



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:16 PM UTC

PDB ID : 6HN5 / pdb_00006hn5
EMDB ID : EMD-0247
Title : Leucine-zippered human insulin receptor ectodomain with single bound insulin
- "upper" membrane-distal part
Authors : Weis, F.; Menting, J.G.; Margetts, M.B.; Chan, S.J.; Xu, Y.; Tennagels, N.;
Wohlfart, P.; Langer, T.; Mueller, C.W.; Dreyer, M.K.; Lawrence, M.C.
Deposited on : 2018-09-14
Resolution : 3.20 Å (reported)
Based on initial model : 4ZXB

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:

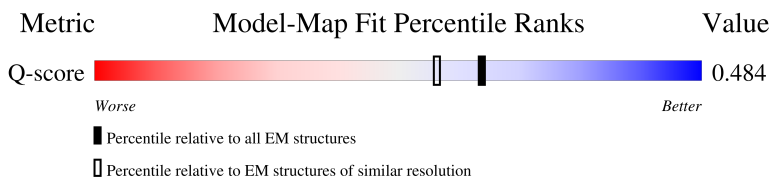
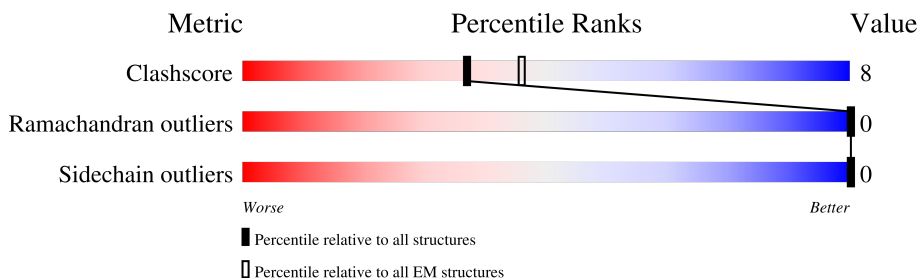
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	21	 90% 10%
2	B	30	 63% 20% 17%
3	E	930	 5% 51% 12% 37%
3	F	930	 28% 7% 65%

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Mol	Chain	Length	Quality of chain
4	C	2	50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7869 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 Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	21	Total	C	N	O	S	0	0
			163	99	25	35	4		

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	25	Total	C	N	O	S	1	0
			212	138	35	37	2		

- Molecule 3 is a protein called Insulin receptor,General control protein GCN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	584	Total	C	N	O	S	1	0
			4715	2984	819	870	42		
3	F	323	Total	C	N	O	S	0	0
			2625	1671	448	495	11		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	variant	UNP P06213
E	421	THR	ILE	variant	UNP P06213
E	465	LYS	GLN	variant	UNP P06213
E	731	ALA	VAL	engineered mutation	UNP P06213
E	732	GLY	THR	engineered mutation	UNP P06213
E	733	ASN	VAL	engineered mutation	UNP P06213
E	734	ASN	ALA	engineered mutation	UNP P06213
F	144	HIS	TYR	variant	UNP P06213
F	421	THR	ILE	variant	UNP P06213
F	465	LYS	GLN	variant	UNP P06213
F	731	ALA	VAL	engineered mutation	UNP P06213
F	732	GLY	THR	engineered mutation	UNP P06213
F	733	ASN	VAL	engineered mutation	UNP P06213

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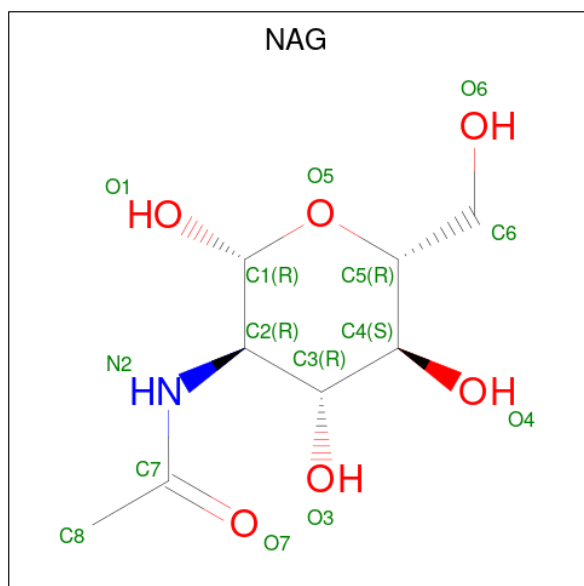
Chain	Residue	Modelled	Actual	Comment	Reference
F	734	ASN	ALA	engineered mutation	UNP P06213

