



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:22 AM UTC

PDB ID : 7SHT / pdb_00007sht
EMDB ID : EMD-25136
Title : Structure of a partially disrupted IgE high affinity receptor complex bound to an omalizumab variant
Authors : Pennington, L.F.; Jardetzky, T.S.
Deposited on : 2021-10-11
Resolution : 7.29 Å (reported)
Based on initial models : 1F6A, 4J4P

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:

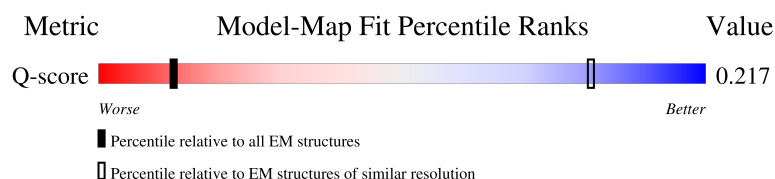
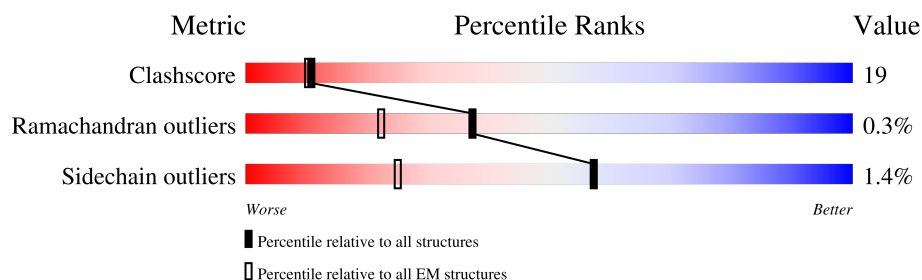
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.29 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.



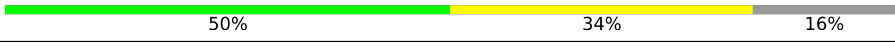
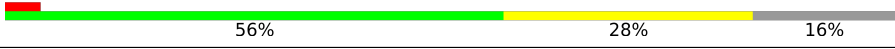
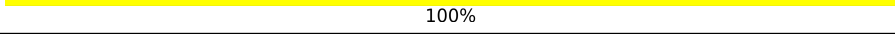
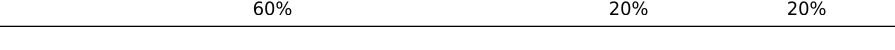
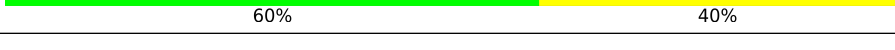
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	397 (6.80 - 7.77)

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	197	13% 52% 31% 15%
2	B	322	14% 54% 43% .
2	D	322	6% 59% 37% ..
3	H	123	6% 57% 40% ..

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Mol	Chain	Length	Quality of chain
3	J	123	
4	K	134	
4	L	134	
5	C	2	
6	E	3	
7	F	5	
7	G	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10062 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 High affinity immunoglobulin epsilon receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	167	Total	C	N	O	S	0	0
			1362	868	222	266	6		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	ALA	-	expression tag	UNP P12319
A	-23	PRO	-	expression tag	UNP P12319
A	-22	MET	-	expression tag	UNP P12319
A	-21	ALA	-	expression tag	UNP P12319
A	-20	GLU	-	expression tag	UNP P12319
A	-19	GLY	-	expression tag	UNP P12319
A	-18	GLY	-	expression tag	UNP P12319
A	-17	GLY	-	expression tag	UNP P12319
A	-16	GLN	-	expression tag	UNP P12319
A	-15	ASN	-	expression tag	UNP P12319
A	-14	HIS	-	expression tag	UNP P12319
A	-13	HIS	-	expression tag	UNP P12319
A	-12	HIS	-	expression tag	UNP P12319
A	-11	HIS	-	expression tag	UNP P12319
A	-10	HIS	-	expression tag	UNP P12319
A	-9	HIS	-	expression tag	UNP P12319
A	-8	HIS	-	expression tag	UNP P12319
A	-7	HIS	-	expression tag	UNP P12319
A	-6	GLY	-	expression tag	UNP P12319
A	-5	GLY	-	expression tag	UNP P12319
A	-4	GLU	-	expression tag	UNP P12319
A	-3	ASN	-	expression tag	UNP P12319
A	-2	LEU	-	expression tag	UNP P12319
A	-1	TYR	-	expression tag	UNP P12319
A	0	PHE	-	expression tag	UNP P12319
A	1	GLN	-	expression tag	UNP P12319
A	2	GLY	-	expression tag	UNP P12319
A	3	GLY	-	expression tag	UNP P12319

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	expression tag	UNP P12319
A	156	CYS	TRP	engineered mutation	UNP P12319

- Molecule 2 is a protein called Immunoglobulin heavy constant epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	316	Total	C	N	O	S	0	0
			2469	1538	440	479	12		
2	D	312	Total	C	N	O	S	0	0
			2440	1525	432	471	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	ALA	-	expression tag	UNP P01854
B	227	SER	-	expression tag	UNP P01854
B	335	CYS	GLY	engineered mutation	UNP P01854
D	226	ALA	-	expression tag	UNP P01854
D	227	SER	-	expression tag	UNP P01854
D	335	CYS	GLY	engineered mutation	UNP P01854

- Molecule 3 is a protein called clone_7 Variable fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			932	589	161	179	3		
3	J	120	Total	C	N	O	S	0	0
			932	589	161	179	3		

- Molecule 4 is a protein called clone_7 Variable fragment light chain.

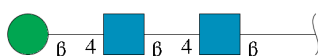
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	112	Total	C	N	O	S	0	0
			848	525	142	178	3		
4	L	112	Total	C	N	O	S	0	0
			848	525	142	178	3		

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



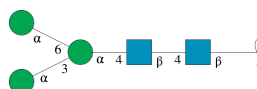
Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



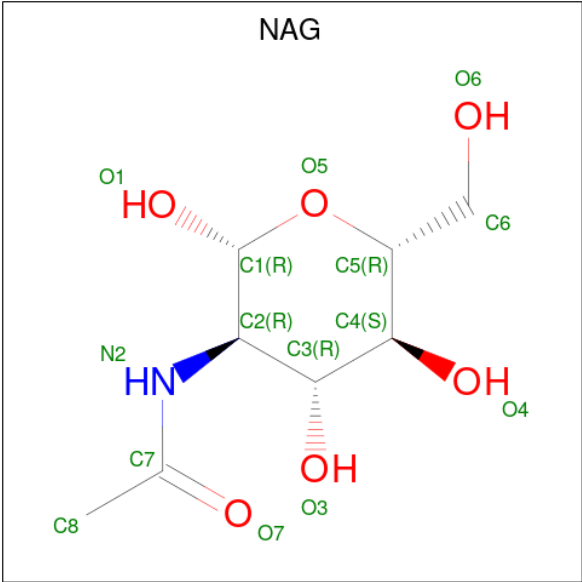
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	3	Total	C	N	O	0	0
			39	22	2	15		

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

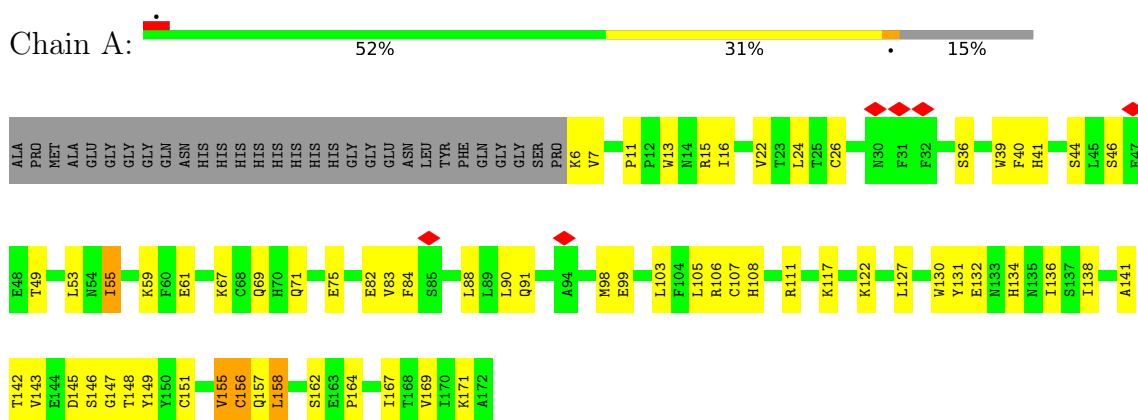


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	H	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	

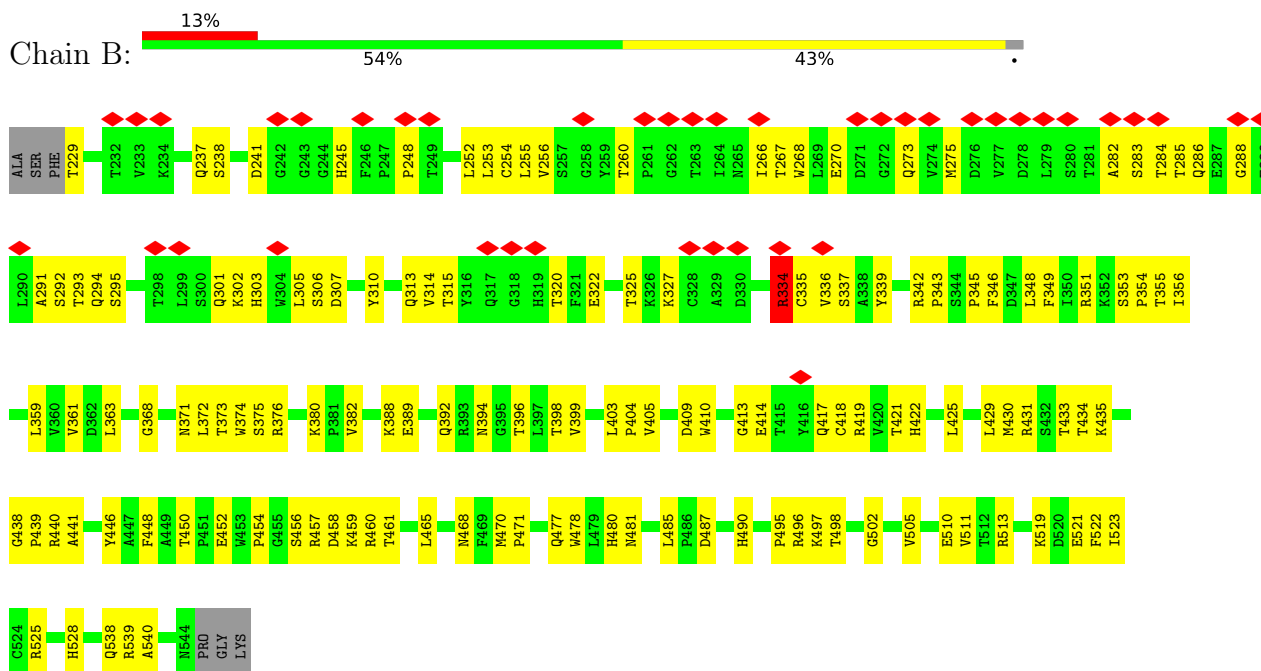
3 Residue-property plots

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.

