:631:TRP:CZ2	2:B:635:ILE:HG13	2.43	0.53
2:B:531:GLY:O	2:B:535:MET:HG2	2.09	0.53
2:F:622:ILE:CB	1:E:34:LEU:CB	2.86	0.53
1:C:265:LEU:HA	1:C:287:GLN:HE21	1.73	0.53
1:C:377:ASN:OD1	1:C:378:CYS:N	2.42	0.53
1:A:35:TRP:CE2	1:A:502:LYS:HD3	2.44	0.53
2:F:632:ASP:O	2:F:636:SER:N	2.41	0.53
1:E:376:PHE:C	5:I:23:U2X:H62	2.29	0.53
5:H:9:ARG:O	5:H:12:SER:OG	2.25	0.53
1:C:421:LYS:NZ	4:M:106:GLU:O	2.32	0.53
1:A:368:ASP:OD2	1:A:369:LEU:N	2.42	0.52
3:J:93:ASN:HD21	3:J:97:ARG:HB2	1.73	0.52
4:M:51:ILE:HD13	4:M:58:ALA:HB2	1.90	0.52
1:E:479:TRP:C	1:E:482:GLU:H	2.12	0.52
1:A:456:ARG:HG2	1:A:468:PHE:CE1	2.45	0.52
3:J:29:VAL:HG11	3:J:90:GLN:HB2	1.92	0.52
1:C:47:ASP:OD2	1:C:48:ALA:N	2.42	0.52
1:A:377:ASN:OD1	1:A:378:CYS:N	2.42	0.52
1:A:378:CYS:HA	7:O:2:NAG:C8	2.38	0.52
5:H:1:MPT:HG	5:H:19:CYS:CB	2.23	0.52
1:A:331:CYS:O	1:A:415:THR:HA	2.09	0.52
4:K:27:ASP:OD2	4:K:28:THR:N	2.41	0.52
4:M:87:ARG:NH2	4:M:90:ASP:OD1	2.39	0.52
1:C:295:ASN:HA	1:C:446:VAL:HG12	1.92	0.52
4:K:101:GLU:OE2	4:K:112:ASN:ND2	2.43	0.52
1:C:457:ASP:OD1	1:C:457:ASP:N	2.41	0.52
2:D:654:GLU:OE1	2:D:654:GLU:N	2.35	0.52
3:L:35:TRP:HD1	3:L:48:ILE:HB	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:54:ARG:HB2	3:L:58:VAL:HG11	1.92	0.51
1:A:281:ALA:O	1:A:282:LYS:NZ	2.28	0.51
1:C:498:PRO:HB3	2:D:610:TRP:CG	2.46	0.51
1:E:479:TRP:O	1:E:483:LEU:N	2.36	0.51
1:C:91:GLU:OE2	1:C:92:GLU:N	2.35	0.51
1:C:258:GLN:NE2	1:C:470:PRO:O	2.37	0.51
4:M:30:ILE:HA	4:M:53:THR:HG21	1.93	0.51
4:M:54:ILE:HD12	4:M:104:ALA:HB1	1.92	0.51
1:C:248:THR:OG1	1:C:249:HIS:N	2.44	0.51
3:L:37:GLN:NE2	3:L:86:TYR:OH	2.44	0.51
1:A:66:HIS:CE1	1:A:111:LEU:HD21	2.45	0.50
1:A:77:THR:OG1	1:A:78:ASP:N	2.43	0.50
3:L:81:GLU:N	3:L:81:GLU:OE1	2.45	0.50
3:J:17:GLU:O	3:J:78:LEU:N	2.40	0.50
7:O:2:NAG:HO3	7:O:2:NAG:C7	2.15	0.50
1:C:280:ASN:HD21	1:C:458:GLY:H	1.59	0.50
4:M:50:ARG:NH2	4:M:112:ASN:O	2.45	0.50
1:C:52:LEU:HB3	1:C:218:CYS:O	2.12	0.50
1:C:276:ASN:HD22	1:C:279:ASN:HD22	1.60	0.50
1:C:267:GLU:N	1:C:267:GLU:OE1	2.45	0.50
1:C:65:LYS:HB3	1:C:115:SER:OG	2.11	0.50
1:A:275:GLU:OE1	1:A:275:GLU:HA	2.11	0.50
1:C:117:LYS:HD2	1:C:203:GLN:OE1	2.12	0.49
3:L:100:PHE:CE2	4:M:45:LEU:HB2	2.47	0.49
1:A:379:GLY:N	7:O:2:NAG:H81	2.27	0.49
2:B:618:ASN:HB3	2:B:621:GLU:HG3	1.94	0.49
3:L:61:ARG:NH2	3:L:82:ASP:OD2	2.33	0.49
4:M:33:SER:OG	4:M:34:PHE:N	2.46	0.49
4:M:73:ASP:OD2	4:M:76:THR:HG22	2.13	0.49
1:C:261:LEU:HD23	1:C:449:ILE:HA	1.94	0.49
1:A:331:CYS:O	1:A:416:LEU:N	2.46	0.49
2:F:589:ASP:O	2:F:592:LEU:N	2.45	0.49
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.95	0.49
3:J:98:TYR:HB2	4:K:47:TRP:CD2	2.48	0.49
1:A:264:SER:O	1:A:287:GLN:NE2	2.46	0.48
4:M:60:TYR:CE2	4:M:70:ILE:HG13	2.47	0.48
1:E:379:GLY:O	8:P:4:MAN:H61	2.13	0.48
3:J:10:THR:HG23	3:J:105:ARG:HB3	1.95	0.48
4:K:105:ASP:OD1	4:K:105:ASP:N	2.44	0.48
1:E:366:GLY:O	5:I:26:CYS:CA	2.62	0.48
2:D:606:THR:OG1	2:D:607:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HG	1:A:127:VAL:HG23	1.96	0.48
1:A:294:ILE:HG22	1:A:447:SER:O	2.14	0.48
4:M:87:ARG:NH2	4:M:89:ASP:OD2	2.47	0.48
1:A:85:HIS:ND1	1:A:86:LEU:O	2.41	0.48
1:A:96:TRP:CD1	1:A:275:GLU:OE1	2.64	0.48
3:J:18:ARG:HB2	3:J:76:SER:HA	1.94	0.48
1:A:269:GLU:OE1	1:A:348:GLN:NE2	2.42	0.48
3:J:49:TYR:O	3:J:53:THR:OG1	2.29	0.48
1:C:64:GLU:HG2	1:C:66:HIS:H	1.79	0.48
3:L:38:GLN:O	3:L:84:ALA:HB1	2.14	0.48
5:G:16:LEU:O	5:G:27:VAL:N	2.47	0.48
4:K:51:ILE:HD13	4:K:58:ALA:HB2	1.96	0.48
1:C:456:ARG:HG2	1:C:457:ASP:H	1.79	0.47
9:A:605:NAG:H83	9:A:605:NAG:H3	1.96	0.47
1:C:52:LEU:HD11	1:C:100:MET:HG2	1.97	0.47
1:A:332:ASN:HA	1:A:414:ILE:O	2.15	0.47
4:K:66:GLY:O	4:K:84:ARG:NH2	2.42	0.47
1:C:261:LEU:HD11	1:C:374:HIS:CE1	2.49	0.47
2:D:531:GLY:O	2:D:535:MET:HG2	2.14	0.47
1:A:96:TRP:CD2	1:A:275:GLU:OE1	2.68	0.47
1:A:272:ILE:HD11	1:A:349:LEU:HD22	1.95	0.47
1:C:46:LYS:NZ	1:C:492:GLU:OE2	2.33	0.47
1:C:393:SER:OG	1:C:395:TRP:NE1	2.47	0.47
2:D:563:GLN:HG2	2:D:566:LEU:HD23	1.97	0.47
1:A:52:LEU:HB3	1:A:218:CYS:O	2.15	0.47
1:A:65:LYS:HE2	1:A:208:VAL:HG11	1.96	0.47
2:B:593:LEU:HB3	2:B:598:CYS:O	2.14	0.47
4:M:87:ARG:NE	4:M:90:ASP:OD2	2.48	0.47
1:C:358:ILE:HG13	1:C:396:ILE:HG13	1.97	0.47
2:B:606:THR:OG1	2:B:607:ASN:N	2.46	0.47
1:C:498:PRO:HB3	2:D:610:TRP:CD1	2.51	0.46
1:A:260:LEU:C	1:A:261:LEU:HD12	2.36	0.46
1:A:358:ILE:O	1:A:465:THR:OG1	2.28	0.46
4:K:60:TYR:CE2	4:K:70:ILE:HG13	2.50	0.46
1:A:112:TRP:CZ2	1:A:255:VAL:HG11	2.50	0.46
4:K:60:TYR:OH	4:K:70:ILE:N	2.47	0.46
3:L:10:THR:HG23	3:L:105:ARG:HB3	1.96	0.46
1:C:126:CYS:HB2	1:C:196:CYS:HB3	1.41	0.46
1:C:291:PRO:HB3	1:C:448:ASN:HB3	1.98	0.46
3:J:54:ARG:NH1	3:J:62:PHE:O	2.48	0.46
1:C:260:LEU:HD12	1:C:260:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:127:SER:OG	4:M:128:SER:N	2.49	0.46
1:A:55:ALA:O	1:A:216:HIS:HB2	2.16	0.46
1:A:259:LEU:HB2	1:A:374:HIS:ND1	2.31	0.46
3:J:32:ASP:O	3:J:33:LEU:HD22	2.16	0.46
1:C:99:ASN:HD21	1:C:103:GLN:NE2	2.14	0.46
2:D:563:GLN:HA	2:D:566:LEU:HB3	1.98	0.46
1:E:54:CYS:CB	1:E:74:CYS:CB	2.94	0.46
1:C:119:CYS:N	1:C:205:CYS:SG	2.89	0.46
3:J:17:GLU:HG3	3:J:18:ARG:H	1.80	0.46
1:C:261:LEU:CD1	1:C:374:HIS:NE2	2.71	0.46
1:A:337:THR:HA	1:A:340:GLU:HG3	1.98	0.46
1:C:360:ARG:HB2	1:C:394:THR:HG23	1.99	0.45
1:A:297:THR:HB	1:A:444:ARG:HG3	1.98	0.45
1:A:271:MET:SD	1:A:271:MET:N	2.87	0.45
4:K:90:ASP:HB2	4:K:126:VAL:HG11	1.99	0.45
1:E:296:CYS:CB	1:E:331:CYS:HA	2.46	0.45
1:A:422:GLN:HE21	1:A:437:PRO:HA	1.81	0.45
1:A:424:ILE:HD11	1:A:435:TYR:CE2	2.50	0.45
2:B:539:VAL:O	2:B:542:ARG:N	2.50	0.45
1:E:35:TRP:N	1:E:499:THR:O	2.48	0.45
1:C:207:LYS:NZ	1:C:436:ALA:HB3	2.31	0.45
4:K:93:VAL:HA	4:K:123:LEU:HA	1.98	0.45
1:C:236:THR:HG22	1:C:237:GLY:N	2.28	0.45
4:M:4:LEU:HB3	4:M:22:CYS:SG	2.57	0.45
4:M:39:GLN:O	4:M:92:ALA:HB1	2.17	0.45
1:E:384:TYR:O	1:E:418:CYS:HA	2.17	0.45
4:M:83:LEU:HD22	4:M:86:LEU:HD23	1.99	0.45
5:G:21:DPR:HA	5:G:23:U2X:HB3	1.99	0.45
1:C:92:GLU:HA	1:C:238:PRO:HA	1.99	0.45
1:C:285:LEU:HD23	1:C:481:SER:HB2	1.99	0.45
1:C:368:ASP:OD1	1:C:369:LEU:N	2.50	0.45
1:A:361:PHE:CB	1:A:391:PHE:HB3	2.47	0.45
1:A:256:SER:OG	1:A:257:THR:N	2.49	0.45
4:K:35:THR:HB	4:K:115:LEU:HD21	1.99	0.45
3:L:105:ARG:HH21	3:L:107:GLU:HG3	1.80	0.45
1:C:261:LEU:HD21	1:C:449:ILE:HG12	1.99	0.44
1:C:335:LYS:HG2	1:C:336:ALA:H	1.80	0.44