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	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: Insulin

Chain A: 



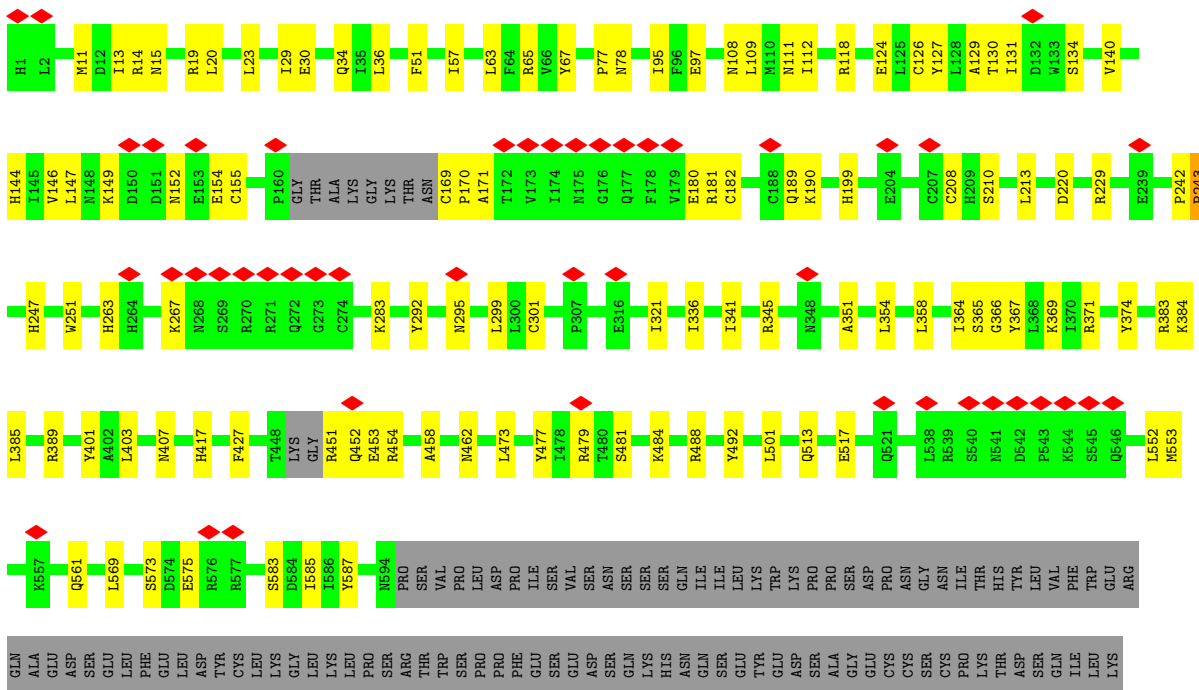
- Molecule 2: Insulin

Chain B: 



- Molecule 3: Insulin receptor, General control protein GCN4

Chain E: 



SER
ASN
ILE
ALA
ARG
MET
LYS
GLN
LEU
GLU
ASP
LYS
VAL
GLU
GLU
LEU
LEU
SER
LYS
ASN
TYR
HIS
LEU
GLU
ASN
GLU
VAL
ALA
ARG
LEU
LYS
LYS
LEU
VAL
GLY
GLU
ARG

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



MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.85	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	299.52, 299.52, 299.52	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/164	0.64	0/220
2	B	0.47	0/218	0.67	0/294
3	E	0.51	0/4832	0.70	0/6548
3	F	0.48	0/2684	0.60	0/3629
All	All	0.50	0/7898	0.66	0/10691

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	243	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	163	0	149	2	0
2	B	212	0	192	6	0
3	E	4715	0	4567	73	0
3	F	2625	0	2561	43	0
4	C	28	0	25	0	0
5	E	84	0	78	1	0
5	F	42	0	39	0	0
All	All	7869	0	7611	117	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 8.