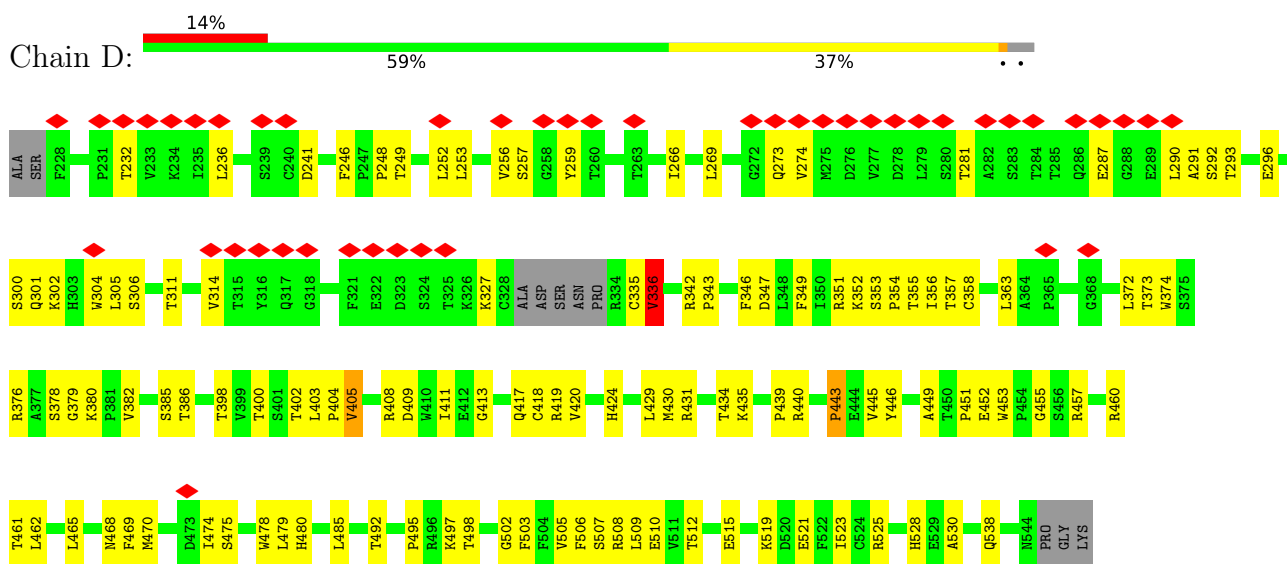
- Molecule 1: High affinity immunoglobulin epsilon receptor subunit alpha



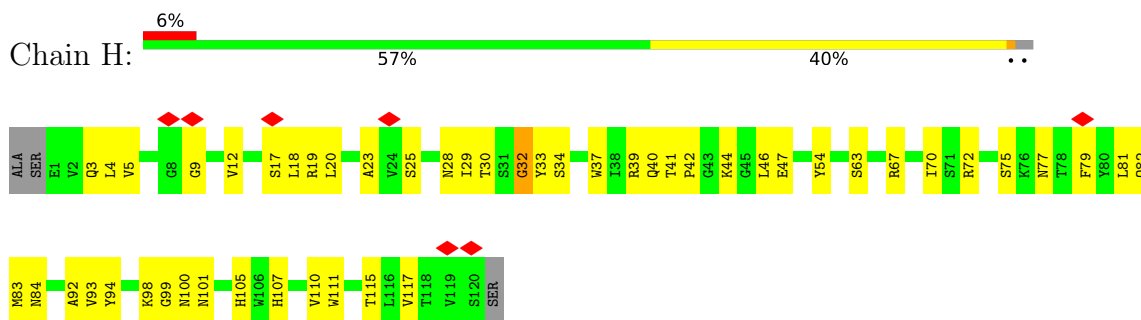
- Molecule 2: Immunoglobulin heavy constant epsilon



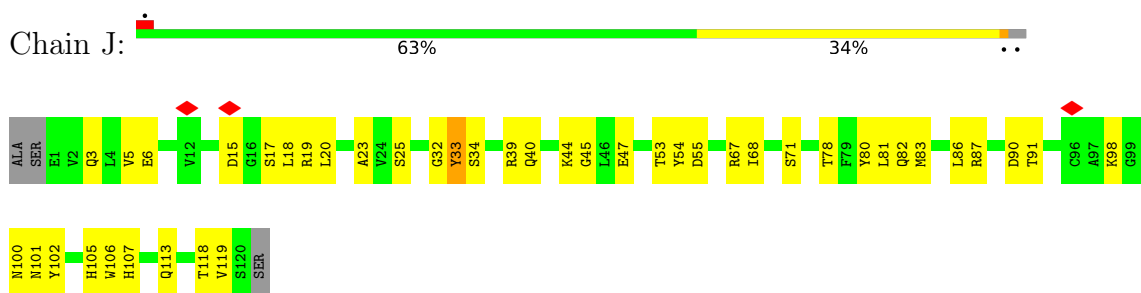
- Molecule 2: Immunoglobulin heavy constant epsilon



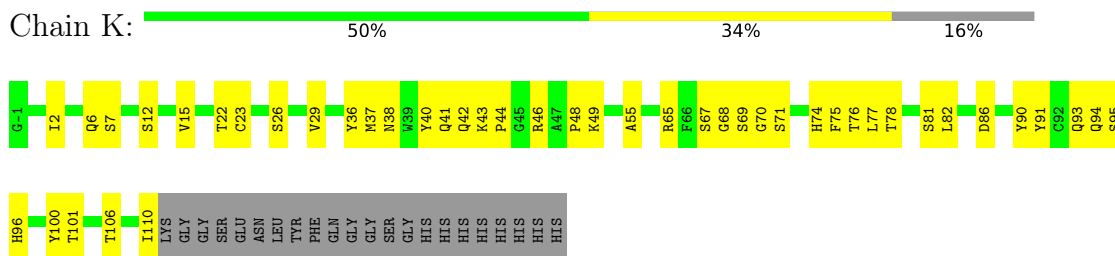
• Molecule 3: clone_7 Variable fragment heavy chain



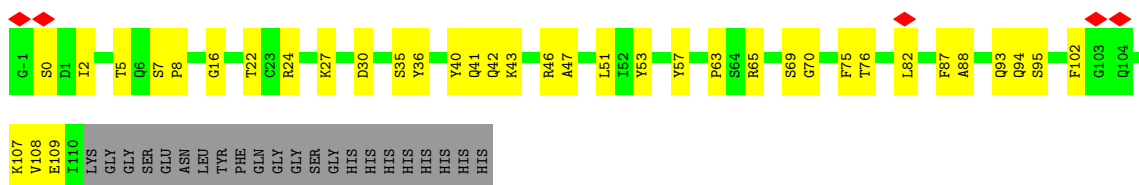
• Molecule 3: clone_7 Variable fragment heavy chain



• Molecule 4: clone_7 Variable fragment light chain



• Molecule 4: clone_7 Variable fragment light chain



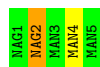
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	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	1.032	Depositor
Minimum map value	-0.468	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	218.1376, 218.1376, 218.1376	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8521, 0.8521, 0.8521	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, BMA, 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	A	0.37	0/1399	0.67	0/1904
2	B	0.33	0/2529	0.65	0/3448
2	D	0.33	0/2499	0.69	2/3405 (0.1%)
3	H	0.33	0/957	0.66	2/1303 (0.2%)
3	J	0.33	0/957	0.72	2/1303 (0.2%)
4	K	0.29	0/867	0.58	0/1177
4	L	0.26	0/867	0.55	0/1177
All	All	0.33	0/10075	0.66	6/13717 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	246	PHE	CB-CA-C	-6.76	103.00	110.98
3	J	34	SER	N-CA-C	6.66	118.90	110.24
2	D	443	PRO	CB-CA-C	-5.79	102.02	111.56
3	H	101	ASN	CB-CA-C	-5.58	99.67	109.71
3	H	32	GLY	CA-C-O	-5.40	115.94	121.61
3	J	32	GLY	CA-C-O	-5.24	116.02	122.15

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	1362	0	1271	52	0
2	B	2469	0	2412	115	0
2	D	2440	0	2382	86	0
3	H	932	0	881	31	0
3	J	932	0	881	31	0
4	K	848	0	798	29	0
4	L	848	0	798	33	0
5	C	28	0	25	0	0
6	E	39	0	34	0	0
7	F	61	0	52	1	0
7	G	61	0	52	0	0
8	A	14	0	13	0	0
8	H	14	0	13	1	0
8	J	14	0	13	0	0
All	All	10062	0	9625	364	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 19.