3:J:20:THR:HG23	3:J:74:THR:HG22	1.98	0.44
2:D:627:THR:N	2:D:630:GLN:HE21	2.13	0.44
1:A:269:GLU:N	1:A:289:ASN:HD21	2.15	0.44
4:M:52:ILE:HG23	4:M:109:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:VAL:HG12	1:A:287:GLN:H	1.81	0.44
1:A:282:LYS:HA	1:A:282:LYS:HD3	1.64	0.44
3:J:45:ARG:NH2	3:J:58:VAL:HG22	2.32	0.44
3:L:25:ALA:O	3:L:69:ALA:HB1	2.18	0.44
4:M:105:ASP:OD1	4:M:105:ASP:N	2.51	0.44
1:C:455:THR:HG21	5:H:18:ARG:HH22	1.83	0.44
2:B:619:LEU:HA	2:B:622:ILE:HD12	2.00	0.44
1:E:261:LEU:HA	1:E:449:ILE:HA	1.99	0.44
3:J:5:THR:N	3:J:24:ARG:O	2.45	0.44
3:L:24:ARG:HD3	3:L:69:ALA:O	2.18	0.44
4:M:71:THR:O	4:M:80:TYR:N	2.50	0.43
2:D:594:GLY:HA2	2:D:599:SER:HB2	2.00	0.43
1:C:292:VAL:HG13	1:C:449:ILE:HB	1.99	0.43
1:C:361:PHE:HB3	1:C:391:PHE:HB3	1.99	0.43
1:A:54:CYS:HB3	1:A:74:CYS:HB3	1.74	0.43
1:E:55:ALA:N	1:E:216:HIS:O	2.51	0.43
1:C:80:ASN:OD1	1:C:80:ASN:N	2.51	0.43
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.53	0.43
3:L:93:ASN:ND2	3:L:97:ARG:O	2.39	0.43
1:A:95:MET:HE3	1:A:484:TYR:HB2	2.00	0.43
4:M:37:VAL:O	4:M:95:PHE:N	2.45	0.43
5:G:21:DPR:HB2	5:G:22:THR:H	1.61	0.43
1:E:379:GLY:N	8:P:2:NAG:H62	2.34	0.43
3:J:98:TYR:HB2	4:K:47:TRP:CG	2.53	0.43
4:M:116:LYS:HG2	4:M:117:HIS:ND1	2.34	0.43
1:E:367:GLY:CA	5:I:26:CYS:CA	2.94	0.43
3:J:6:GLN:H	3:J:102:GLN:NE2	2.17	0.42
3:L:59:PRO:HD2	3:L:62:PHE:HE2	1.84	0.42
5:H:21:DPR:HB2	5:H:22:THR:H	1.60	0.42
1:C:335:LYS:C	1:C:337:THR:H	2.23	0.42
3:J:6:GLN:HA	3:J:23:CYS:HA	2.01	0.42
4:M:67:ARG:HA	4:M:84:ARG:HE	1.84	0.42
1:A:69:TRP:CE3	1:A:111:LEU:HD13	2.55	0.42
3:J:7:SER:HA	3:J:8:PRO:HA	1.83	0.42
3:L:5:THR:OG1	3:L:24:ARG:HB3	2.19	0.42
4:M:38:ARG:HD3	4:M:94:TYR:CE1	2.55	0.42
1:E:360:ARG:O	1:E:467:THR:HA	2.20	0.42
2:D:641:ILE:O	2:D:645:LEU:HG	2.20	0.42
1:C:68:VAL:O	1:C:71:THR:HG22	2.20	0.42
1:A:93:PHE:CE1	1:A:228:CYS:HB2	2.54	0.42
3:J:6:GLN:H	3:J:102:GLN:HE22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:O	1:A:358:ILE:HG13	2.20	0.42
3:L:2:ILE:HA	3:L:26:SER:OG	2.19	0.42
4:M:38:ARG:HA	4:M:94:TYR:HA	2.01	0.42
1:E:335:LYS:C	1:E:337:THR:H	2.22	0.42
2:B:625:ASN:OD1	2:B:625:ASN:N	2.53	0.42
1:E:119:CYS:O	1:E:202:THR:HA	2.20	0.41
1:C:36:VAL:HG12	2:D:610:TRP:HD1	1.85	0.41
1:C:87:GLU:N	1:C:87:GLU:OE1	2.53	0.41
1:C:326:ILE:HD12	1:C:326:ILE:HA	1.90	0.41
1:A:55:ALA:N	1:A:216:HIS:O	2.53	0.41
1:C:439:ILE:HG13	1:C:440:GLN:H	1.85	0.41
1:A:54:CYS:HB2	1:A:74:CYS:HA	2.02	0.41
1:A:343:GLY:O	1:A:346:VAL:HG12	2.20	0.41
2:B:651:ASN:HA	2:B:654:GLU:CD	2.41	0.41
3:J:96:PRO:HD2	4:K:59:HIS:CD2	2.56	0.41
6:N:2:NAG:H4	6:N:3:BMA:H2	1.59	0.41
1:C:254:VAL:HG11	1:C:261:LEU:O	2.20	0.41
1:C:358:ILE:HD12	1:C:396:ILE:HA	2.02	0.41
1:A:326:ILE:C	1:A:327:ARG:HH11	2.24	0.41
1:A:339:ASN:ND2	9:A:604:NAG:C7	2.83	0.41
4:K:29:PHE:CD2	4:K:74:LYS:HA	2.55	0.41
4:K:85:ASN:ND2	4:K:85:ASN:O	2.54	0.41
4:K:94:TYR:N	4:K:122:THR:O	2.38	0.41
1:C:259:LEU:HD23	1:C:452:LEU:HB3	2.03	0.41
1:C:297:THR:OG1	1:C:444:ARG:HG2	2.20	0.41
1:A:373:THR:HG22	1:A:374:HIS:N	2.34	0.41
3:L:11:LEU:HD23	3:L:19:ALA:HB1	2.01	0.41
2:F:627:THR:O	2:F:631:TRP:N	2.47	0.41
1:C:447:SER:HA	9:C:601:NAG:H81	2.03	0.41
1:A:391:PHE:N	1:A:391:PHE:CD2	2.88	0.41
1:A:485:LYS:O	1:A:486:TYR:CG	2.71	0.41
3:J:70:GLU:N	3:J:70:GLU:OE1	2.53	0.41
4:M:91:THR:HG21	4:M:126:VAL:N	2.35	0.41
1:C:335:LYS:HE2	1:C:335:LYS:HB3	1.81	0.41
1:A:33:ASN:OD1	1:A:33:ASN:N	2.54	0.41
1:A:263:GLY:C	1:A:450:THR:OG1	2.58	0.41
3:J:38:GLN:O	3:J:85:VAL:HG22	2.21	0.41
3:J:45:ARG:HH21	3:J:58:VAL:HG22	1.86	0.41
1:C:276:ASN:ND2	1:C:279:ASN:HD22	2.18	0.40
1:C:373:THR:OG1	1:C:374:HIS:N	2.52	0.40
1:C:473:GLY:O	5:H:23:U2X:HD21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:HB2	1:A:442:VAL:HG23	2.03	0.40
1:A:439:ILE:HG12	1:A:440:GLN:H	1.86	0.40
1:A:446:VAL:HG22	1:A:446:VAL:O	2.22	0.40
2:B:535:MET:O	2:B:539:VAL:HG23	2.21	0.40
1:A:428:GLN:H	1:A:428:GLN:HG3	1.65	0.40
4:K:11:VAL:HG12	4:K:125:THR:OG1	2.21	0.40
1:A:425:ASN:O	5:G:23:U2X:HE11	2.21	0.40
9:A:605:NAG:C3	9:A:605:NAG:C8	2.98	0.40
3:J:93:ASN:ND2	3:J:97:ARG:HE	2.19	0.40
4:K:60:TYR:HE2	4:K:70:ILE:HG13	1.86	0.40
2:D:572:GLY:O	2:D:576:LEU:N	2.54	0.40
1:A:261:LEU:HD11	1:A:374:HIS:HE1	1.87	0.40
2:B:533:ALA:HA	2:B:536:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/479 (74%)	304 (86%)	48 (14%)	1 (0%)	37	70
1	C	348/479 (73%)	298 (86%)	50 (14%)	0	100	100
1	E	343/479 (72%)	283 (82%)	60 (18%)	0	100	100
2	B	119/153 (78%)	110 (92%)	9 (8%)	0	100	100
2	D	122/153 (80%)	110 (90%)	12 (10%)	0	100	100
2	F	124/153 (81%)	113 (91%)	11 (9%)	0	100	100
3	J	104/214 (49%)	93 (89%)	10 (10%)	1 (1%)	13	46
3	L	107/214 (50%)	99 (92%)	7 (6%)	1 (1%)	14	48
4	K	128/239 (54%)	117 (91%)	11 (9%)	0	100	100
4	M	128/239 (54%)	118 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	24/28 (86%)	21 (88%)	2 (8%)	1 (4%)	2	21
5	H	24/28 (86%)	22 (92%)	1 (4%)	1 (4%)	2	21
5	I	24/28 (86%)	24 (100%)	0	0	100	100
All	All	1948/2886 (68%)	1712 (88%)	231 (12%)	5 (0%)	38	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ILE
3	J	30	SER
3	L	30	SER
5	G	22	THR
5	H	22	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/427 (74%)	315 (99%)	3 (1%)	75	83
1	C	317/427 (74%)	316 (100%)	1 (0%)	91	92
1	E	3/427 (1%)	3 (100%)	0	100	100
2	B	105/129 (81%)	105 (100%)	0	100	100
2	D	105/129 (81%)	104 (99%)	1 (1%)	73	81
3	J	87/184 (47%)	87 (100%)	0	100	100
3	L	90/184 (49%)	90 (100%)	0	100	100
4	K	107/203 (53%)	107 (100%)	0	100	100
4	M	107/203 (53%)	107 (100%)	0	100	100
5	G	20/20 (100%)	20 (100%)	0	100	100
5	H	20/20 (100%)	20 (100%)	0	100	100
All	All	1279/2353 (54%)	1274 (100%)	5 (0%)	88	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	203	GLN
2	D	585	ARG
1	A	271	MET
1	A	448	ASN
1	A	501	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	ASN
1	C	279	ASN
1	C	352	HIS
1	C	422	GLN
2	D	543	ASN
2	D	630	GLN
1	A	33	ASN
1	A	66	HIS
1	A	72	HIS
1	A	258	GLN
2	B	630	GLN
3	J	93	ASN
4	K	112	ASN
3	L	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	U2X	H	23	5	19,20,21	0.52	0	20,25,27	0.84	1 (5%)
5	DPR	H	21	5	6,7,8	0.56	0	7,8,10	1.45	1 (14%)
5	U2X	G	23	5	19,20,21	0.54	0	20,25,27	0.90	1 (5%)
5	DPR	G	21	5	6,7,8	0.55	0	7,8,10	1.58	1 (14%)
5	DPR	I	21	5	6,7,8	0.76	0	7,8,10	1.13	0
5	U2X	I	23	5	19,20,21	2.54	4 (21%)	20,25,27	1.42	5 (25%)