All (117) 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)
3:E:263:HIS:O	3:E:267:LYS:HB2	1.89	0.73
3:E:146:VAL:HG12	3:E:147:LEU:HG	1.75	0.69
3:F:363:GLU:HG2	3:F:387:LEU:HB3	1.78	0.66
3:E:561:GLN:HE21	3:E:587:TYR:HB3	1.60	0.65
3:E:65:ARG:NH2	3:E:97:GLU:OE2	2.29	0.65
3:E:111:ASN:HD22	3:E:213:LEU:HD11	1.61	0.65
3:F:487:LEU:O	3:F:550:GLY:HA3	1.97	0.64
3:F:504:MET:SD	3:F:567:LYS:NZ	2.66	0.64
3:E:401:TYR:HA	3:E:427:PHE:HB3	1.80	0.63
2:B:10:HIS:O	2:B:14:ALA:HB3	1.99	0.62
3:E:208:CYS:HA	3:E:220:ASP:H	1.65	0.62
3:E:134:SER:HA	3:E:140:VAL:HG21	1.83	0.60
3:E:247:HIS:HB2	3:E:283:LYS:HG2	1.84	0.60
3:E:341:ILE:HG12	3:E:369:LYS:HB3	1.85	0.59
3:E:131:ILE:O	3:E:189:GLN:NE2	2.35	0.58
3:E:129:ALA:O	3:E:181:ARG:NH1	2.38	0.57
3:E:479:ARG:NH1	3:E:481:SER:OG	2.37	0.57
3:E:513:GLN:HE21	3:E:561:GLN:HE22	1.52	0.57
3:F:369:LYS:HE2	3:F:371:ARG:HB2	1.86	0.57
3:E:34:GLN:HB3	3:E:36:LEU:HD22	1.87	0.57
3:E:473:LEU:HD21	3:E:492:TYR:HB2	1.86	0.56
3:E:213:LEU:HB2	3:E:229:ARG:HB3	1.86	0.56
3:E:78:ASN:HA	3:E:108:ASN:HD22	1.71	0.55
3:E:29:ILE:HD12	3:E:57:ILE:HG12	1.88	0.55
3:E:77:PRO:O	3:E:108:ASN:ND2	2.38	0.55
3:E:364:ILE:HG22	3:E:366:GLY:H	1.72	0.54
3:E:484:LYS:HA	3:E:553:MET:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:292:TYR:HB3	3:E:301:CYS:HB3	1.89	0.54
3:E:13:ILE:HG23	3:E:19:ARG:HB2	1.91	0.53
3:E:30:GLU:HG2	3:E:251:TRP:HE1	1.72	0.53
3:E:152:ASN:ND2	3:E:154:GLU:OE1	2.42	0.53
3:F:562:TYR:O	3:F:587:TYR:HA	2.08	0.53
3:E:374:TYR:O	3:E:407:ASN:ND2	2.40	0.53
3:F:344:ILE:HG21	3:F:350:LEU:HD21	1.90	0.53
3:F:400:PHE:HB3	3:F:426:LEU:HD13	1.91	0.53
3:F:355:GLU:OE2	3:F:383:ARG:NH2	2.42	0.52
3:E:78:ASN:OD1	3:E:108:ASN:ND2	2.43	0.52
3:E:484:LYS:HD3	3:E:552:LEU:HD21	1.92	0.51
3:F:487:LEU:HD11	3:F:564:ILE:HD13	1.92	0.51
3:F:442:MET:O	3:F:446:SER:CB	2.58	0.51
3:F:379:LEU:O	3:F:412:TRP:NE1	2.42	0.51
3:F:425:LYS:HG2	3:F:453:GLU:HB3	1.93	0.51
3:F:412:TRP:HZ3	3:F:419:LEU:HD22	1.76	0.51
3:E:573:SER:HB3	3:E:575:GLU:HG2	1.91	0.50
3:F:501:LEU:HD21	3:F:699:SER:HB2	1.92	0.50
3:F:442:MET:O	3:F:446:SER:OG	2.28	0.50