All (364) 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:B:322:GLU:HB3	4:L:24:ARG:NH2	1.61	1.12
1:A:143:VAL:HG13	1:A:171:LYS:NZ	1.74	1.02
2:B:334:ARG:CG	2:B:336:VAL:HG23	1.91	1.01
2:B:322:GLU:HB3	4:L:24:ARG:HH22	1.19	0.99
2:B:337:SER:O	2:B:361:VAL:HG22	1.63	0.98
1:A:143:VAL:HG13	1:A:171:LYS:HZ3	1.22	0.97
2:B:334:ARG:HD2	2:B:336:VAL:HG23	1.51	0.91
2:B:334:ARG:CD	2:B:336:VAL:HG23	2.01	0.90
1:A:156:CYS:HG	2:D:335:CYS:HG	0.85	0.83
2:B:334:ARG:HD2	2:B:336:VAL:CG2	2.16	0.76
2:B:322:GLU:CB	4:L:24:ARG:HH22	1.98	0.75
2:D:335:CYS:O	2:D:336:VAL:HG13	1.91	0.70
4:K:70:GLY:HA3	4:K:75:PHE:HA	1.74	0.70
3:H:5:VAL:HB	3:H:23:ALA:HB3	1.73	0.68
1:A:148:THR:HG22	1:A:164:PRO:HB2	1.74	0.68
2:D:347:ASP:HA	2:D:351:ARG:HB3	1.74	0.68
1:A:7:VAL:HA	1:A:26:CYS:HA	1.77	0.67
2:B:237:GLN:HE22	2:B:252:LEU:HA	1.60	0.67
1:A:98:MET:HE3	1:A:99:GLU:H	1.61	0.66
3:J:5:VAL:HB	3:J:23:ALA:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:GLN:HE21	2:B:525:ARG:HE	1.43	0.65
2:B:392:GLN:HE21	2:B:394:ASN:H	1.45	0.65
4:K:42:GLN:HA	4:K:48:PRO:HA	1.77	0.64
1:A:143:VAL:CG1	1:A:171:LYS:NZ	2.56	0.64
2:D:479:LEU:HB2	2:D:523:ILE:HB	1.80	0.64
3:H:20:LEU:HB2	3:H:81:LEU:HB3	1.78	0.64
2:B:266:ILE:HG12	2:B:314:VAL:HG13	1.80	0.63
2:B:334:ARG:HH11	2:B:336:VAL:HB	1.63	0.63
2:D:439:PRO:O	2:D:440:ARG:NH1	2.32	0.63
4:L:5:THR:HB	4:L:24:ARG:HB2	1.81	0.63
4:L:70:GLY:HA3	4:L:75:PHE:HA	1.81	0.63
2:B:313:GLN:HE21	2:B:322:GLU:HG3	1.64	0.62
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.79	0.62
2:B:422:HIS:HB3	2:B:425:LEU:HD13	1.81	0.62
2:B:446:TYR:HB2	2:B:465:LEU:HD23	1.81	0.62
1:A:130:TRP:NE1	1:A:132:GLU:OE1	2.32	0.62
4:L:87:PHE:HA	4:L:108:VAL:HG13	1.82	0.62
2:B:373:THR:HB	2:B:419:ARG:HB3	1.80	0.62
3:J:39:ARG:HB3	3:J:47:GLU:HB3	1.82	0.61
2:B:334:ARG:HG2	2:B:336:VAL:HG23	1.81	0.61
3:J:3:GLN:HB2	3:J:25:SER:HB2	1.83	0.61
4:L:42:GLN:NE2	4:L:46:ARG:O	2.32	0.61
1:A:105:LEU:HB2	1:A:136:ILE:HB	1.82	0.61
2:B:355:THR:HA	2:B:404:PRO:HA	1.82	0.61
2:B:268:TRP:HB3	2:B:275:MET:HE3	1.83	0.60
2:B:334:ARG:O	2:B:335:CYS:HB2	2.00	0.60
4:L:41:GLN:HE22	4:L:43:LYS:HG2	1.66	0.60
2:D:372:LEU:HA	2:D:420:VAL:HA	1.84	0.60
2:D:497:LYS:HA	2:D:503:PHE:HA	1.83	0.60
2:D:429:LEU:HD21	2:D:431:ARG:HH21	1.67	0.60
3:H:82:GLN:NE2	3:H:84:ASN:OD1	2.34	0.60
1:A:143:VAL:HG13	1:A:171:LYS:HZ1	1.65	0.60
4:K:94:GLN:HE21	4:K:101:THR:HG23	1.66	0.60
2:B:458:ASP:HB3	2:B:513:ARG:HB2	1.84	0.60
2:B:334:ARG:HG3	2:B:336:VAL:HG23	1.82	0.59
4:K:65:ARG:NH1	4:K:81:SER:O	2.35	0.59
2:B:282:ALA:HA	2:B:295:SER:HA	1.85	0.59
2:B:342:ARG:NH2	2:B:434:THR:O	2.36	0.59
1:A:122:LYS:HD2	1:A:149:TYR:HE2	1.67	0.58
2:B:286:GLN:HA	2:B:291:ALA:HA	1.85	0.58
2:D:269:LEU:HB2	2:D:311:THR:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:0:SER:O	4:L:27:LYS:NZ	2.36	0.58
2:D:376:ARG:HG2	2:D:378:SER:H	1.68	0.58
4:K:6:GLN:HA	4:K:23:CYS:HA	1.84	0.58
2:B:363:LEU:O	2:B:396:THR:OG1	2.22	0.57
1:A:59:LYS:NZ	1:A:61:GLU:OE1	2.38	0.57
2:B:345:PRO:HA	2:B:348:LEU:HB2	1.86	0.57
2:B:452:GLU:OE1	2:B:460:ARG:NH2	2.38	0.57
2:D:480:HIS:ND1	2:D:521:GLU:O	2.35	0.57
2:B:238:SER:HA	2:D:236:LEU:HD22	1.87	0.56
2:B:337:SER:C	2:B:361:VAL:HG22	2.29	0.56
2:D:376:ARG:HH21	2:D:382:VAL:HG12	1.69	0.56
4:K:42:GLN:NE2	4:K:46:ARG:O	2.38	0.56
1:A:103:LEU:HB3	1:A:138:ILE:HB	1.86	0.56
2:D:351:ARG:NH1	2:D:353:SER:OG	2.39	0.56
2:D:452:GLU:HB2	2:D:457:ARG:HG2	1.87	0.56
2:B:523:ILE:HD13	2:B:538:GLN:HB2	1.88	0.56
2:D:373:THR:HB	2:D:419:ARG:HB3	1.88	0.56
2:D:373:THR:N	2:D:419:ARG:O	2.38	0.56
2:D:498:THR:N	2:D:502:GLY:O	2.37	0.56
2:B:339:TYR:N	2:B:359:LEU:O	2.39	0.55
2:D:452:GLU:OE1	2:D:460:ARG:NH2	2.39	0.55
4:K:93:GLN:NE2	4:K:94:GLN:O	2.39	0.55
2:B:468:ASN:HA	2:B:502:GLY:HA3	1.87	0.55
2:B:487:ASP:OD1	2:B:487:ASP:N	2.39	0.55
3:H:40:GLN:N	3:H:93:VAL:O	2.39	0.55
3:J:82:GLN:NE2	3:J:83:MET:O	2.38	0.55
4:L:16:GLY:H	4:L:82:LEU:HB3	1.70	0.55
1:A:143:VAL:CG1	1:A:171:LYS:HZ1	2.19	0.55
3:H:42:PRO:HD3	3:H:92:ALA:HA	1.88	0.55
3:J:19:ARG:HH22	3:J:80:TYR:HB2	1.70	0.55
2:B:450:THR:HB	2:B:460:ARG:HB3	1.88	0.55
4:K:37:MET:HB3	4:K:55:ALA:HB2	1.88	0.55
2:B:351:ARG:NH1	2:B:353:SER:OG	2.40	0.55
3:H:17:SER:OG	3:H:82:GLN:NE2	2.40	0.55
1:A:15:ARG:HB3	1:A:84:PHE:HE1	1.72	0.55
1:A:111:ARG:NH1	2:D:424:HIS:O	2.39	0.55
3:J:18:LEU:O	3:J:82:GLN:NE2	2.39	0.55
4:K:71:SER:N	4:K:74:HIS:O	2.38	0.55
1:A:24:LEU:HB2	1:A:53:LEU:HB3	1.88	0.54
2:B:487:ASP:O	2:B:490:HIS:ND1	2.40	0.54
2:B:371:ASN:HB2	2:B:421:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:PRO:O	2:B:457:ARG:NH2	2.40	0.54
3:H:72:ARG:HA	3:H:79:PHE:HA	1.90	0.54
4:L:22:THR:HG22	4:L:24:ARG:HG3	1.89	0.54
4:K:38:ASN:ND2	4:K:95:SER:OG	2.40	0.54
3:J:20:LEU:HD12	3:J:81:LEU:HD22	1.90	0.54
1:A:88:LEU:HD11	1:A:155:VAL:HG21	1.89	0.54
2:B:441:ALA:N	2:B:470:MET:O	2.38	0.54
3:H:39:ARG:HB3	3:H:47:GLU:HB2	1.90	0.54
3:J:67:ARG:HG3	3:J:68:ILE:HG12	1.90	0.54
2:B:337:SER:HB3	2:B:361:VAL:CG2	2.38	0.54
2:D:287:GLU:HG2	2:D:290:LEU:HB3	1.90	0.54
3:J:40:GLN:NE2	3:J:44:LYS:O	2.41	0.54
4:L:30:ASP:OD1	4:L:35:SER:OG	2.23	0.54
2:D:355:THR:HA	2:D:404:PRO:HA	1.89	0.53
2:D:417:GLN:HE21	2:D:431:ARG:H	1.55	0.53
2:D:495:PRO:HA	2:D:505:VAL:HG22	1.90	0.53
2:B:376:ARG:HH21	2:B:382:VAL:HG12	1.72	0.53
4:L:107:LYS:NZ	4:L:109:GLU:OE2	2.42	0.53
3:J:19:ARG:NH2	3:J:71:SER:OG	2.42	0.53
4:L:69:SER:N	4:L:76:THR:O	2.41	0.53
2:B:256:VAL:HG21	2:B:314:VAL:HG21	1.91	0.53
2:B:417:GLN:NE2	2:B:418:CYS:O	2.42	0.53
2:B:478:TRP:HZ3	2:B:522:PHE:HB3	1.74	0.53
4:K:40:TYR:HB2	4:K:91:TYR:HB2	1.91	0.53
2:D:281:THR:O	2:D:296:GLU:N	2.42	0.52
3:J:19:ARG:HE	3:J:82:GLN:HB2	1.74	0.52
1:A:122:LYS:HB2	1:A:127:LEU:HD22	1.91	0.52
2:D:409:ASP:OD1	2:D:409:ASP:N	2.39	0.52
2:B:448:PHE:HZ	2:D:451:PRO:HD3	1.74	0.52
2:D:468:ASN:N	2:D:503:PHE:O	2.40	0.52
3:J:68:ILE:HG23	3:J:83:MET:HA	1.92	0.52
2:D:354:PRO:HB2	2:D:405:VAL:HB	1.91	0.52
2:B:446:TYR:OH	2:D:452:GLU:O	2.28	0.52
3:J:40:GLN:NE2	3:J:45:GLY:O	2.43	0.52
2:D:358:CYS:O	2:D:400:THR:OG1	2.25	0.52
3:J:17:SER:OG	3:J:82:GLN:NE2	2.43	0.52
2:B:409:ASP:O	2:B:414:GLU:N	2.42	0.52
2:B:478:TRP:HB3	2:B:485:LEU:HD12	1.92	0.52
3:J:33:TYR:HB3	3:J:98:LYS:HE2	1.92	0.52
3:H:28:ASN:OD1	3:H:30:THR:OG1	2.27	0.51
2:B:284:THR:HA	2:B:293:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:VAL:HG11	3:H:18:LEU:HD22	1.92	0.51
4:L:63:PRO:HB2	4:L:65:ARG:HG2	1.92	0.51
2:D:385:SER:OG	2:D:386:THR:N	2.41	0.51
2:B:270:GLU:O	2:B:273:GLN:NE2	2.44	0.51
2:D:349:PHE:O	2:D:352:LYS:NZ	2.37	0.51
1:A:88:LEU:HB3	1:A:162:SER:HB2	1.93	0.51
2:D:419:ARG:NE	2:D:430:MET:SD	2.75	0.51
2:D:461:THR:OG1	2:D:510:GLU:OE1	2.29	0.51
2:D:479:LEU:N	2:D:523:ILE:O	2.40	0.51
1:A:16:ILE:HG13	1:A:83:VAL:HA	1.92	0.51
1:A:151:CYS:HB3	1:A:162:SER:HB3	1.92	0.51
1:A:134:HIS:HD2	1:A:136:ILE:HD11	1.76	0.51
2:D:378:SER:OG	2:D:380:LYS:NZ	2.39	0.51
2:B:229:THR:OG1	2:B:260:THR:N	2.44	0.50
2:D:507:SER:OG	2:D:508:ARG:N	2.43	0.50
4:K:22:THR:HG21	4:K:74:HIS:NE2	2.26	0.50
2:B:458:ASP:OD1	2:B:513:ARG:NH1	2.37	0.50
2:D:478:TRP:HB3	2:D:485:LEU:HD12	1.93	0.50
4:K:6:GLN:HG2	4:K:23:CYS:HB3	1.93	0.50
2:B:363:LEU:HD13	2:B:398:THR:HA	1.94	0.50
4:K:7:SER:N	4:K:22:THR:O	2.45	0.50
4:K:43:LYS:HG3	4:K:46:ARG:HH21	1.77	0.50
1:A:145:ASP:O	1:A:149:TYR:OH	2.30	0.50
2:B:248:PRO:HA	2:B:301:GLN:HB2	1.93	0.49
3:J:55:ASP:OD1	3:J:55:ASP:N	2.41	0.49
2:B:334:ARG:NH1	2:B:336:VAL:N	2.60	0.49
2:D:462:LEU:O	2:D:509:LEU:N	2.42	0.49
3:H:19:ARG:HA	3:H:82:GLN:HA	1.93	0.49
1:A:22:VAL:HG12	1:A:55:ILE:HB	1.95	0.49
1:A:142:THR:OG1	1:A:145:ASP:OD1	2.30	0.49
1:A:13:TRP:HB3	1:A:91:GLN:HE22	1.77	0.49
2:D:409:ASP:O	2:D:413:GLY:N	2.45	0.49
2:D:528:HIS:CD2	2:D:530:ALA:H	2.30	0.49
1:A:69:GLN:HB3	1:A:75:GLU:HG3	1.95	0.49
2:D:346:PHE:O	2:D:351:ARG:N	2.41	0.49
3:J:101:ASN:HB2	3:J:106:TRP:CZ2	2.47	0.49
2:D:453:TRP:HD1	2:D:455:GLY:H	1.61	0.48
3:H:63:SER:O	3:H:67:ARG:NH2	2.45	0.48
3:J:91:THR:HG23	3:J:118:THR:HA	1.95	0.48
4:K:67:SER:O	4:K:78:THR:N	2.43	0.48
2:B:322:GLU:CB	4:L:24:ARG:NH2	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:HB3	1:A:134:HIS:CE1	2.47	0.48
1:A:15:ARG:HA	1:A:82:GLU:HB2	1.94	0.48