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	U2X	H	23	5	-	6/10/19/21	0/2/2/2
5	DPR	H	21	5	-	0/0/9/11	0/1/1/1
5	U2X	G	23	5	-	6/10/19/21	0/2/2/2
5	DPR	G	21	5	-	0/0/9/11	0/1/1/1
5	DPR	I	21	5	-	0/0/9/11	0/1/1/1
5	U2X	I	23	5	-	2/10/19/21	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	23	U2X	CE2-CD2	8.00	1.51	1.38
5	I	23	U2X	CE1-CD1	5.12	1.47	1.38
5	I	23	U2X	CE1-CZ	2.84	1.44	1.38
5	I	23	U2X	C4-C3	2.42	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	21	DPR	CB-CA-C	-3.31	108.12	112.66
5	I	23	U2X	C1-C2-C3	-2.97	105.83	112.08
5	I	23	U2X	C2-C3-C7	2.88	119.11	111.42
5	H	21	DPR	CB-CA-C	-2.76	108.87	112.66
5	G	23	U2X	C7-OH-CZ	-2.53	112.28	117.85
5	H	23	U2X	C7-OH-CZ	-2.10	113.23	117.85
5	I	23	U2X	C4-C3-C7	2.07	116.94	111.42
5	I	23	U2X	C6-C1-C2	-2.06	107.18	111.42
5	I	23	U2X	CD2-CG-CD1	2.00	121.21	118.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	23	U2X	C-CA-CB-CG
5	H	23	U2X	C-CA-CB-CG
5	H	23	U2X	C2-C3-C7-OH
5	G	23	U2X	CA-CB-CG-CD1
5	G	23	U2X	CA-CB-CG-CD2
5	H	23	U2X	C4-C3-C7-OH
5	G	23	U2X	N-CA-CB-CG
5	H	23	U2X	N-CA-CB-CG
5	I	23	U2X	CE1-CZ-OH-C7
5	H	23	U2X	CA-CB-CG-CD1
5	H	23	U2X	CA-CB-CG-CD2
5	I	23	U2X	CE2-CZ-OH-C7
5	G	23	U2X	CE1-CZ-OH-C7
5	G	23	U2X	CE2-CZ-OH-C7