3:E:126:CYS:SG	3:E:127:TYR:N	2.67	0.50
3:E:351:ALA:HA	3:E:354:LEU:HB2	1.93	0.49
3:F:331:ARG:HG2	3:F:357:ASN:HA	1.93	0.49
3:F:327:ALA:O	3:F:330:LEU:HB2	2.12	0.49
3:E:369:LYS:HD3	3:E:371:ARG:HD2	1.95	0.49
3:E:501:LEU:N	3:E:569:LEU:O	2.41	0.49
3:F:484:LYS:HB3	3:F:552:LEU:HD11	1.96	0.48
2:B:24:PHE:HD2	3:E:15:ASN:HD21	1.62	0.48
3:E:365:SER:HA	3:E:389:ARG:HB2	1.96	0.48
3:F:314:LEU:HD12	3:F:338:GLY:HA3	1.96	0.47
3:E:403:LEU:HB2	3:E:427:PHE:HE2	1.78	0.47
1:A:16:LEU:HD11	2:B:6:LEU:HD22	1.97	0.47
3:E:484:LYS:HB3	3:E:552:LEU:HD11	1.96	0.47
3:F:327:ALA:HA	3:F:330:LEU:HD13	1.97	0.47
3:E:118:ARG:HH22	3:F:702:ARG:HA	1.80	0.47
3:E:369:LYS:HG3	3:E:401:TYR:CD2	2.51	0.46
3:E:126:CYS:HB2	3:E:155:CYS:HB2	1.58	0.46
3:F:436:LEU:HA	3:F:439:ILE:HD12	1.96	0.46
3:E:118:ARG:HG3	3:E:144[B]:HIS:HB3	1.96	0.46
3:E:109:LEU:HD21	3:E:112:ILE:HD11	1.97	0.46
3:F:481:SER:O	3:F:591:ASP:N	2.45	0.46
3:E:65:ARG:NH1	3:E:67:TYR:OH	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:336:ILE:HB	3:E:364:ILE:HG12	1.97	0.45
3:F:436:LEU:HD23	3:F:439:ILE:HD12	1.98	0.45
2:B:10:HIS:O	2:B:14:ALA:CB	2.64	0.45
2:B:26[A]:TYR:OH	3:E:19:ARG:NH1	2.50	0.45
3:F:535:ASP:OD1	3:F:535:ASP:N	2.48	0.45
3:F:467:SER:HA	3:F:578:THR:HG21	1.98	0.44
3:F:521:GLN:HG3	3:F:522:ASP:H	1.81	0.44
3:E:130:THR:O	3:E:182:CYS:N	2.50	0.44
3:F:442:MET:O	3:F:446:SER:HB3	2.17	0.44
3:E:118:ARG:HG3	3:E:144[A]:HIS:HB3	2.00	0.44
3:E:451:ARG:HB3	3:E:453:GLU:HG2	2.00	0.44
3:F:363:GLU:OE1	3:F:389:ARG:NH2	2.51	0.44
3:E:295:ASN:O	3:E:299:LEU:N	2.40	0.44
3:F:377:VAL:HB	3:F:522:ASP:HA	2.00	0.44
3:F:485:ILE:HB	3:F:553:MET:HE3	1.99	0.44
3:E:171:ALA:HA	3:E:180:GLU:HA	2.00	0.43
3:F:493:TRP:CE3	3:F:497:PHE:HB2	2.53	0.43
3:E:11:MET:HG3	3:E:23:LEU:HD21	2.00	0.43
3:E:199:HIS:ND1	3:E:210:SER:O	2.46	0.43
3:E:452:GLN:HE22	3:E:454:ARG:HD3	1.83	0.43
3:E:383:ARG:HG3	3:E:384:LYS:HE3	2.00	0.43
3:E:190:LYS:HD3	5:E:1004:NAG:H81	2.01	0.43
3:F:378:SER:OG	3:F:522:ASP:OD1	2.34	0.43
3:F:553:MET:HB3	3:F:556:LEU:HD11	1.99	0.42
3:E:20:LEU:HB3	3:E:51:PHE:HZ	1.83	0.42
3:E:477:TYR:HB3	3:E:488:ARG:HB2	2.01	0.42