1:A:146:SER:OG	1:A:167:ILE:O	2.30	0.48
2:B:480:HIS:HB3	2:B:485:LEU:HD21	1.96	0.48
3:J:53:THR:OG1	3:J:54:TYR:N	2.46	0.48
2:B:334:ARG:NH1	2:B:336:VAL:H	2.12	0.48
2:D:374:TRP:HA	2:D:418:CYS:HA	1.96	0.48
2:B:461:THR:HA	2:B:510:GLU:HA	1.96	0.48
2:B:254:CYS:SG	2:B:295:SER:OG	2.66	0.48
2:D:443:PRO:HB3	2:D:469:PHE:CD2	2.48	0.48
2:B:368:GLY:O	2:B:422:HIS:NE2	2.47	0.48
2:D:248:PRO:O	2:D:301:GLN:N	2.46	0.48
3:J:100:ASN:N	3:J:107:HIS:O	2.47	0.48
4:L:41:GLN:HE21	4:L:88:ALA:HB3	1.78	0.48
1:A:40:PHE:N	1:A:67:LYS:O	2.42	0.47
1:A:146:SER:HB2	1:A:169:VAL:HG12	1.97	0.47
2:B:237:GLN:NE2	2:B:252:LEU:HA	2.26	0.47
3:J:33:TYR:CD2	3:J:100:ASN:HA	2.50	0.47
2:B:339:TYR:HB2	2:B:359:LEU:HB2	1.96	0.47
2:D:357:THR:HA	2:D:402:THR:HA	1.95	0.47
3:H:17:SER:HA	3:H:84:ASN:HA	1.96	0.47
3:H:75:SER:HA	8:H:201:NAG:H3	1.95	0.47
4:L:41:GLN:HB2	4:L:51:LEU:HD11	1.96	0.47
1:A:106:ARG:HH12	1:A:108:HIS:HB2	1.78	0.47
2:B:346:PHE:O	2:B:351:ARG:N	2.39	0.47
2:B:496:ARG:HH22	2:B:497:LYS:HG2	1.80	0.47
2:D:266:ILE:HG23	2:D:314:VAL:HG22	1.97	0.47
3:J:20:LEU:HB2	3:J:81:LEU:HB3	1.97	0.47
2:B:480:HIS:HE1	2:B:519:LYS:HB3	1.80	0.47
2:D:269:LEU:N	2:D:311:THR:O	2.46	0.47
2:B:303:HIS:O	2:B:306:SER:OG	2.33	0.47
2:B:375:SER:N	2:B:417:GLN:O	2.47	0.47
4:L:2:ILE:HG23	4:L:27:LYS:H	1.80	0.47
1:A:103:LEU:HD23	1:A:138:ILE:HD12	1.96	0.47
2:D:302:LYS:HA	2:D:305:LEU:HB2	1.97	0.47
2:D:492:THR:HA	2:D:507:SER:HA	1.96	0.47
3:H:18:LEU:O	3:H:83:MET:N	2.45	0.47
2:B:430:MET:O	4:L:57:TYR:OH	2.29	0.46
2:B:439:PRO:HD2	2:B:470:MET:HE2	1.95	0.46
2:D:446:TYR:HD1	2:D:465:LEU:HD11	1.79	0.46
2:D:408:ARG:HA	2:D:408:ARG:HD2	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:68:GLY:HA2	4:K:77:LEU:HA	1.96	0.46
3:J:39:ARG:NE	3:J:47:GLU:OE2	2.48	0.46
1:A:59:LYS:HG3	1:A:61:GLU:H	1.80	0.46
2:B:285:THR:OG1	2:B:292:SER:O	2.27	0.46
2:D:256:VAL:HG21	2:D:314:VAL:HG21	1.97	0.46
2:D:525:ARG:HG3	2:D:538:GLN:HB3	1.98	0.46
4:K:12:SER:OG	4:K:110:ILE:O	2.34	0.46
2:B:302:LYS:HA	2:B:305:LEU:HB2	1.97	0.46
2:B:310:TYR:N	2:B:325:THR:O	2.46	0.46
3:H:9:GLY:HA2	3:H:117:VAL:HG22	1.98	0.46
3:J:87:ARG:N	3:J:90:ASP:OD2	2.44	0.46
2:B:470:MET:HE3	2:B:471:PRO:HG3	1.98	0.46
2:B:519:LYS:HE3	2:B:521:GLU:H	1.80	0.46
3:J:15:ASP:N	3:J:86:LEU:O	2.42	0.46
1:A:155:VAL:O	1:A:158:LEU:N	2.48	0.46
2:B:342:ARG:NH2	2:B:433:THR:OG1	2.47	0.46
2:B:372:LEU:HD21	2:B:374:TRP:HE1	1.81	0.46
2:B:286:GLN:NE2	2:B:288:GLY:O	2.50	0.45
2:B:441:ALA:O	2:B:528:HIS:NE2	2.38	0.45
2:D:232:THR:OG1	2:D:257:SER:OG	2.31	0.45
3:J:23:ALA:HA	3:J:78:THR:HG23	1.97	0.45
4:L:93:GLN:NE2	4:L:94:GLN:O	2.50	0.45
4:L:43:LYS:HB3	4:L:46:ARG:HH11	1.80	0.45
2:D:269:LEU:O	2:D:311:THR:N	2.49	0.45
2:D:363:LEU:HD13	2:D:398:THR:HA	1.98	0.45
4:K:42:GLN:NE2	4:K:43:LYS:O	2.50	0.45
2:D:512:THR:HG1	2:D:515:GLU:CD	2.24	0.45
3:H:33:TYR:HB3	3:H:99:GLY:O	2.17	0.45
2:D:249:THR:HG22	2:D:300:SER:HA	1.99	0.45
3:H:105:HIS:ND1	4:L:95:SER:O	2.49	0.45
2:B:513:ARG:HA	2:B:513:ARG:HD2	1.87	0.45
2:D:257:SER:HA	2:D:292:SER:HA	1.98	0.45
2:B:345:PRO:O	2:B:349:PHE:N	2.42	0.45
4:K:93:GLN:HE21	4:K:100:TYR:HB3	1.82	0.45
1:A:90:LEU:HG	1:A:151:CYS:HB2	1.98	0.45
2:D:449:ALA:HA	2:D:462:LEU:HD22	1.98	0.45
2:B:376:ARG:NH2	2:B:380:LYS:O	2.50	0.44
2:D:356:ILE:N	2:D:403:LEU:O	2.49	0.44
3:H:100:ASN:HB2	3:H:107:HIS:CD2	2.52	0.44
1:A:106:ARG:NH2	1:A:107:CYS:O	2.51	0.44
2:D:266:ILE:HG13	2:D:314:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:SER:OG	2:B:459:LYS:O	2.31	0.44
4:K:69:SER:N	4:K:76:THR:O	2.43	0.44
2:B:310:TYR:O	2:B:325:THR:N	2.44	0.44
2:B:480:HIS:CE1	2:B:519:LYS:HB3	2.53	0.44
4:L:5:THR:N	4:L:24:ARG:O	2.51	0.44
1:A:6:LYS:HD2	1:A:6:LYS:HA	1.73	0.44
2:D:241:ASP:OD1	2:D:241:ASP:N	2.42	0.44
1:A:90:LEU:HA	1:A:107:CYS:HA	1.98	0.44
2:D:259:TYR:O	2:D:291:ALA:N	2.51	0.44
3:H:94:TYR:HB2	3:H:115:THR:HG23	2.00	0.44
2:B:495:PRO:HA	2:B:505:VAL:HG22	2.00	0.44
4:K:86:ASP:O	4:K:90:TYR:OH	2.33	0.44
2:D:480:HIS:CE1	2:D:519:LYS:HB3	2.53	0.43
3:H:46:LEU:HB2	4:L:102:PHE:CD2	2.53	0.43
2:B:460:ARG:O	2:B:511:VAL:N	2.43	0.43
3:H:4:LEU:HD11	3:H:110:VAL:HG22	2.00	0.43
2:B:354:PRO:HG2	2:B:405:VAL:HB	2.01	0.43
2:B:307:ASP:HA	2:B:327:LYS:HB3	2.01	0.43
2:B:434:THR:OG1	2:B:435:LYS:N	2.52	0.43
2:B:285:THR:O	2:B:292:SER:N	2.51	0.43
2:D:434:THR:OG1	2:D:435:LYS:N	2.52	0.43
4:K:44:PRO:O	4:K:46:ARG:NH2	2.51	0.43
1:A:99:GLU:HA	1:A:141:ALA:HB3	1.99	0.43
1:A:36:SER:OG	1:A:49:THR:O	2.33	0.43
2:B:438:GLY:O	2:B:440:ARG:NH1	2.52	0.43
3:H:70:ILE:HA	3:H:81:LEU:HA	2.00	0.43
1:A:16:ILE:HD11	1:A:83:VAL:HG22	2.00	0.43
2:B:480:HIS:CE1	2:B:481:ASN:HB2	2.54	0.43
3:H:111:TRP:HB2	4:L:47:ALA:HB1	2.00	0.43
4:L:53:TYR:CZ	4:L:57:TYR:HB3	2.54	0.42
2:D:248:PRO:HA	2:D:301:GLN:HE21	1.84	0.42
4:L:36:TYR:O	4:L:95:SER:N	2.46	0.42
2:B:301:GLN:HE21	2:B:305:LEU:HD11	1.85	0.42
2:D:356:ILE:O	2:D:403:LEU:N	2.47	0.42
2:B:523:ILE:HG23	2:B:539:ARG:H	1.84	0.42
4:K:36:TYR:HB2	4:K:96:HIS:HB2	2.01	0.42
2:B:539:ARG:NH2	2:B:540:ALA:O	2.53	0.42
1:A:11:PRO:HB2	1:A:13:TRP:HD1	1.85	0.42
1:A:24:LEU:HD11	1:A:55:ILE:HG12	2.01	0.42
2:B:283:SER:HB2	2:B:294:GLN:HG3	2.01	0.42
2:B:410:TRP:C	2:B:413:GLY:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:PHE:N	2:D:475:SER:OG	2.48	0.42
3:H:29:ILE:HG12	3:H:77:ASN:HA	2.01	0.42
2:B:363:LEU:HD13	2:B:399:VAL:H	1.85	0.42
4:K:67:SER:N	4:K:78:THR:O	2.51	0.42
7:F:2:NAG:H82	7:F:2:NAG:H2	1.89	0.42
2:B:241:ASP:OD1	2:B:245:HIS:N	2.53	0.42
2:D:363:LEU:HB2	2:D:398:THR:HA	2.01	0.42
3:J:33:TYR:CB	3:J:98:LYS:HE2	2.50	0.42
2:D:259:TYR:OH	2:D:293:THR:OG1	2.34	0.42
2:B:480:HIS:CE1	2:B:519:LYS:HE2	2.55	0.41
2:D:273:GLN:NE2	2:D:274:VAL:O	2.53	0.41
3:H:98:LYS:HB2	3:H:98:LYS:HE3	1.83	0.41
2:B:409:ASP:N	2:B:409:ASP:OD1	2.52	0.41
2:D:386:THR:OG1	2:D:402:THR:N	2.50	0.41
4:L:7:SER:HA	4:L:8:PRO:HA	1.93	0.41
4:L:107:LYS:HE3	4:L:107:LYS:HB3	1.85	0.41
1:A:117:LYS:HE3	1:A:131:TYR:HD1	1.84	0.41
3:J:6:GLU:H	3:J:113:GLN:HE22	1.67	0.41
3:J:83:MET:HB2	3:J:86:LEU:HD21	2.02	0.41
4:K:41:GLN:O	4:K:49:LYS:N	2.54	0.41
1:A:147:GLY:O	1:A:167:ILE:N	2.47	0.41
2:B:315:THR:HA	2:B:320:THR:HA	2.01	0.41
2:D:474:ILE:HG12	2:D:528:HIS:HA	2.02	0.41
2:B:389:GLU:HG3	2:B:399:VAL:HG22	2.02	0.41
2:D:376:ARG:HB3	2:D:379:GLY:H	1.86	0.41
3:H:37:TRP:HD1	3:H:70:ILE:HD12	1.85	0.41
3:J:91:THR:OG1	3:J:119:VAL:N	2.44	0.41
2:B:337:SER:O	2:B:361:VAL:CG2	2.50	0.41
2:B:380:LYS:NZ	3:H:32:GLY:HA3	2.35	0.41
2:B:498:THR:N	2:B:502:GLY:O	2.41	0.41
2:D:465:LEU:HA	2:D:506:PHE:HD1	1.85	0.41
4:K:2:ILE:HG23	4:K:26:SER:H	1.86	0.41
1:A:13:TRP:HB3	1:A:91:GLN:NE2	2.34	0.41
3:H:41:THR:HB	3:H:44:LYS:HB3	2.02	0.41
1:A:41:HIS:O	1:A:44:SER:OG	2.31	0.41
2:B:241:ASP:OD1	2:B:241:ASP:N	2.51	0.41
2:B:343:PRO:HD3	2:B:356:ILE:HD12	2.03	0.41
2:B:356:ILE:N	2:B:403:LEU:O	2.45	0.41
2:D:342:ARG:HA	2:D:343:PRO:HD3	1.89	0.41
2:D:408:ARG:HA	2:D:411:ILE:HD12	2.03	0.41
4:L:43:LYS:HB2	4:L:46:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:CD1	1:A:132:GLU:H	2.39	0.41
2:D:497:LYS:HE2	2:D:497:LYS:HB2	1.95	0.41
4:L:40:TYR:HE2	4:L:93:GLN:HB3	1.85	0.41
2:B:267:THR:HG23	2:B:313:GLN:HB3	2.03	0.41
2:B:388:LYS:O	2:B:399:VAL:HA	2.21	0.41
2:B:429:LEU:HD11	2:B:431:ARG:HE	1.86	0.41
2:D:302:LYS:O	2:D:306:SER:N	2.53	0.41
2:D:508:ARG:NH2	2:D:510:GLU:HB2	2.36	0.41
2:D:470:MET:HB2	2:D:470:MET:HE3	1.77	0.40
3:H:32:GLY:HA2	3:H:54:TYR:CD1	2.57	0.40
3:J:102:TYR:N	3:J:105:HIS:O	2.49	0.40
4:L:41:GLN:HB3	4:L:51:LEU:HD21	2.02	0.40
1:A:39:TRP:N	1:A:46:SER:OG	2.47	0.40
4:K:29:VAL:HB	4:K:96:HIS:ND1	2.35	0.40
2:D:304:TRP:CZ2	2:D:327:LYS:HA	2.57	0.40
4:K:15:VAL:HA	4:K:82:LEU:HB3	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	A	165/197 (84%)	142 (86%)	22 (13%)	1 (1%)	21	59
2	B	314/322 (98%)	286 (91%)	27 (9%)	1 (0%)	36	72
2	D	308/322 (96%)	279 (91%)	28 (9%)	1 (0%)	36	72
3	H	118/123 (96%)	110 (93%)	8 (7%)	0	100	100
3	J	118/123 (96%)	105 (89%)	12 (10%)	1 (1%)	16	54
4	K	110/134 (82%)	97 (88%)	13 (12%)	0	100	100
4	L	110/134 (82%)	103 (94%)	7 (6%)	0	100	100
All	All	1243/1355 (92%)	1122 (90%)	117 (9%)	4 (0%)	37	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	336	VAL
1	A	71	GLN
2	B	334	ARG
3	J	33	TYR