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	23	U2X	2	0
5	H	21	DPR	2	0
5	G	23	U2X	2	0
5	G	21	DPR	2	0
5	I	23	U2X	12	0

5.5 Carbohydrates [i](#)

15 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	$\# Z > 2$
6	NAG	N	1	1,6	14,14,15	0.32	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	2	6	14,14,15	0.30	0	17,19,21	0.60	0
6	BMA	N	3	6	11,11,12	0.29	0	15,15,17	1.02	1 (6%)
6	MAN	N	4	6	11,11,12	0.30	0	15,15,17	1.04	2 (13%)
6	MAN	N	5	6	11,11,12	0.21	0	15,15,17	0.85	0
6	MAN	N	6	6	11,11,12	0.23	0	15,15,17	0.68	0
7	NAG	O	1	1,7	14,14,15	2.60	1 (7%)	17,19,21	2.07	3 (17%)
7	NAG	O	2	7	14,14,15	0.31	0	17,19,21	0.84	1 (5%)
7	BMA	O	3	7	11,11,12	0.25	0	15,15,17	0.67	0
7	MAN	O	4	7	11,11,12	0.54	0	15,15,17	1.94	4 (26%)
7	MAN	O	5	7	11,11,12	0.23	0	15,15,17	0.74	0
8	NAG	P	1	1,8	14,14,15	0.32	0	17,19,21	1.03	0
8	NAG	P	2	8	14,14,15	0.29	0	17,19,21	0.62	0
8	BMA	P	3	8	11,11,12	0.22	0	15,15,17	0.78	0
8	MAN	P	4	8	11,11,12	0.22	0	15,15,17	0.52	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
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
6	MAN	N	6	6	-	1/2/19/22	0/1/1/1
7	NAG	O	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	O	2	7	-	4/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
7	MAN	O	4	7	-	2/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	0/1/1/1
8	NAG	P	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	2/6/23/26	0/1/1/1
8	BMA	P	3	8	-	2/2/19/22	0/1/1/1
8	MAN	P	4	8	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	1	NAG	C1-C2	9.68	1.65	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	1	NAG	O5-C1-C2	-6.57	101.12	111.29
7	O	4	MAN	O3-C3-C2	-4.32	101.25	110.05
7	O	1	NAG	C1-O5-C5	4.26	117.90	112.19
7	O	4	MAN	O3-C3-C4	3.65	118.97	110.38
7	O	4	MAN	O4-C4-C5	-3.16	101.55	109.32
7	O	4	MAN	C2-C3-C4	-2.57	106.33	110.86
7	O	2	NAG	C1-O5-C5	2.42	115.43	112.19
7	O	1	NAG	C4-C3-C2	-2.35	107.58	111.02
6	N	4	MAN	C2-C3-C4	-2.34	106.75	110.86
6	N	3	BMA	O5-C5-C6	2.26	112.06	107.66
6	N	4	MAN	O3-C3-C4	-2.24	105.09	110.38

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C3-C2-N2-C7
7	O	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C3-C2-N2-C7
8	P	1	NAG	C8-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2
7	O	3	BMA	C4-C5-C6-O6
7	O	1	NAG	C8-C7-N2-C2
6	N	3	BMA	O5-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
8	P	4	MAN	O5-C5-C6-O6
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
8	P	4	MAN	C4-C5-C6-O6
8	P	3	BMA	O5-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6

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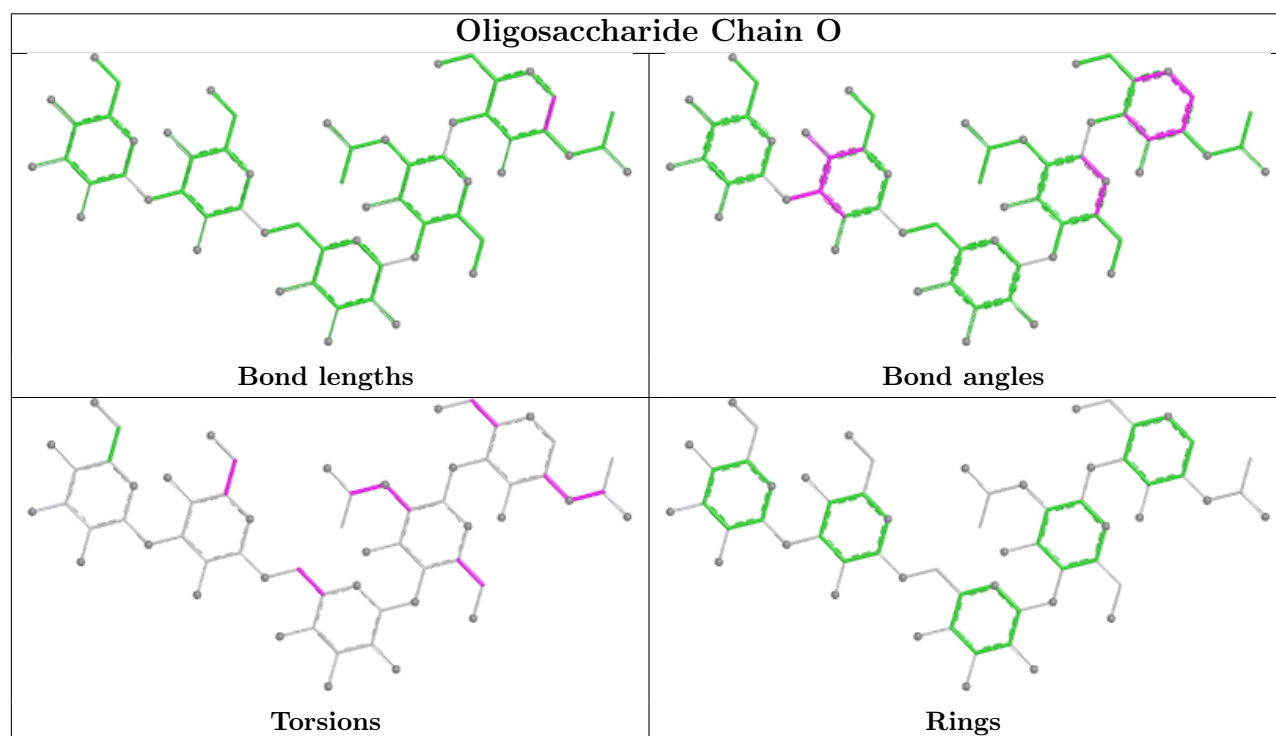
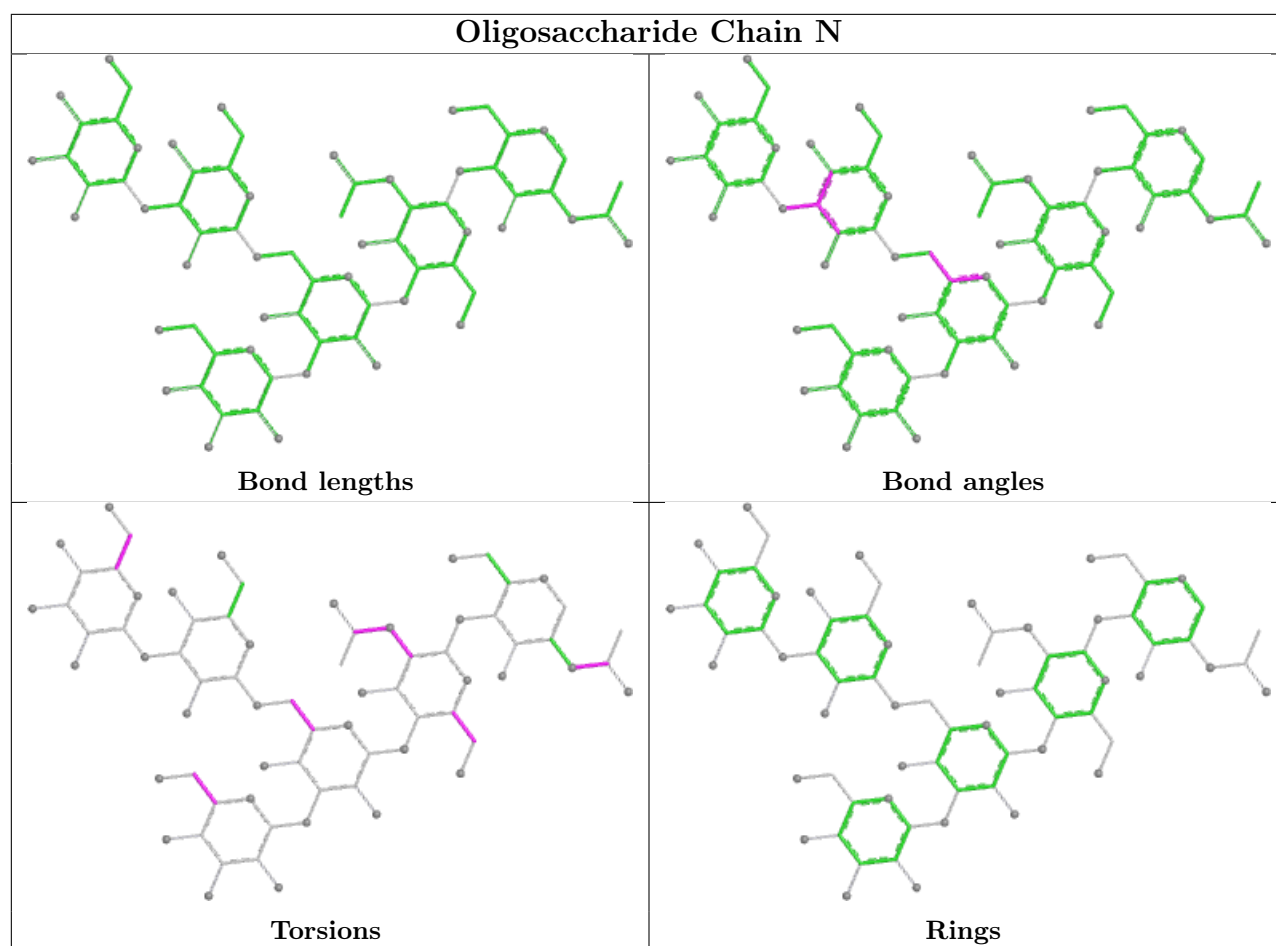
Mol	Chain	Res	Type	Atoms
7	O	2	NAG	O5-C5-C6-O6
6	N	6	MAN	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
8	P	2	NAG	C8-C7-N2-C2
8	P	3	BMA	C4-C5-C6-O6
8	P	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	2	NAG	C3-C2-N2-C7
6	N	1	NAG	O7-C7-N2-C2
7	O	4	MAN	C4-C5-C6-O6