3:E:345:ARG:HD3	3:F:704:THR:HG21	2.01	0.42
3:F:344:ILE:O	3:F:374:TYR:N	2.51	0.42
3:E:14:ARG:HH22	3:F:713:VAL:HG13	1.85	0.42
3:E:517:GLU:HA	3:E:585:ILE:HD11	2.01	0.42
3:F:465:LYS:HA	3:F:572:PHE:CZ	2.55	0.42
3:E:242:PRO:HA	3:E:243:PRO:HD3	1.71	0.42
3:E:13:ILE:HG21	3:E:20:LEU:HG	2.01	0.41
3:F:477:TYR:HE2	3:F:486:LEU:HD23	1.85	0.41
3:E:367:TYR:HE2	3:E:369:LYS:HE3	1.84	0.41
3:E:473:LEU:HB2	3:E:583:SER:HB3	2.02	0.41
3:F:707:ASP:O	3:F:711:ASN:ND2	2.53	0.41
3:E:111:ASN:ND2	3:E:213:LEU:HD11	2.34	0.41
3:E:385:LEU:O	3:E:417:HIS:NE2	2.47	0.41
3:E:63:LEU:HD12	3:E:95:ILE:HD12	2.03	0.41
3:E:169:CYS:HA	3:E:170:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:458:ALA:O	3:E:462:ASN:ND2	2.51	0.41
3:F:369:LYS:HE2	3:F:371:ARG:HD3	2.03	0.41
3:F:513:GLN:HE21	3:F:561:GLN:HE22	1.69	0.41
3:E:321:ILE:HD13	3:E:358:LEU:HD11	2.03	0.41
1:A:20:CYS:HB3	2:B:19:CYS:HB3	1.77	0.40
3:E:124:GLU:HA	3:E:149:LYS:HB2	2.02	0.40
3:F:582:LYS:HE2	3:F:582:LYS:HB3	1.89	0.40
3:E:14:ARG:HH11	3:E:14:ARG:HD3	1.73	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	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
2	B	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
3	E	579/930 (62%)	513 (89%)	66 (11%)	0	100	100
3	F	317/930 (34%)	285 (90%)	32 (10%)	0	100	100
All	All	939/1911 (49%)	837 (89%)	102 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	20/20 (100%)	20 (100%)	0	100	100
2	B	22/26 (85%)	22 (100%)	0	100	100
3	E	533/843 (63%)	533 (100%)	0	100	100
3	F	289/843 (34%)	289 (100%)	0	100	100
All	All	864/1732 (50%)	864 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
3	E	15	ASN
3	E	78	ASN
3	E	108	ASN
3	E	209	HIS
3	E	230	ASN
3	E	295	ASN
3	E	313	HIS
3	E	546	GLN
3	E	561	GLN
3	E	589	GLN
3	F	405	ASN
3	F	407	ASN
3	F	547	ASN
3	F	561	GLN
3	F	711	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1	4,3	14,14,15	0.66	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	C	2	4	14,14,15	0.59	0	17,19,21	0.60	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-2.34	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	O4-C4-C5	-2.47	103.23	109.32