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	152/173 (88%)	147 (97%)	5 (3%)	33	55
2	B	281/285 (99%)	278 (99%)	3 (1%)	65	76
2	D	277/285 (97%)	272 (98%)	5 (2%)	51	68
3	H	99/101 (98%)	98 (99%)	1 (1%)	68	78
3	J	99/101 (98%)	99 (100%)	0	100	100
4	K	95/113 (84%)	94 (99%)	1 (1%)	65	76
4	L	95/113 (84%)	95 (100%)	0	100	100
All	All	1098/1171 (94%)	1083 (99%)	15 (1%)	57	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	155	VAL
1	A	156	CYS
1	A	157	GLN
1	A	158	LEU
2	B	253	LEU
2	B	255	LEU
2	B	334	ARG
2	D	252	LEU
2	D	253	LEU
2	D	336	VAL
2	D	405	VAL

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Mol	Chain	Res	Type
2	D	445	VAL
3	H	34	SER
4	K	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	72	GLN
1	A	91	GLN
2	B	313	GLN
2	B	319	HIS
2	B	392	GLN
2	B	467	GLN
2	D	251	GLN
2	D	301	GLN
2	D	535	GLN
3	H	13	GLN
3	H	40	GLN
3	H	82	GLN
3	H	100	ASN
3	J	82	GLN
3	J	100	ASN
3	J	105	HIS
4	K	38	ASN
4	K	93	GLN
4	L	41	GLN
4	L	74	HIS
4	L	83	GLN
4	L	93	GLN

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 [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$
5	NAG	C	1	5,1	14,14,15	0.30	0	17,19,21	1.29	2 (11%)
5	NAG	C	2	5	14,14,15	0.41	0	17,19,21	1.12	2 (11%)
6	NAG	E	1	6,1	14,14,15	0.56	0	17,19,21	2.04	6 (35%)
6	NAG	E	2	6	14,14,15	0.36	0	17,19,21	0.68	0
6	BMA	E	3	6	11,11,12	0.29	0	15,15,17	0.58	0
7	NAG	F	1	2,7	14,14,15	0.45	0	17,19,21	0.92	0
7	NAG	F	2	7	14,14,15	0.31	0	17,19,21	1.24	2 (11%)
7	MAN	F	3	7	11,11,12	0.23	0	15,15,17	0.64	0
7	MAN	F	4	7	11,11,12	0.37	0	15,15,17	0.93	1 (6%)
7	MAN	F	5	7	11,11,12	0.20	0	15,15,17	0.55	0
7	NAG	G	1	2,7	14,14,15	0.46	0	17,19,21	1.37	3 (17%)
7	NAG	G	2	7	14,14,15	0.42	0	17,19,21	1.50	1 (5%)
7	MAN	G	3	7	11,11,12	0.25	0	15,15,17	0.73	0
7	MAN	G	4	7	11,11,12	0.32	0	15,15,17	0.73	0
7	MAN	G	5	7	11,11,12	0.19	0	15,15,17	0.49	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
5	NAG	C	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	E	2	6	-	4/6/23/26	0/1/1/1
6	BMA	E	3	6	-	2/2/19/22	0/1/1/1
7	NAG	F	1	2,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	F	2	7	-	4/6/23/26	0/1/1/1
7	MAN	F	3	7	-	2/2/19/22	1/1/1/1
7	MAN	F	4	7	-	0/2/19/22	0/1/1/1
7	MAN	F	5	7	-	0/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	G	2	7	-	4/6/23/26	0/1/1/1
7	MAN	G	3	7	-	2/2/19/22	1/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2	NAG	C1-O5-C5	-5.03	105.44	112.19
6	E	1	NAG	C2-N2-C7	4.83	129.38	122.90
6	E	1	NAG	C4-C3-C2	3.48	116.12	111.02
5	C	1	NAG	O5-C1-C2	3.48	116.68	111.29
7	F	2	NAG	C4-C3-C2	-3.30	106.18	111.02
6	E	1	NAG	O5-C1-C2	-3.29	106.19	111.29
7	G	1	NAG	C4-C3-C2	2.91	115.28	111.02
7	G	1	NAG	C1-O5-C5	-2.81	108.42	112.19
7	G	1	NAG	C3-C4-C5	2.79	115.28	110.23
7	F	2	NAG	O5-C1-C2	-2.65	107.19	111.29
6	E	1	NAG	C1-C2-N2	2.44	114.28	110.43
5	C	2	NAG	C2-N2-C7	-2.40	119.68	122.90
6	E	1	NAG	C3-C4-C5	2.31	114.42	110.23
5	C	2	NAG	C4-C3-C2	2.25	114.32	111.02
5	C	1	NAG	C1-O5-C5	2.23	115.18	112.19
6	E	1	NAG	O7-C7-N2	2.15	125.77	121.98
7	F	4	MAN	C1-C2-C3	2.05	112.63	109.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C1-C2-N2-C7
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	E	1	NAG	C1-C2-N2-C7
7	F	2	NAG	C8-C7-N2-C2
7	F	2	NAG	O7-C7-N2-C2
6	E	3	BMA	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6
7	G	3	MAN	C4-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
7	G	4	MAN	C4-C5-C6-O6
7	G	3	MAN	O5-C5-C6-O6
7	G	2	NAG	O7-C7-N2-C2
6	E	1	NAG	O5-C5-C6-O6
6	E	1	NAG	C4-C5-C6-O6
7	F	1	NAG	O5-C5-C6-O6
7	G	4	MAN	O5-C5-C6-O6
7	G	5	MAN	O5-C5-C6-O6
6	E	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
6	E	3	BMA	C4-C5-C6-O6
7	F	3	MAN	C4-C5-C6-O6
6	E	2	NAG	C8-C7-N2-C2
7	F	1	NAG	C4-C5-C6-O6
7	G	5	MAN	C4-C5-C6-O6
7	F	3	MAN	O5-C5-C6-O6
6	E	2	NAG	O7-C7-N2-C2
5	C	1	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	F	2	NAG	O5-C5-C6-O6
7	F	2	NAG	C4-C5-C6-O6
6	E	1	NAG	C8-C7-N2-C2
6	E	1	NAG	O7-C7-N2-C2
7	G	1	NAG	C1-C2-N2-C7
7	G	2	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	3	MAN	C1-C2-C3-C4-C5-O5
7	G	3	MAN	C1-C2-C3-C4-C5-O5

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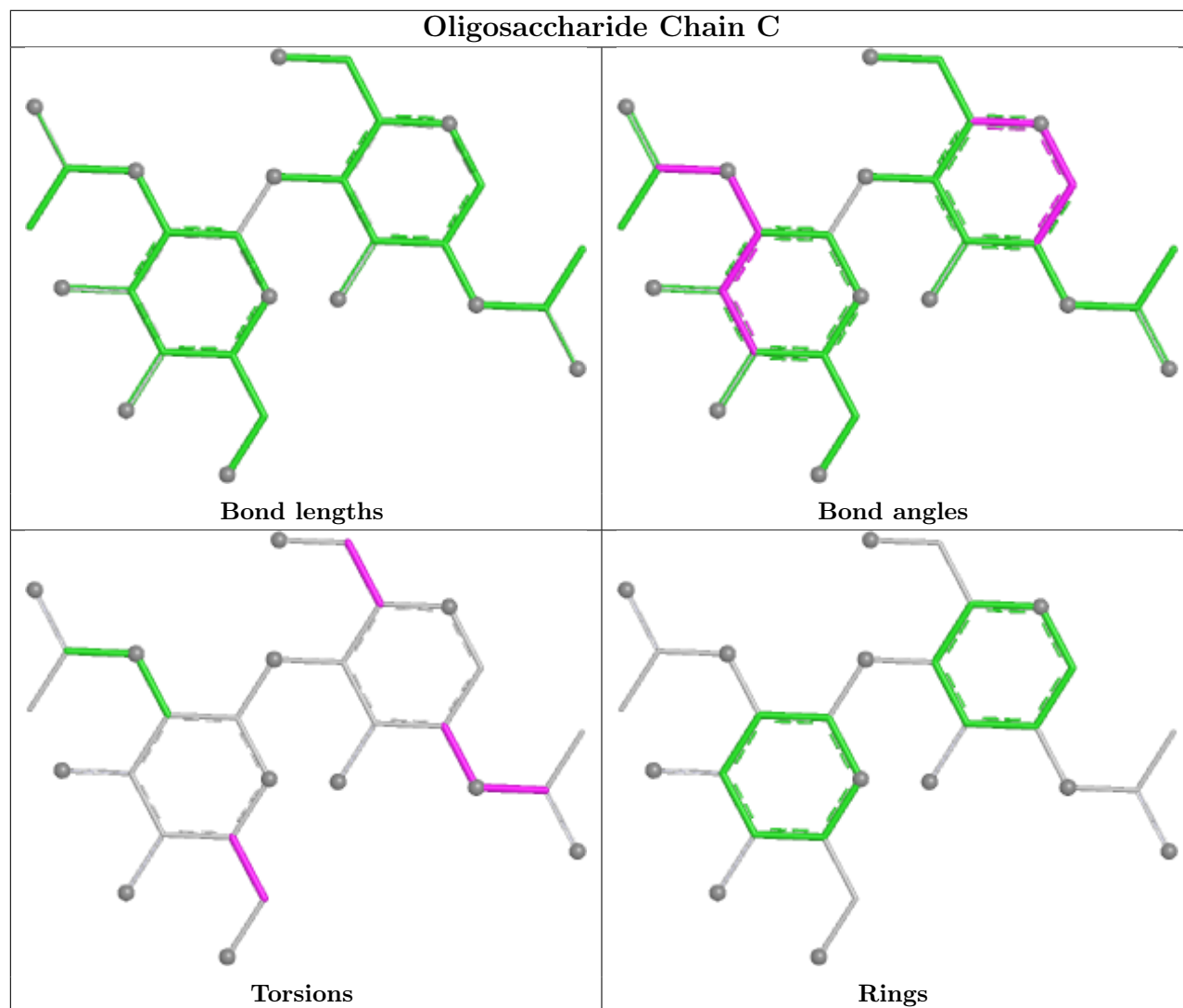
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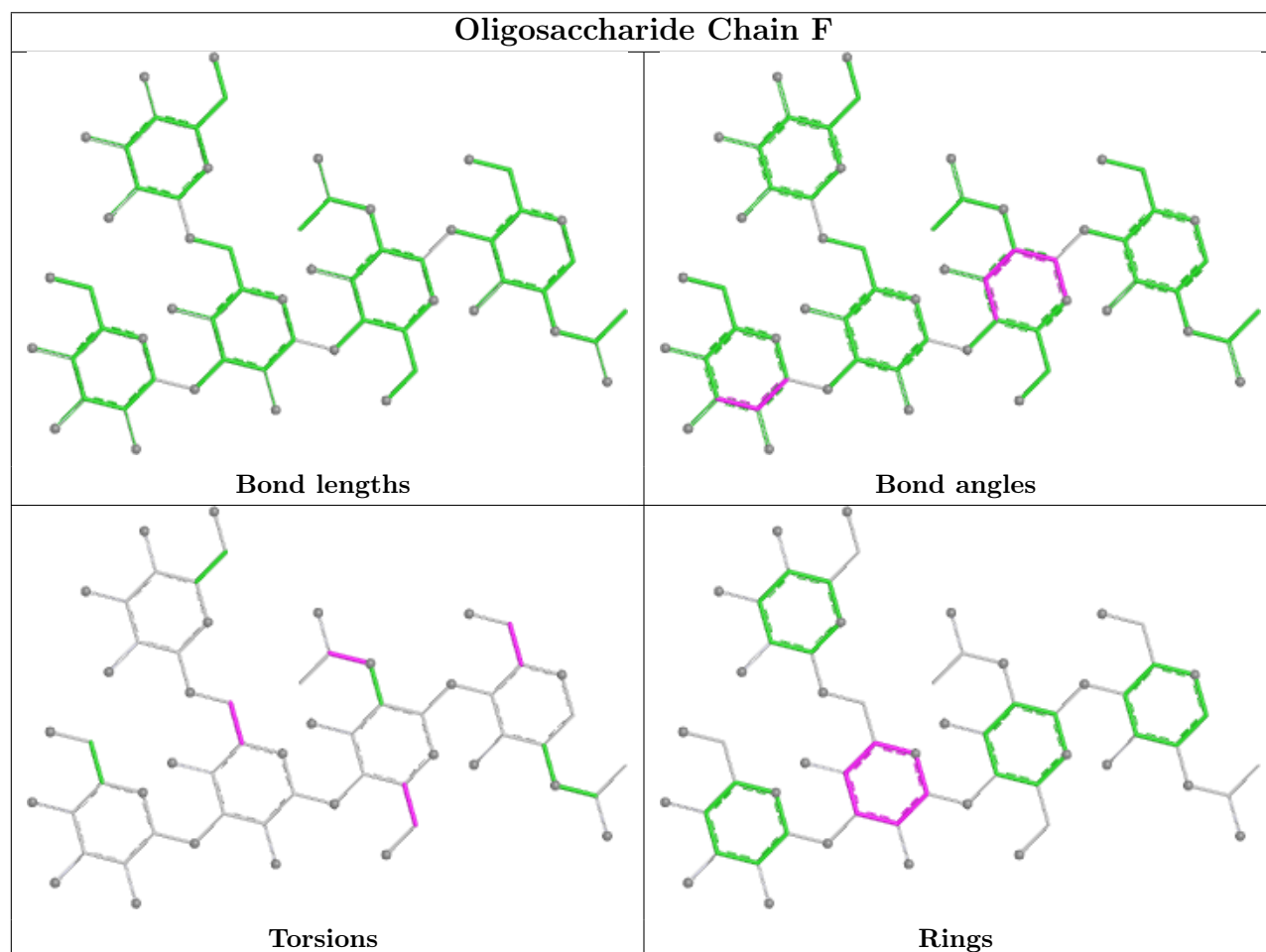
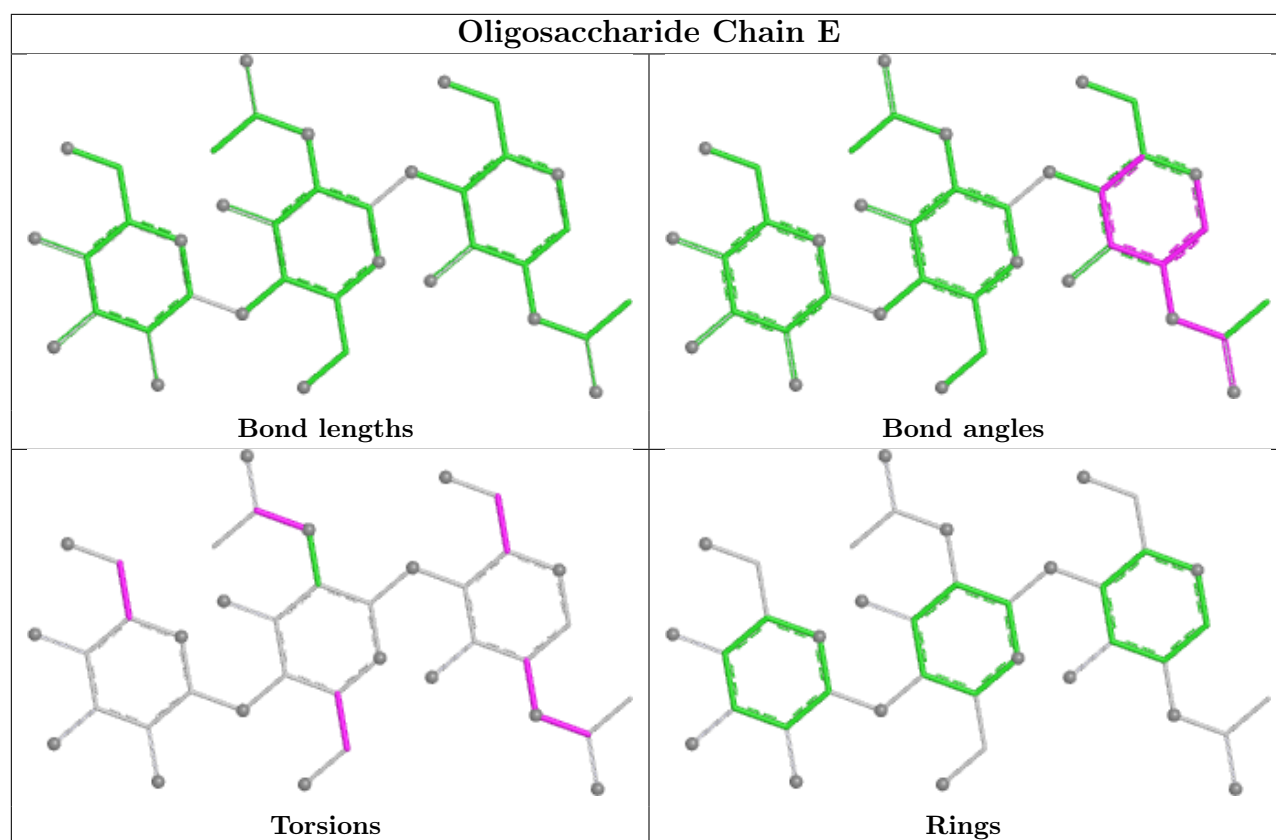
Mol	Chain	Res	Type	Atoms
7	G	5	MAN	C1-C2-C3-C4-C5-O5