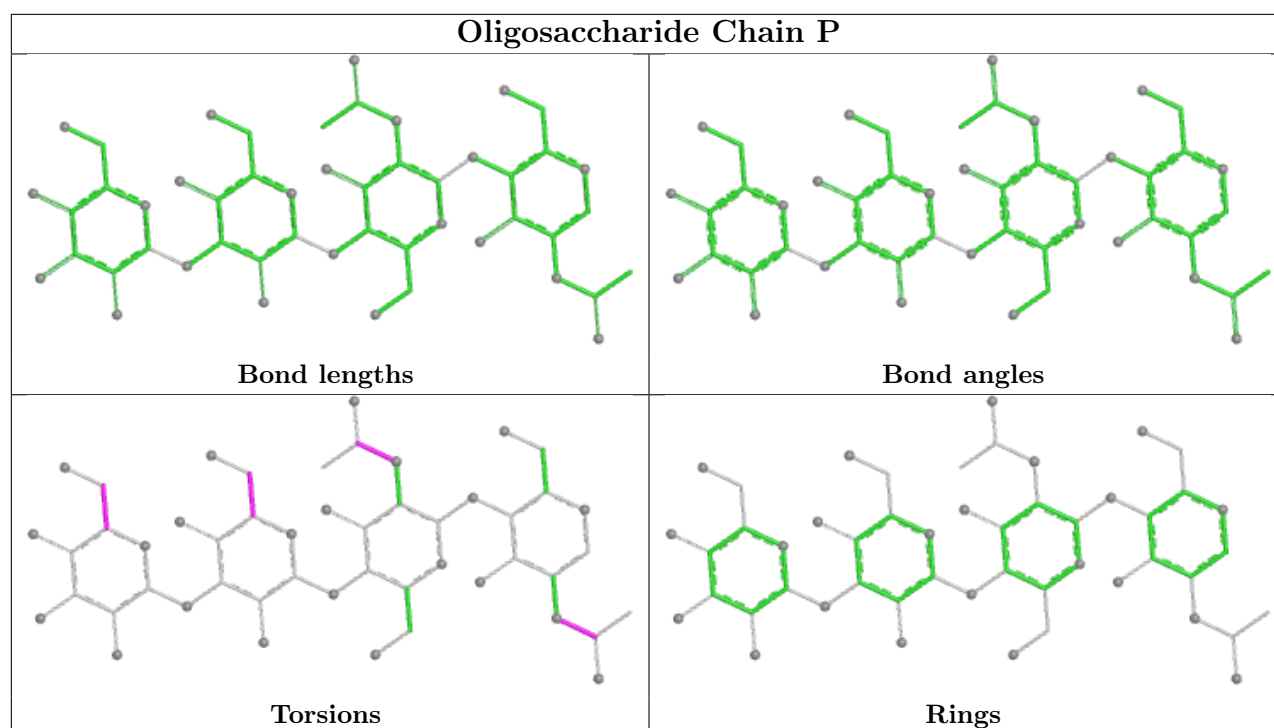
There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	3	BMA	1	0
6	N	4	MAN	1	0
8	P	4	MAN	1	0
7	O	2	NAG	6	0
8	P	2	NAG	1	0
8	P	1	NAG	1	0
6	N	2	NAG	2	0
7	O	4	MAN	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.





5.6 Ligand geometry [i](#)

8 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$
9	NAG	A	604	1	14,14,15	0.28	0	17,19,21	0.67	0
9	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.74	0
9	NAG	A	603	1	14,14,15	0.26	0	17,19,21	0.70	0
9	NAG	A	606	1	14,14,15	0.27	0	17,19,21	0.57	0
9	NAG	A	605	1	14,14,15	0.28	0	17,19,21	0.75	0
9	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.69	0
9	NAG	E	601	1	14,14,15	0.70	1 (7%)	17,19,21	0.77	1 (5%)
9	NAG	C	601	1	14,14,15	0.34	0	17,19,21	0.85	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	604	1	-	3/6/23/26	0/1/1/1
9	NAG	A	601	1	-	0/6/23/26	0/1/1/1
9	NAG	A	603	1	-	2/6/23/26	0/1/1/1
9	NAG	A	606	1	-	2/6/23/26	0/1/1/1
9	NAG	A	605	1	-	4/6/23/26	0/1/1/1
9	NAG	A	602	1	-	0/6/23/26	0/1/1/1
9	NAG	E	601	1	-	2/6/23/26	0/1/1/1
9	NAG	C	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	601	NAG	C1-C2	2.08	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	601	NAG	C1-O5-C5	2.47	115.50	112.19
9	C	601	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	605	NAG	C3-C2-N2-C7
9	A	605	NAG	C8-C7-N2-C2
9	A	605	NAG	O7-C7-N2-C2
9	E	601	NAG	O5-C5-C6-O6
9	E	601	NAG	C4-C5-C6-O6
9	A	604	NAG	O5-C5-C6-O6
9	A	603	NAG	C8-C7-N2-C2
9	A	604	NAG	C8-C7-N2-C2
9	A	606	NAG	C4-C5-C6-O6
9	A	603	NAG	O7-C7-N2-C2
9	A	606	NAG	O5-C5-C6-O6
9	A	604	NAG	O7-C7-N2-C2
9	A	605	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	604	NAG	1	0
9	A	605	NAG	4	0
9	E	601	NAG	1	0
9	C	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

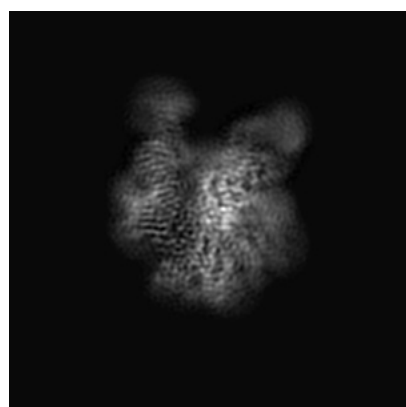
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23465. These allow visual inspection of the internal detail of the map and identification of artifacts.

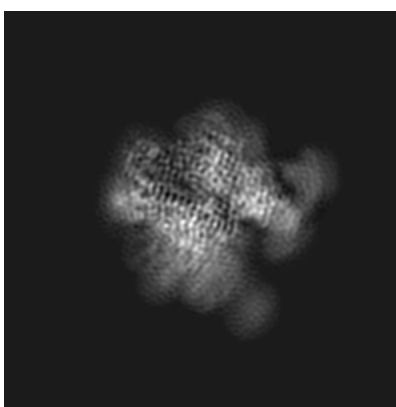
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

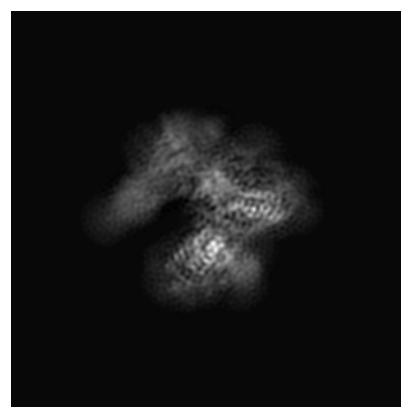
6.1.1 Primary map



X



Y

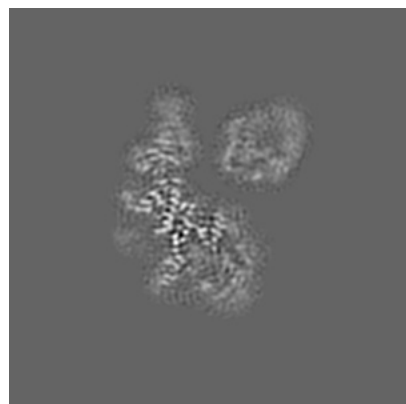


Z

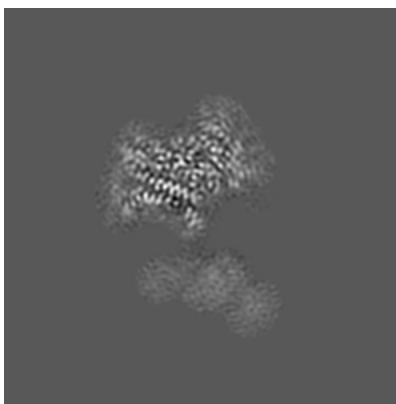
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