There are no chirality outliers.

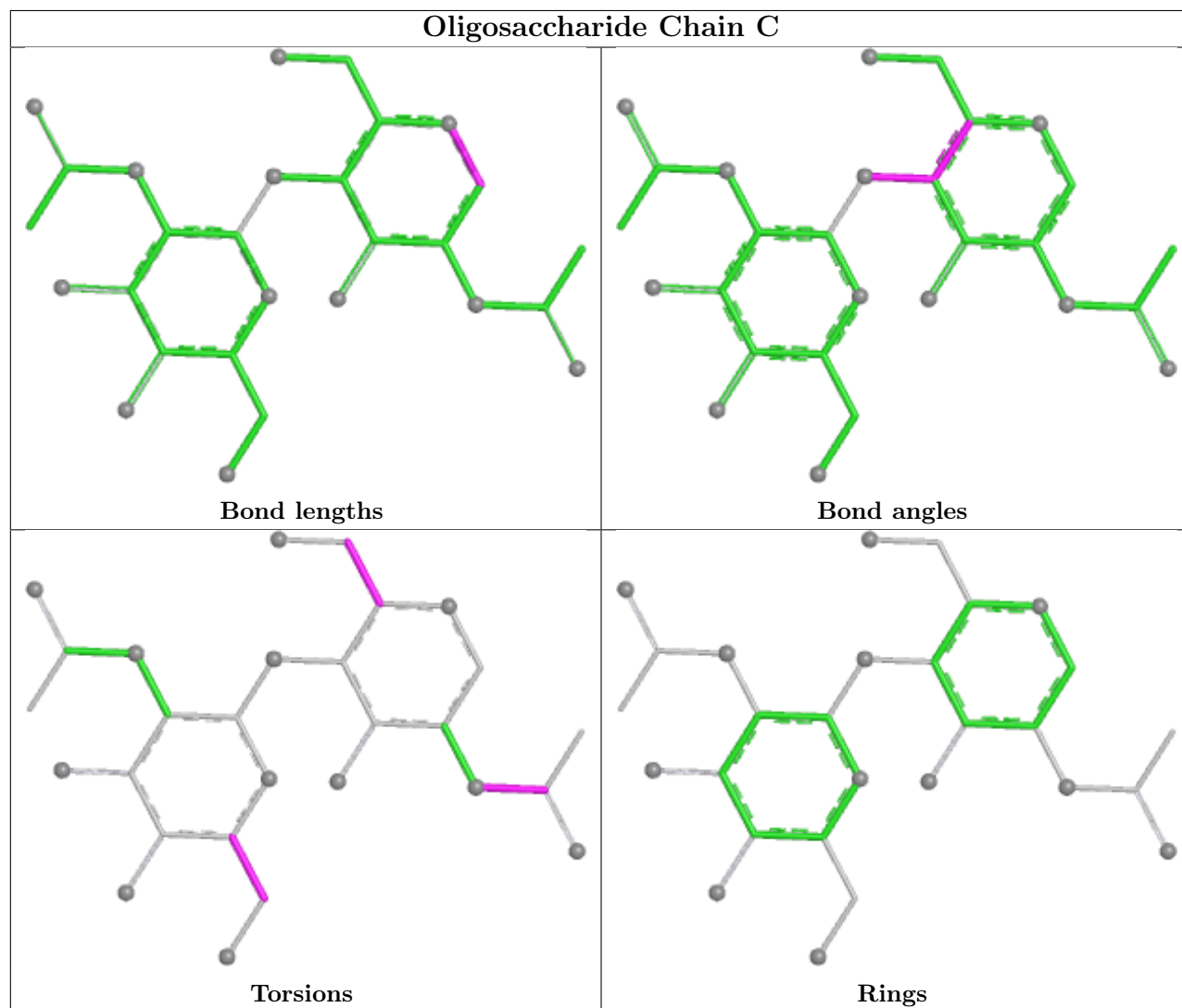
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	C	1	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1006	3	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	E	1004	3	14,14,15	0.20	0	17,19,21	1.31	3 (17%)
5	NAG	F	1003	3	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
5	NAG	E	1007	3	14,14,15	0.79	1 (7%)	17,19,21	2.40	4 (23%)
5	NAG	E	1008	3	14,14,15	0.35	0	17,19,21	1.36	3 (17%)
5	NAG	F	1002	3	14,14,15	0.71	1 (7%)	17,19,21	2.40	3 (17%)
5	NAG	E	1001	3	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
5	NAG	E	1005	3	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
5	NAG	F	1001	3	14,14,15	0.22	0	17,19,21	0.51	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	E	1006	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1004	3	-	4/6/23/26	0/1/1/1
5	NAG	F	1003	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1007	3	-	6/6/23/26	0/1/1/1
5	NAG	E	1008	3	-	4/6/23/26	0/1/1/1
5	NAG	F	1002	3	-	6/6/23/26	0/1/1/1
5	NAG	E	1001	3	-	4/6/23/26	0/1/1/1
5	NAG	E	1005	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1001	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1007	NAG	C1-C2	2.34	1.55	1.52
5	F	1002	NAG	C1-C2	2.05	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1002	NAG	C2-N2-C7	8.39	134.14	122.90
5	E	1007	NAG	C2-N2-C7	8.32	134.04	122.90
5	E	1007	NAG	C1-C2-N2	3.99	116.72	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1002	NAG	C1-C2-N2	3.97	116.69	110.43
5	E	1008	NAG	C1-O5-C5	3.38	116.72	112.19
5	E	1008	NAG	C2-N2-C7	3.35	127.39	122.90
5	E	1004	NAG	C2-N2-C7	3.31	127.33	122.90
5	E	1001	NAG	C2-N2-C7	3.22	127.22	122.90
5	E	1004	NAG	C1-O5-C5	3.03	116.25	112.19
5	F	1003	NAG	C1-O5-C5	2.48	115.52	112.19
5	E	1008	NAG	C1-C2-N2	2.19	113.88	110.43
5	E	1004	NAG	C1-C2-N2	2.17	113.85	110.43
5	E	1007	NAG	C1-O5-C5	2.15	115.07	112.19
5	F	1002	NAG	C8-C7-N2	2.15	119.69	116.12
5	E	1005	NAG	C1-O5-C5	2.15	115.07	112.19
5	E	1007	NAG	C8-C7-N2	2.14	119.67	116.12