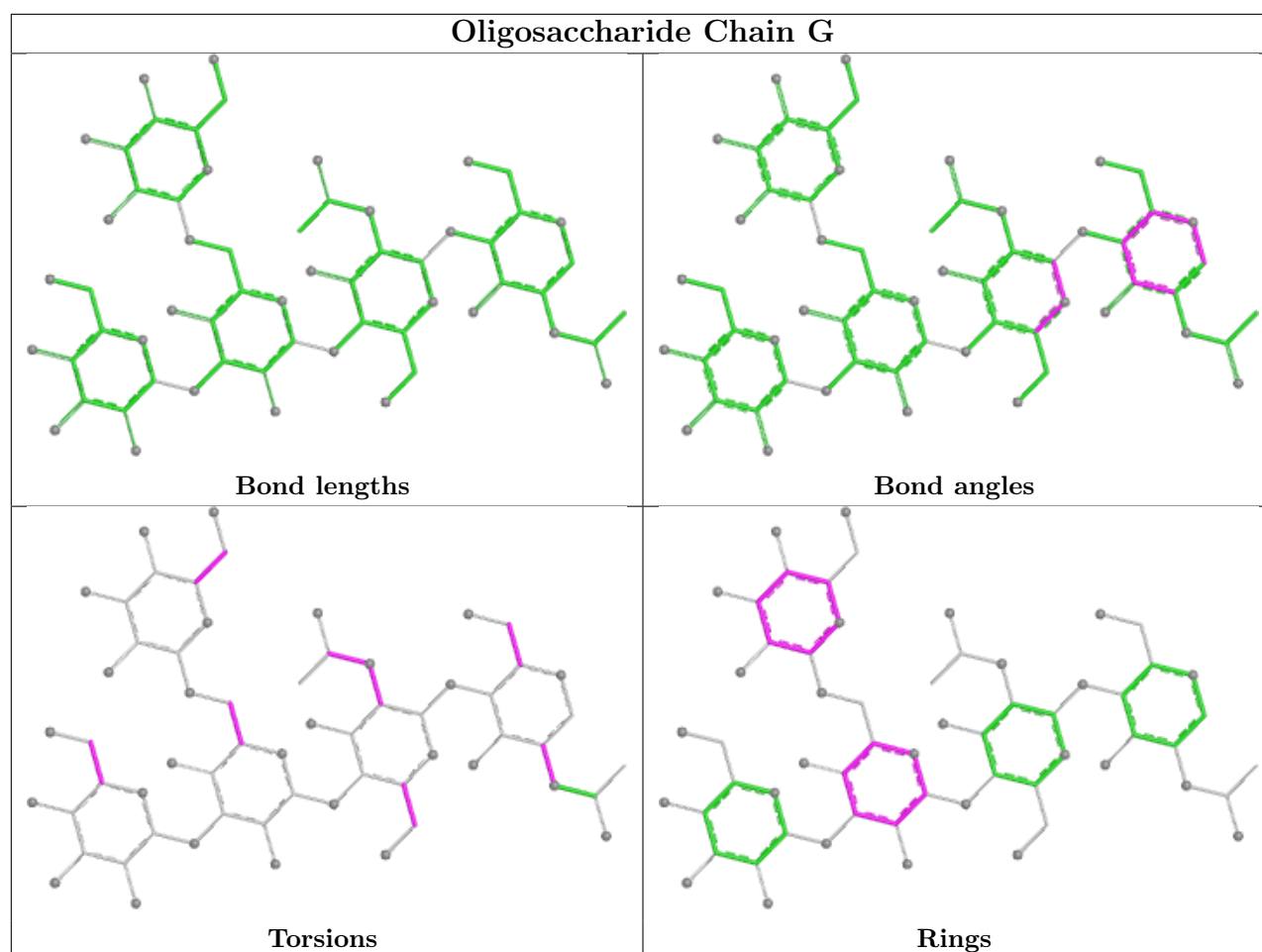
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	2	NAG	1	0

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







5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
8	NAG	H	201	3	14,14,15	0.20	0	17,19,21	0.38	0
8	NAG	A	201	1	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
8	NAG	J	201	3	14,14,15	0.31	0	17,19,21	0.54	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
8	NAG	H	201	3	-	2/6/23/26	0/1/1/1
8	NAG	A	201	1	-	5/6/23/26	0/1/1/1
8	NAG	J	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	201	NAG	C2-N2-C7	3.59	127.72	122.90
8	A	201	NAG	C1-C2-N2	3.01	115.18	110.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	201	NAG	C1-C2-N2-C7
8	A	201	NAG	C8-C7-N2-C2
8	A	201	NAG	O7-C7-N2-C2
8	H	201	NAG	C4-C5-C6-O6
8	H	201	NAG	O5-C5-C6-O6
8	A	201	NAG	C4-C5-C6-O6
8	A	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	201	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.

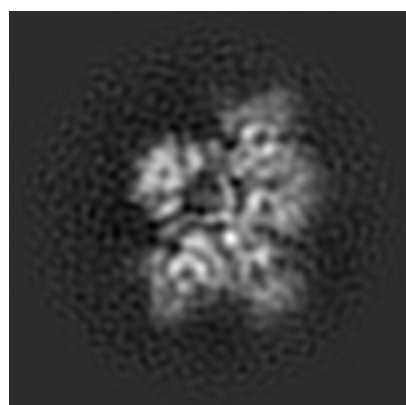
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25136. These allow visual inspection of the internal detail of the map and identification of artifacts.

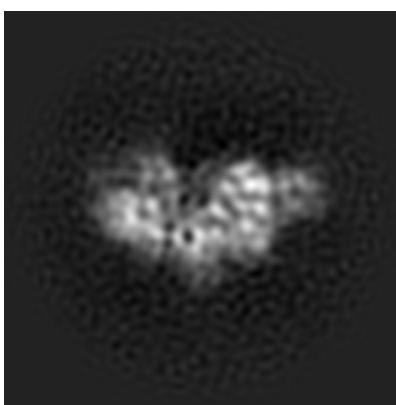
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

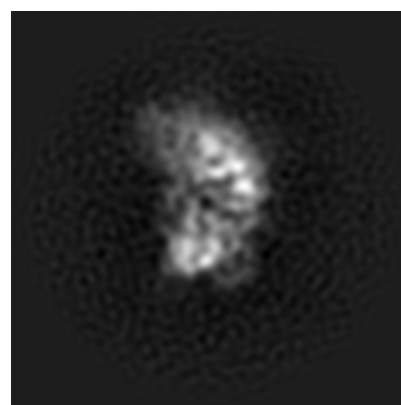
6.1.1 Primary map



X



Y

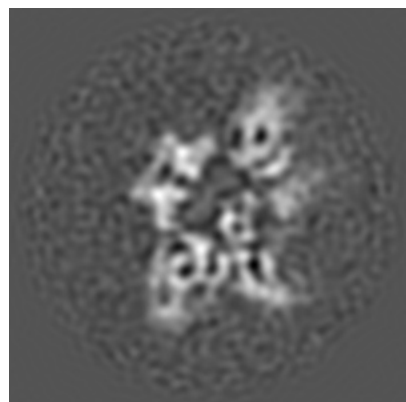


Z

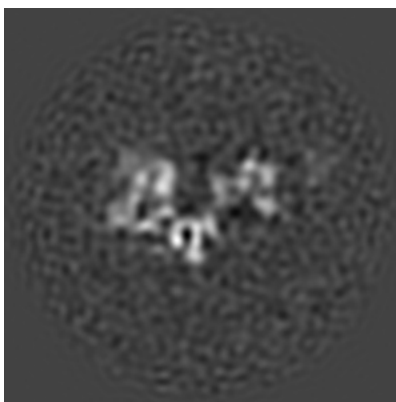
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

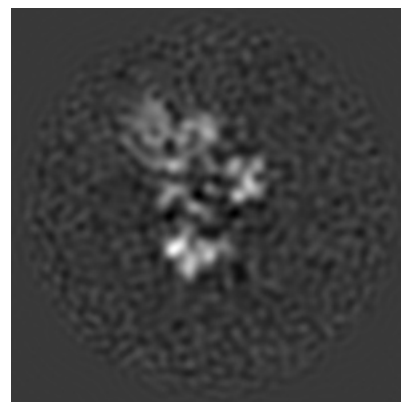
6.2.1 Primary map



X Index: 128



Y Index: 128

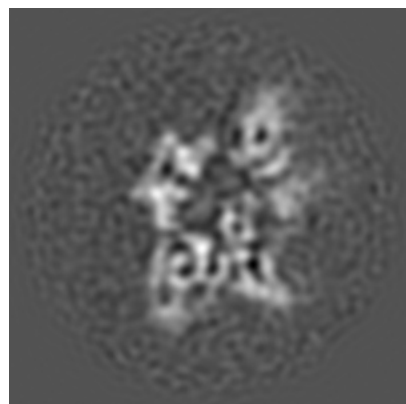


Z Index: 128

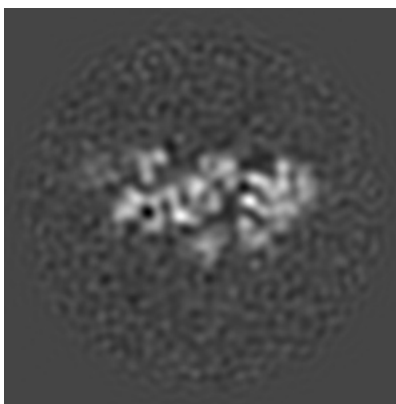
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