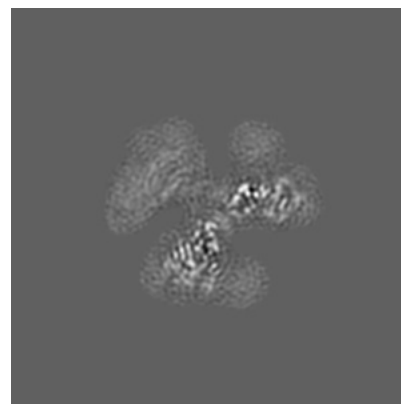
6.2.1 Primary map



X Index: 128



Y Index: 128

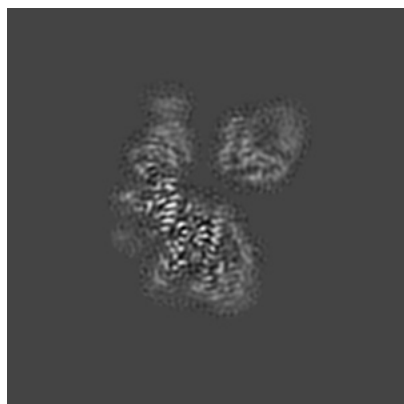


Z Index: 128

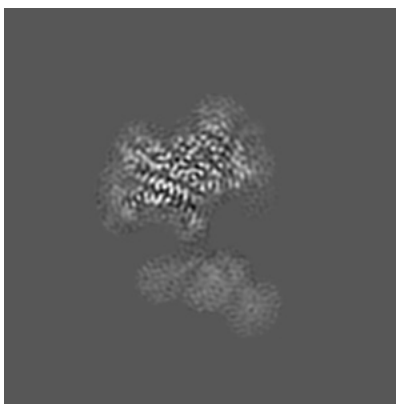
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

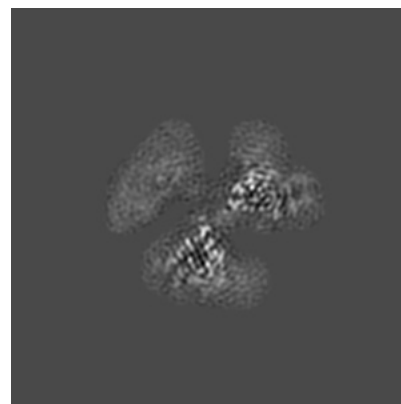
6.3.1 Primary map



X Index: 130



Y Index: 129

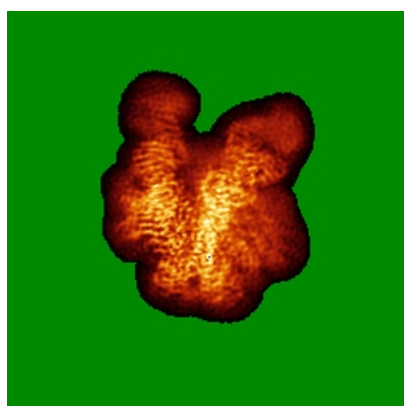


Z Index: 132

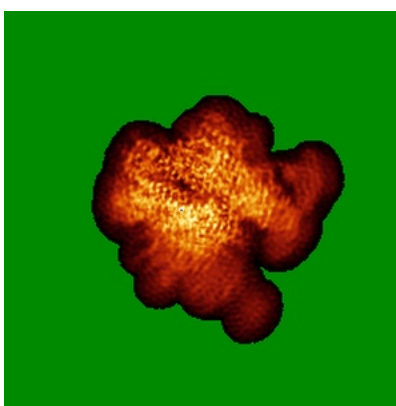
The images above show the largest variance slices of the map in three orthogonal directions.

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

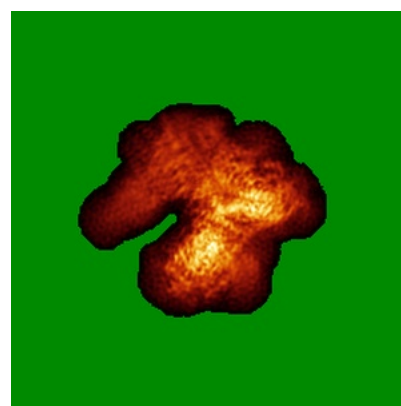
6.4.1 Primary map



X



Y

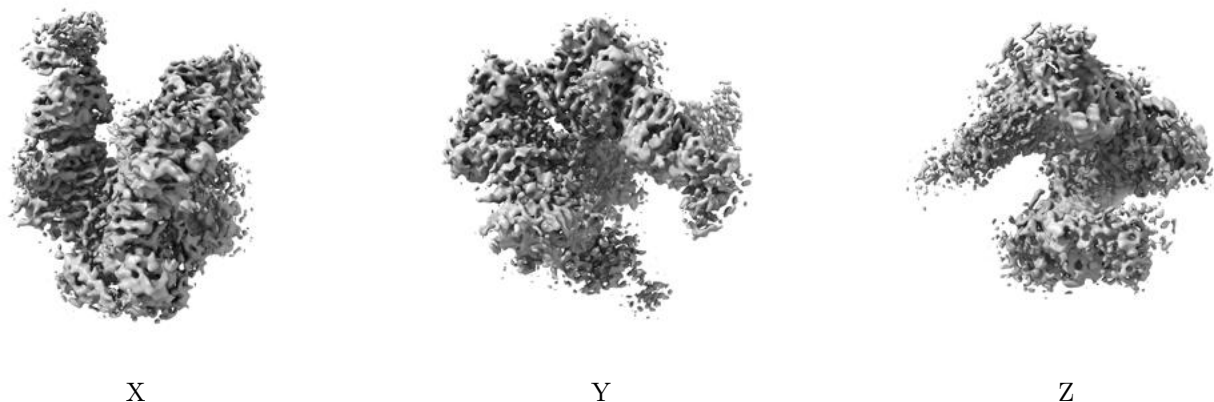


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

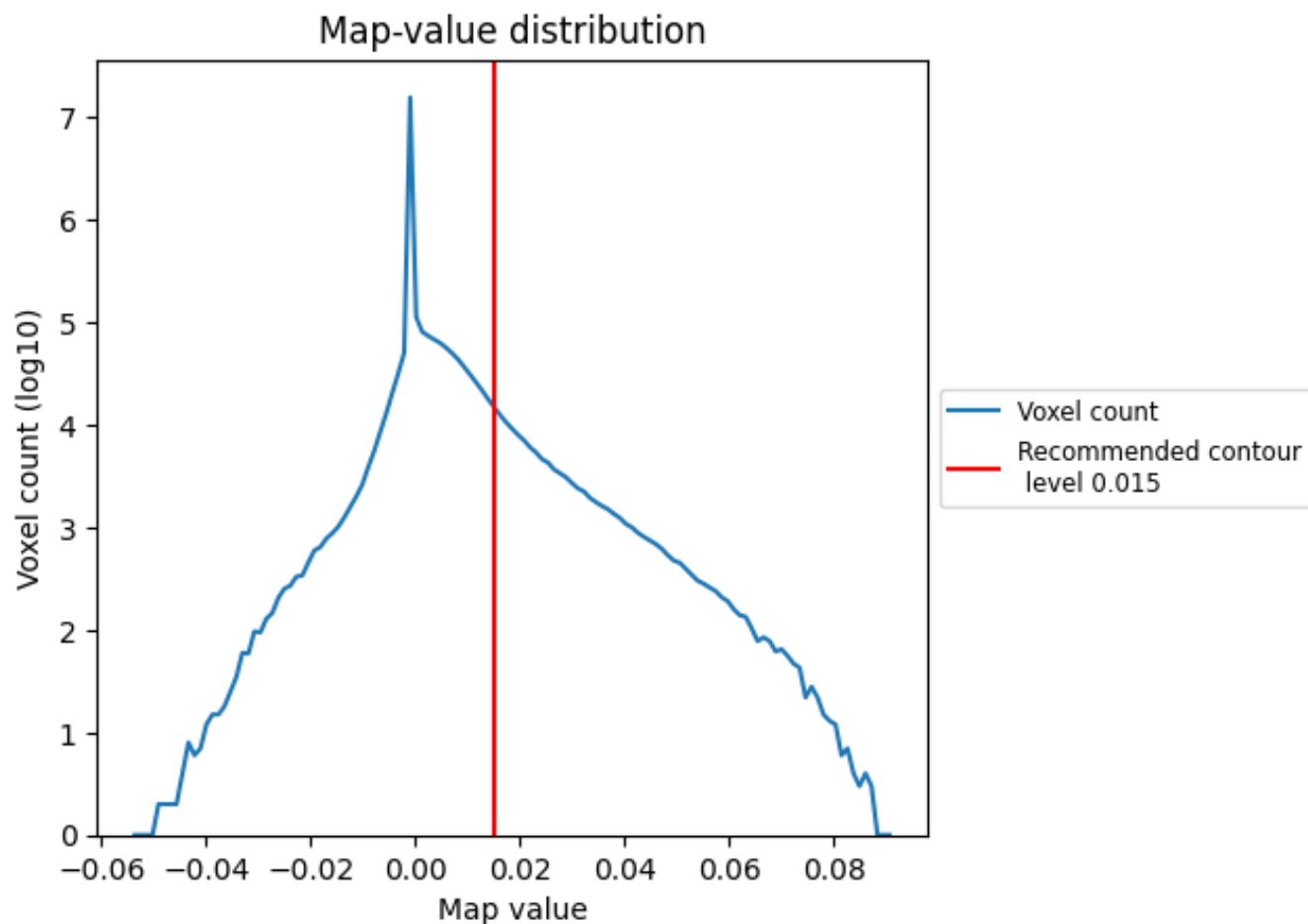
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