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1008	NAG	O5-C5-C6-O6
5	F	1003	NAG	O5-C5-C6-O6
5	E	1006	NAG	O5-C5-C6-O6
5	E	1007	NAG	O5-C5-C6-O6
5	E	1004	NAG	O5-C5-C6-O6
5	E	1008	NAG	C4-C5-C6-O6
5	F	1003	NAG	C4-C5-C6-O6
5	F	1002	NAG	O5-C5-C6-O6
5	F	1001	NAG	O5-C5-C6-O6
5	E	1001	NAG	C4-C5-C6-O6
5	E	1004	NAG	C4-C5-C6-O6
5	E	1006	NAG	C4-C5-C6-O6
5	E	1007	NAG	C4-C5-C6-O6
5	F	1002	NAG	C4-C5-C6-O6
5	F	1001	NAG	C4-C5-C6-O6
5	E	1005	NAG	C8-C7-N2-C2
5	E	1005	NAG	O7-C7-N2-C2
5	E	1007	NAG	C8-C7-N2-C2
5	E	1007	NAG	O7-C7-N2-C2
5	F	1002	NAG	C8-C7-N2-C2
5	F	1002	NAG	O7-C7-N2-C2
5	E	1001	NAG	O5-C5-C6-O6
5	E	1001	NAG	C1-C2-N2-C7
5	E	1004	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	E	1007	NAG	C1-C2-N2-C7
5	E	1008	NAG	C1-C2-N2-C7
5	F	1002	NAG	C1-C2-N2-C7
5	E	1001	NAG	C3-C2-N2-C7
5	E	1004	NAG	C3-C2-N2-C7
5	E	1007	NAG	C3-C2-N2-C7
5	E	1008	NAG	C3-C2-N2-C7
5	F	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1004	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.