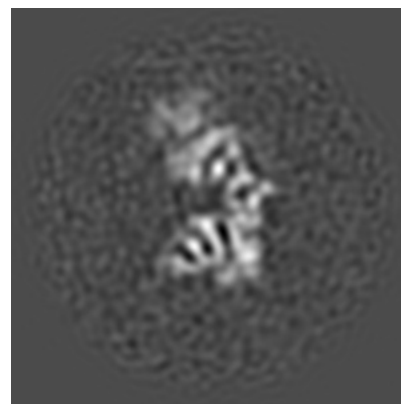
6.3.1 Primary map



X Index: 127



Y Index: 153

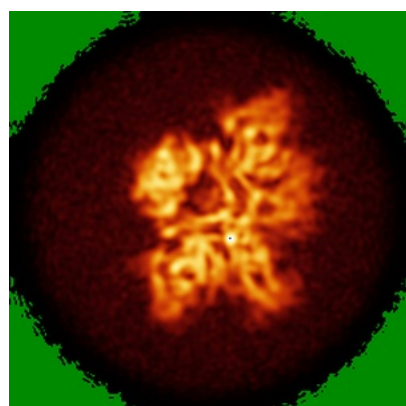


Z Index: 155

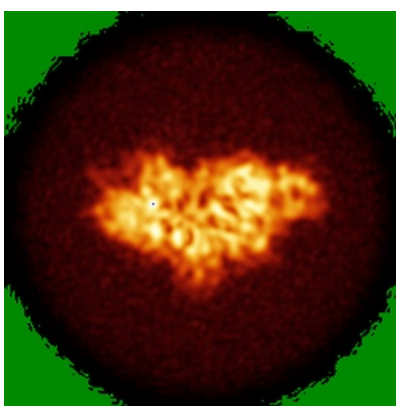
The images above show the largest variance slices of the map in three orthogonal directions.

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

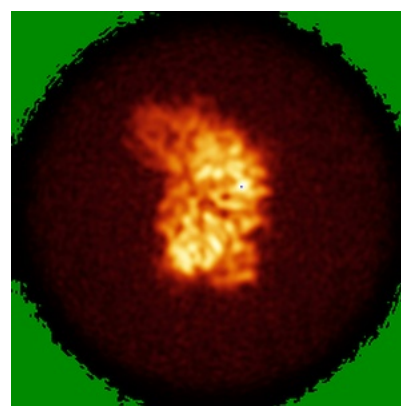
6.4.1 Primary map



X



Y

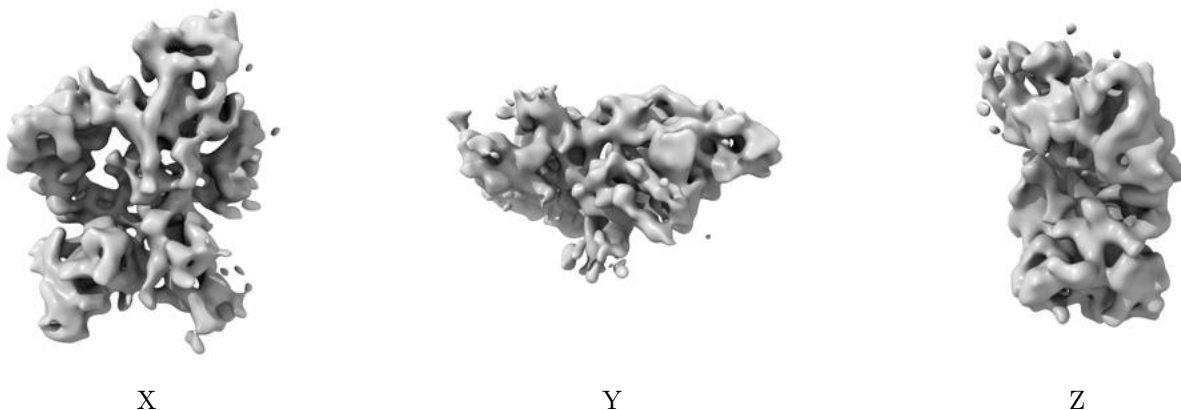


Z

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

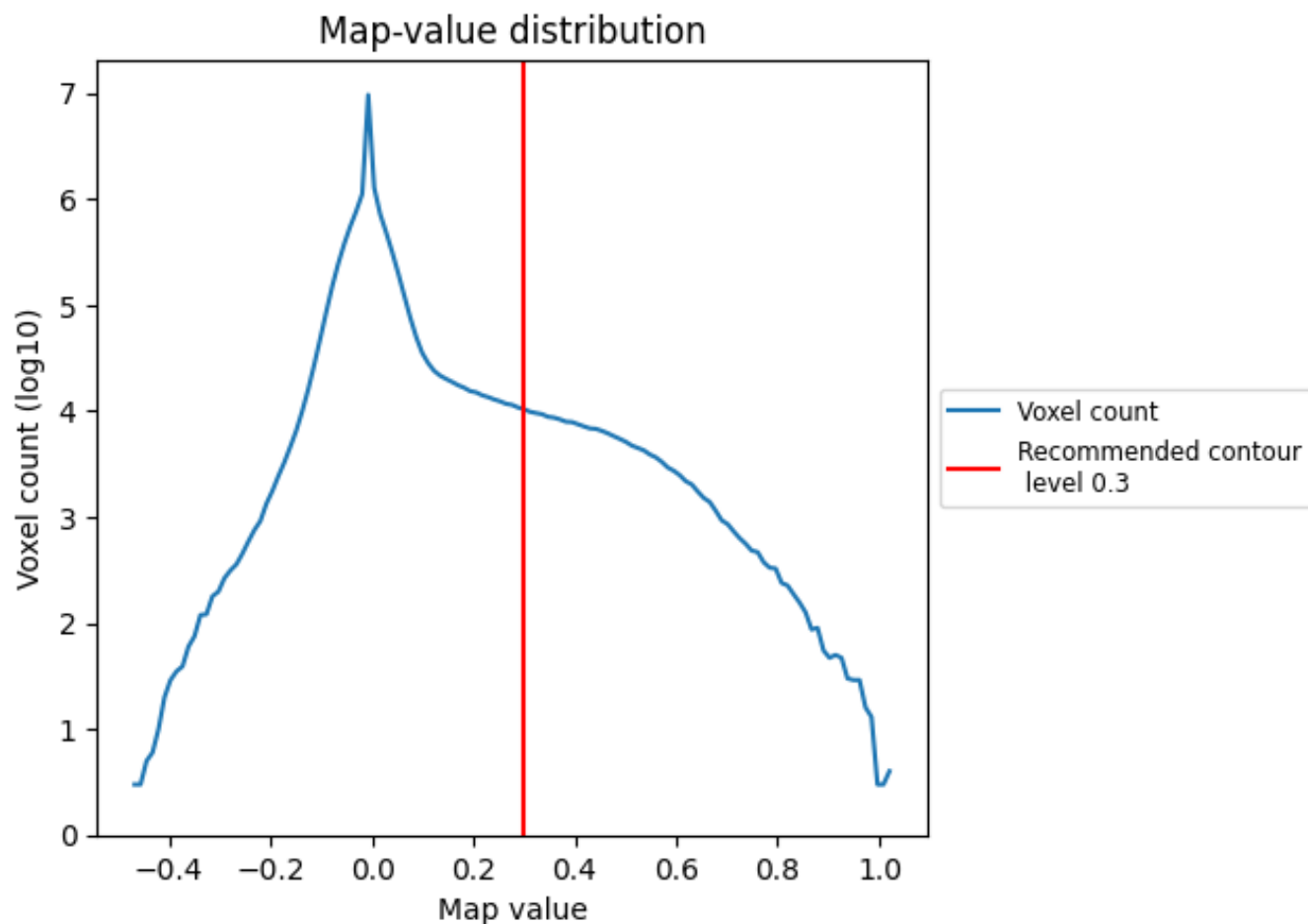
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

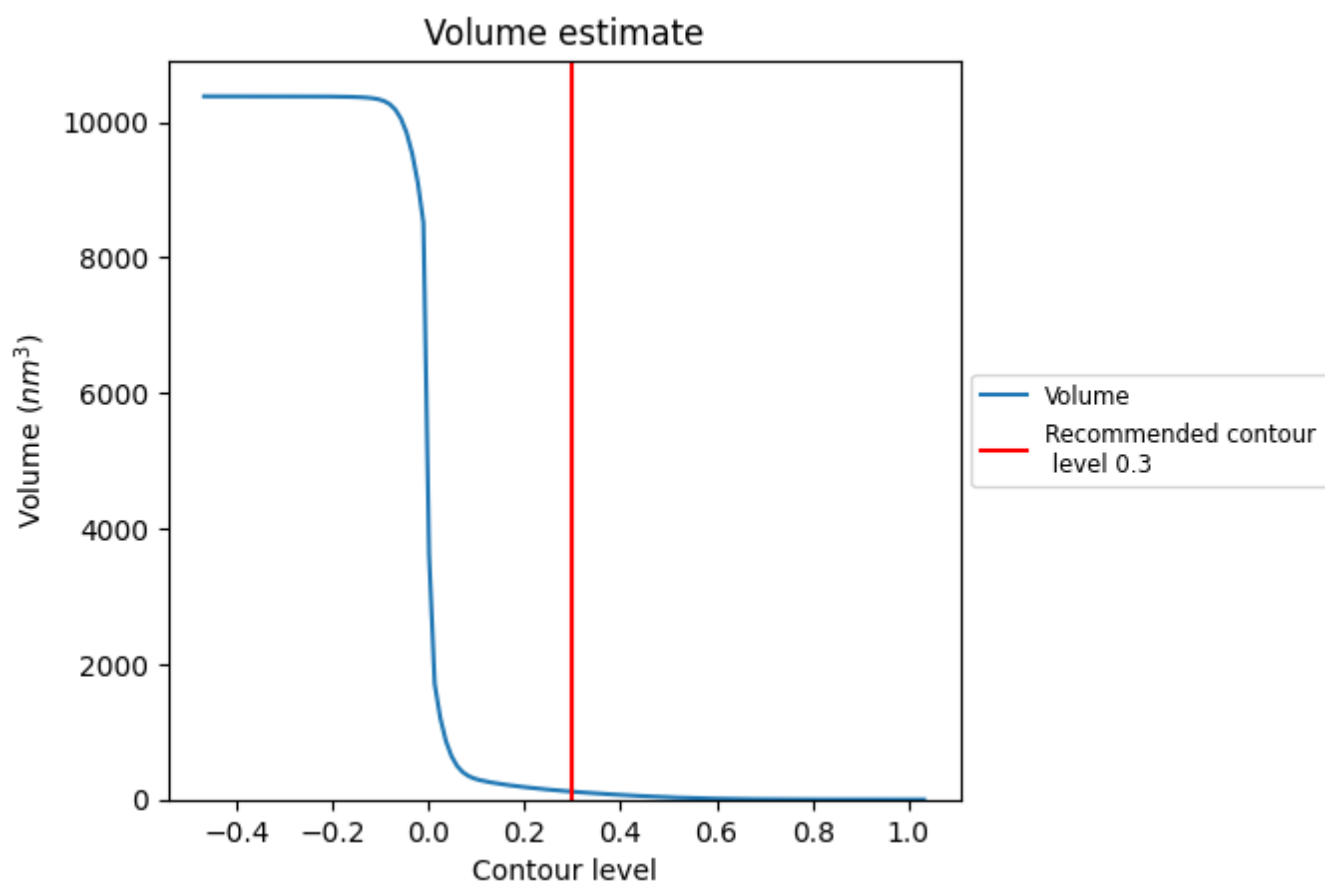
This section contains the results of statistical analysis of the map.

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.