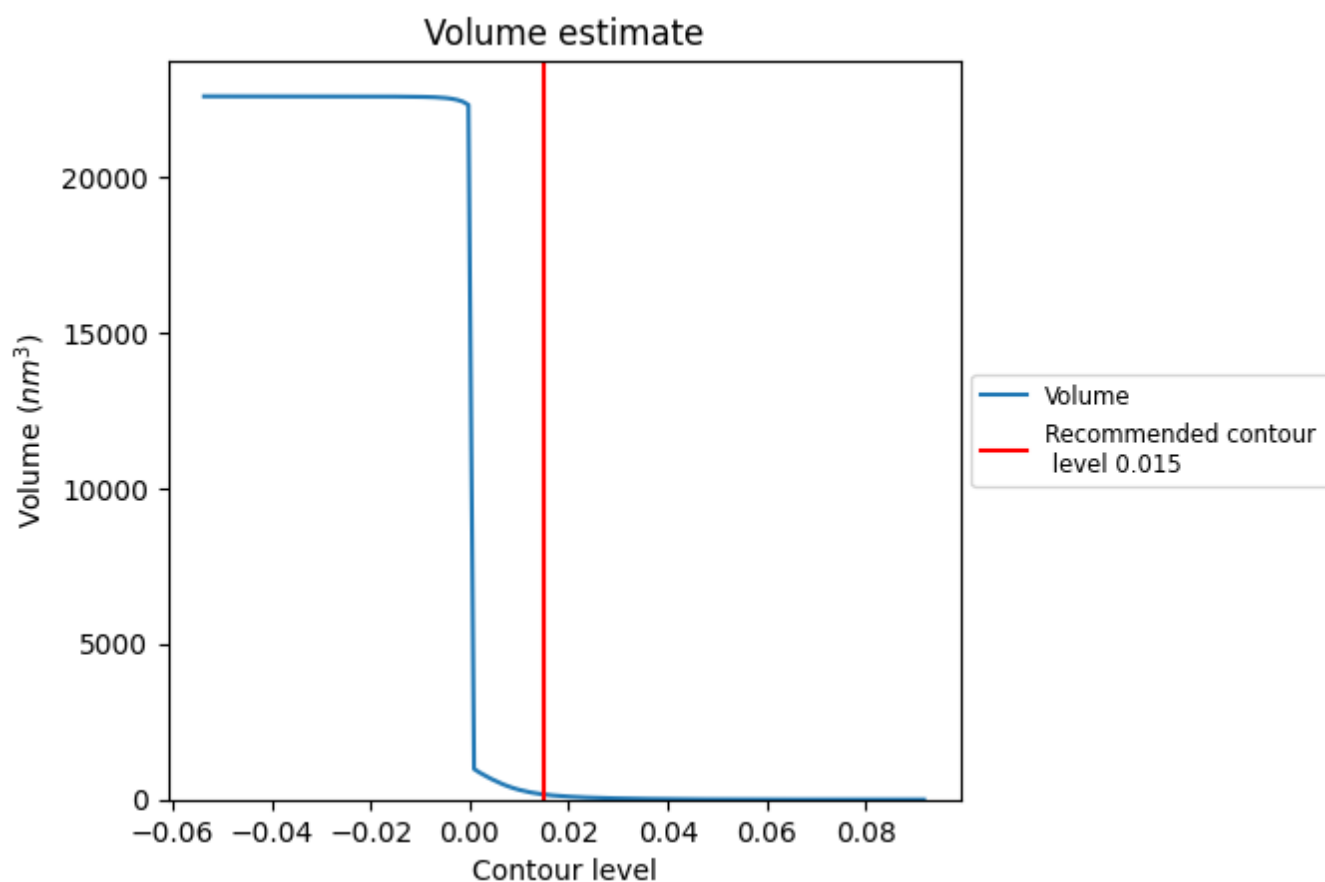
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

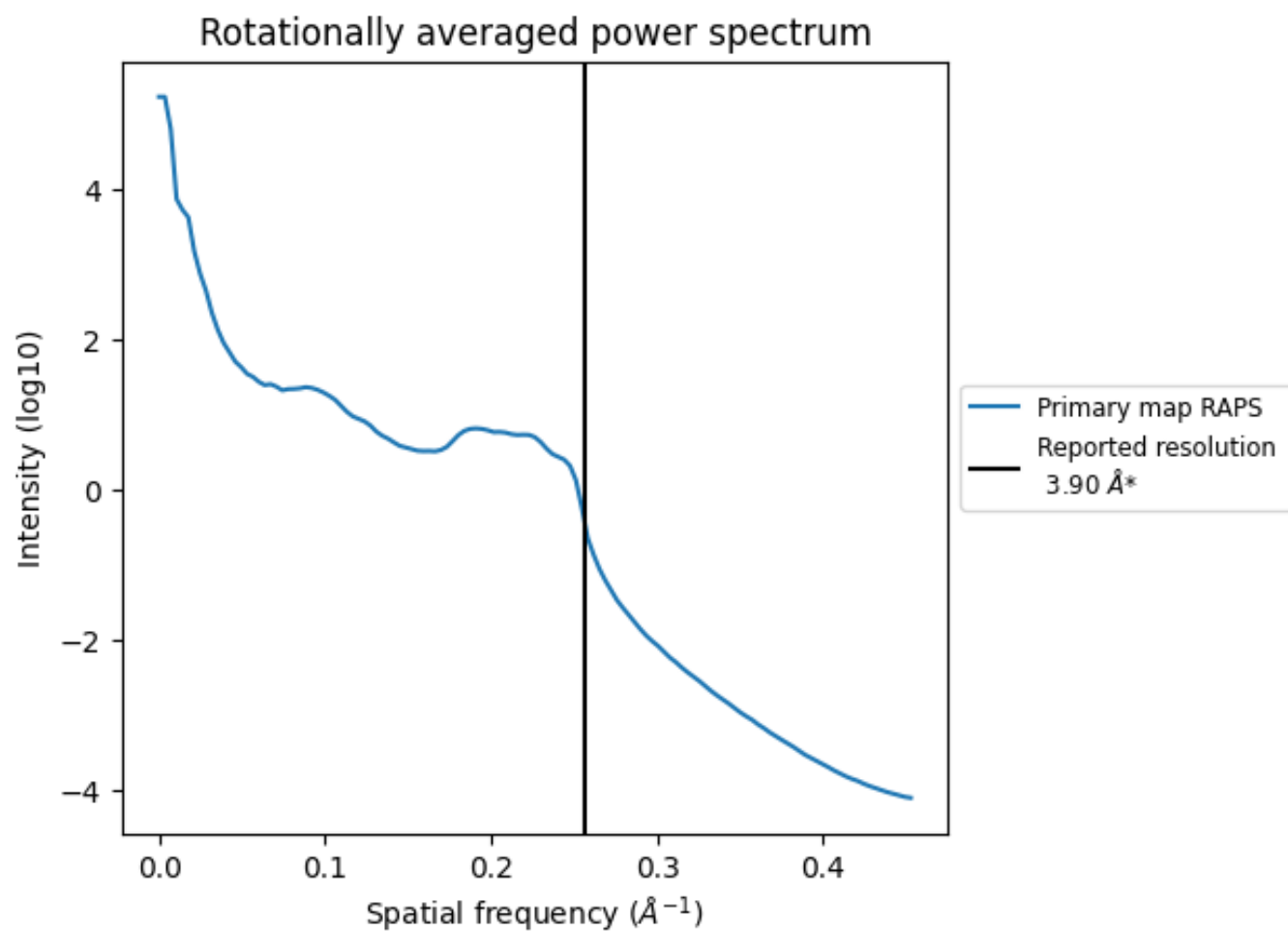
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm³; this corresponds to an approximate mass of 149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

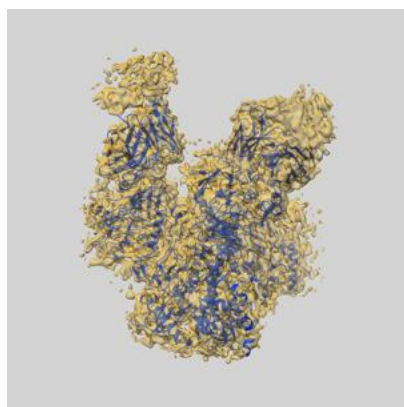
8 Fourier-Shell correlation ⓘ

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

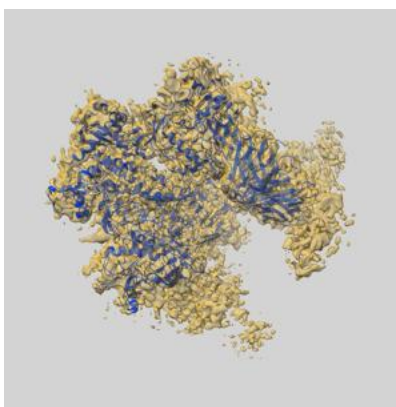
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23465 and PDB model 7LOK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

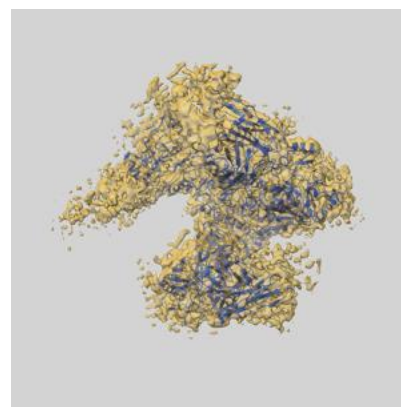
9.1 Map-model overlay [i](#)



X



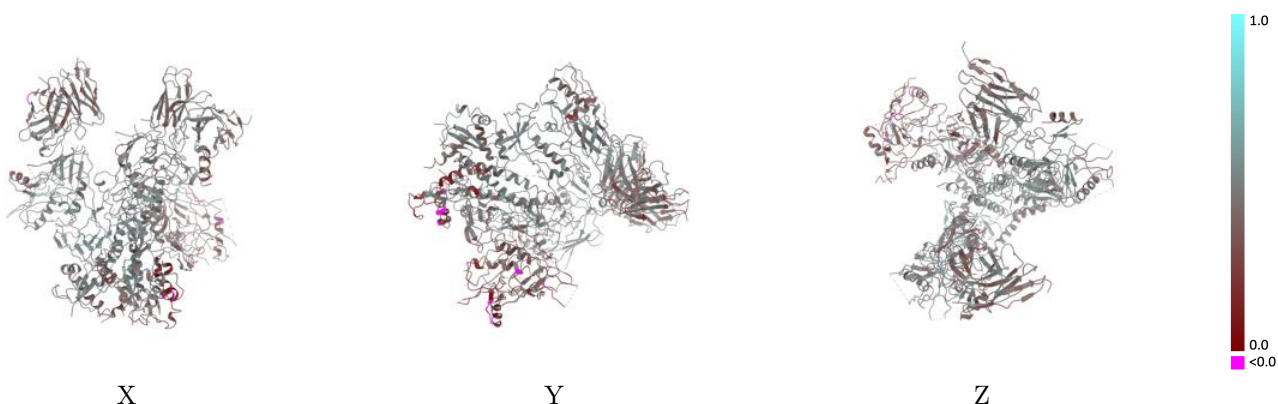
Y



Z

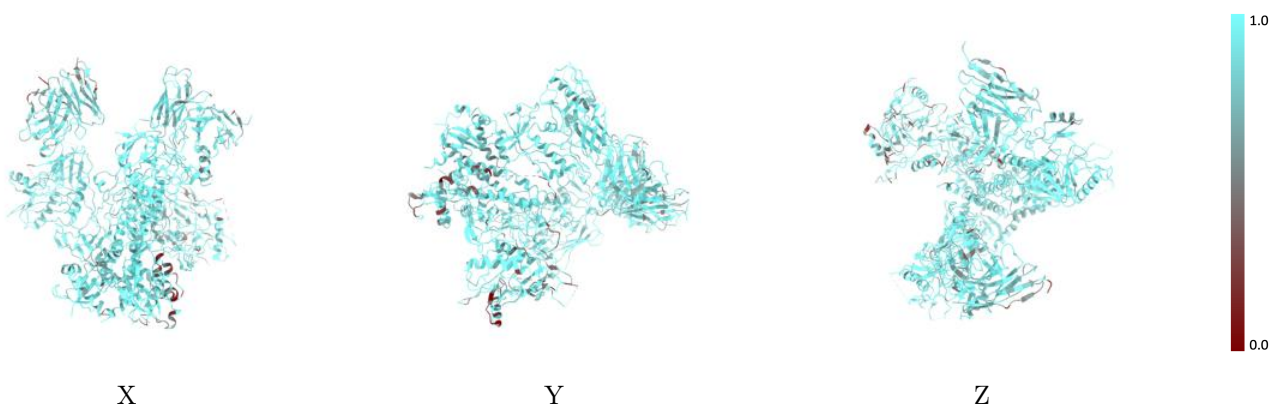
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



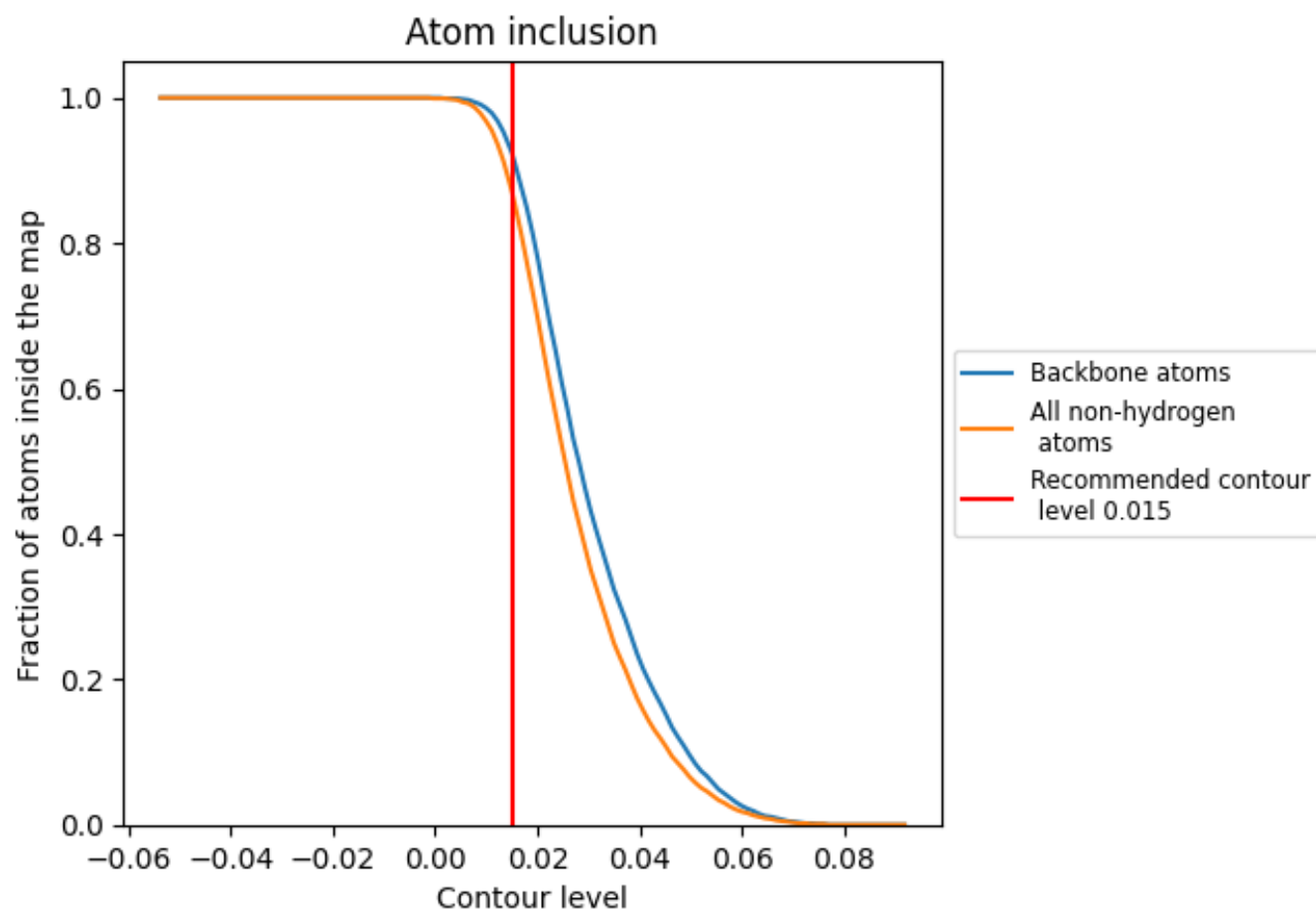
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.4500
A	 0.9180	 0.4950
B	 0.8950	 0.4690
C	 0.9240	 0.4890
D	 0.8870	 0.4600
E	 0.8450	 0.3930
F	 0.7760	 0.3520
G	 0.8630	 0.4310
H	 0.8280	 0.4180
I	 0.6080	 0.2590
J	 0.8010	 0.4150
K	 0.8110	 0.4460
L	 0.8550	 0.4220
M	 0.8620	 0.4470
N	 0.8060	 0.4320
O	 0.7540	 0.3350
P	 0.7600	 0.3650