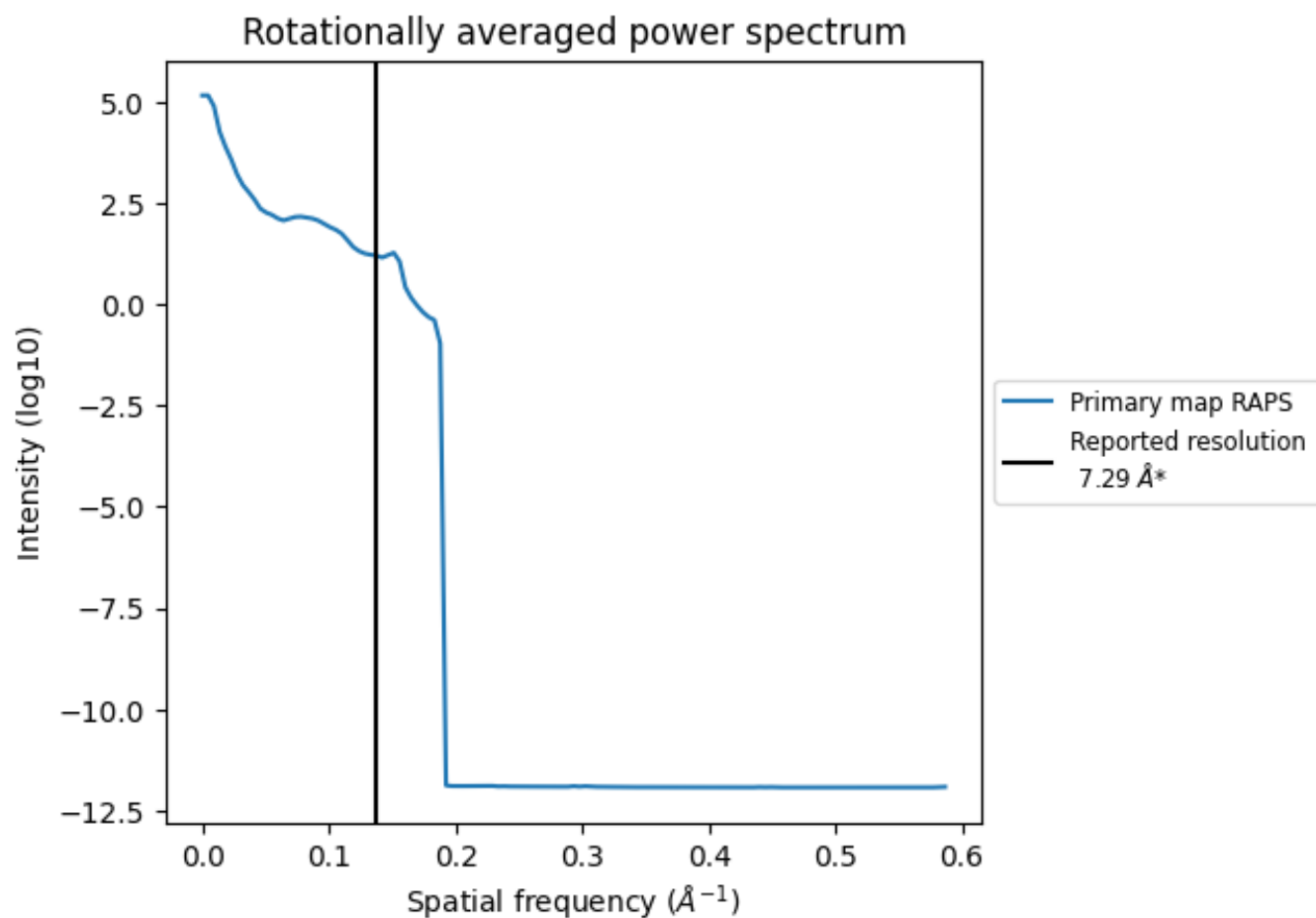
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 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 0.137 Å⁻¹

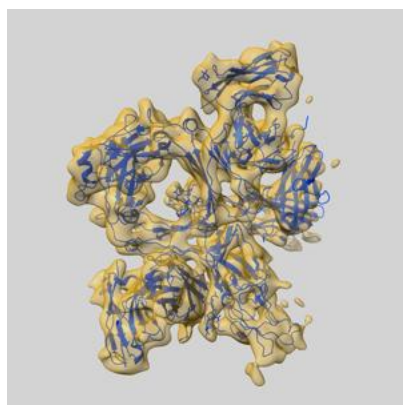
8 Fourier-Shell correlation

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

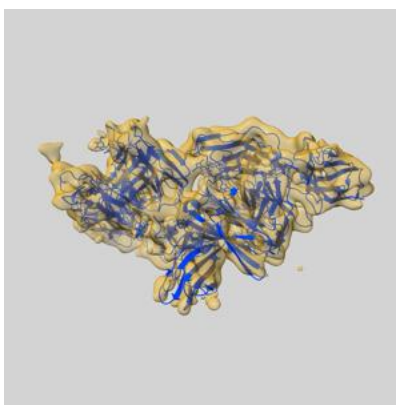
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25136 and PDB model 7SHT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

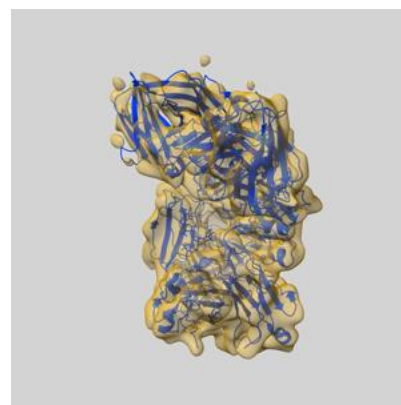
9.1 Map-model overlay [i](#)



X



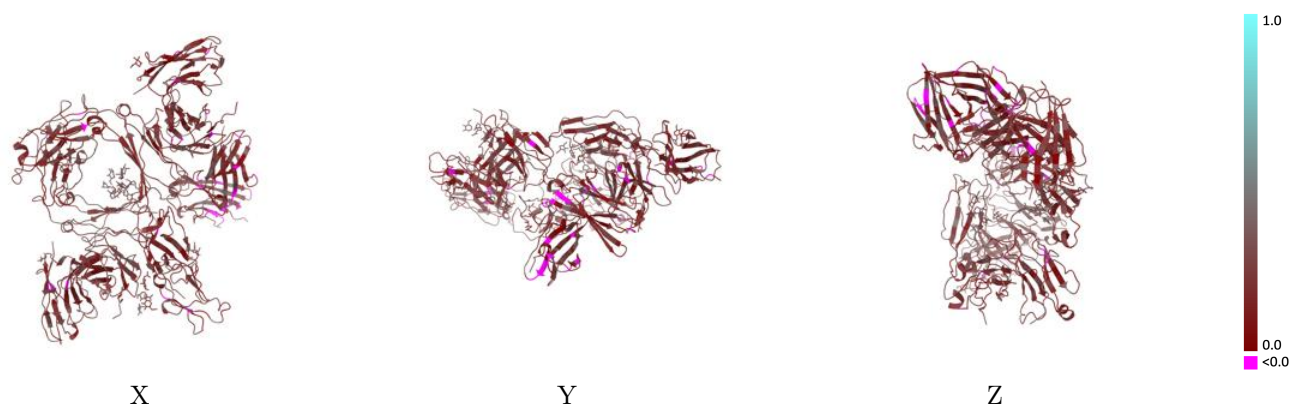
Y



Z

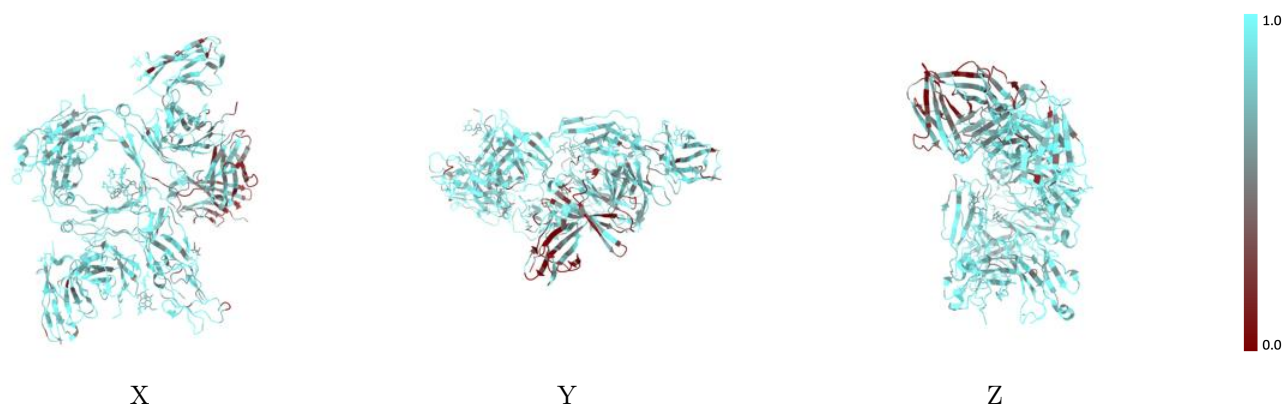
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



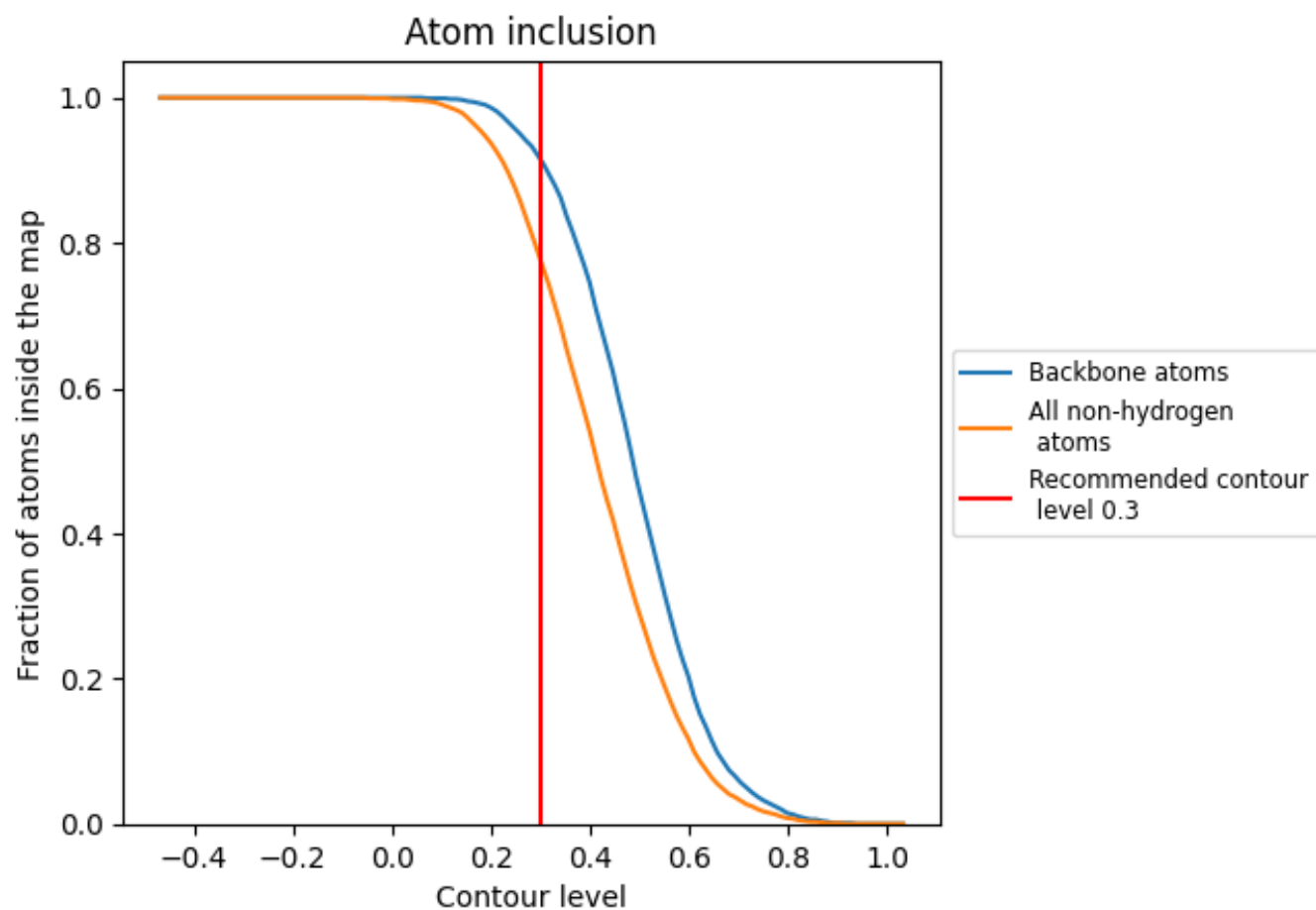
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.2170
A	0.8150	0.2090
B	0.7470	0.2140
C	0.6790	0.3220
D	0.7210	0.2190
E	0.8210	0.3250
F	0.8690	0.3740
G	0.7380	0.3340
H	0.8070	0.1990
J	0.8440	0.2170
K	0.8490	0.2320
L	0.7680	0.2160