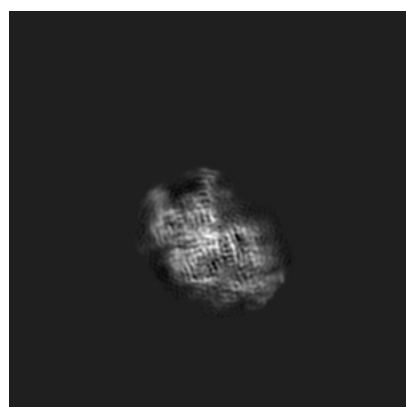
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0247. These allow visual inspection of the internal detail of the map and identification of artifacts.

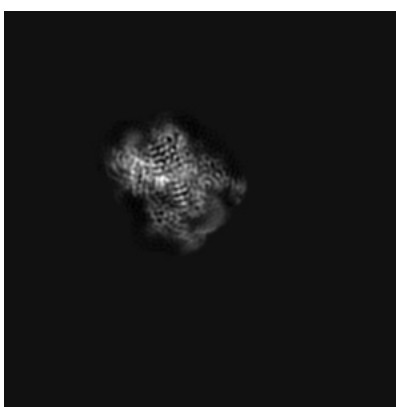
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

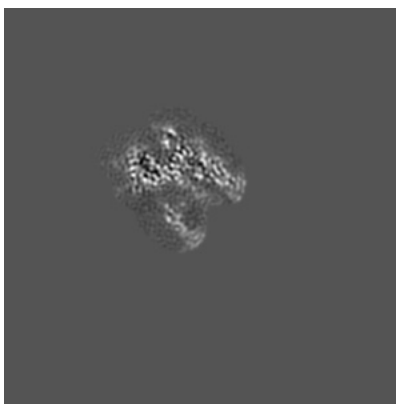
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

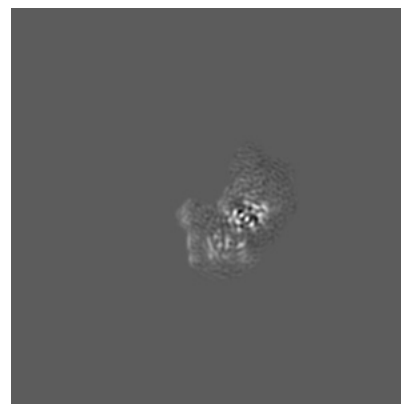
6.2.1 Primary map



X Index: 144



Y Index: 144

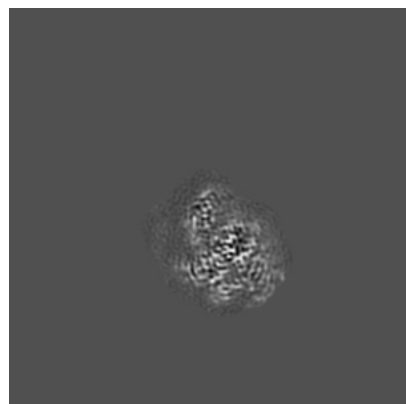


Z Index: 144

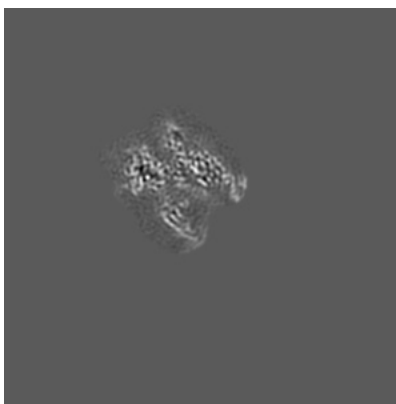
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

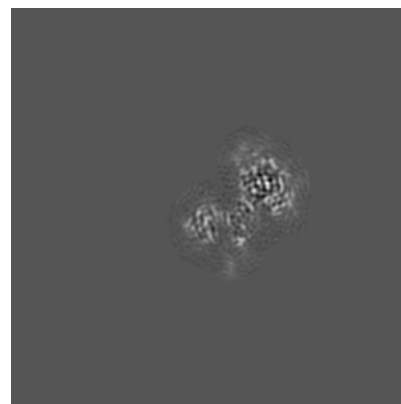
6.3.1 Primary map



X Index: 176



Y Index: 141

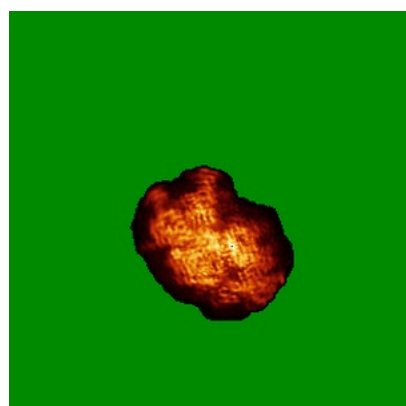


Z Index: 116

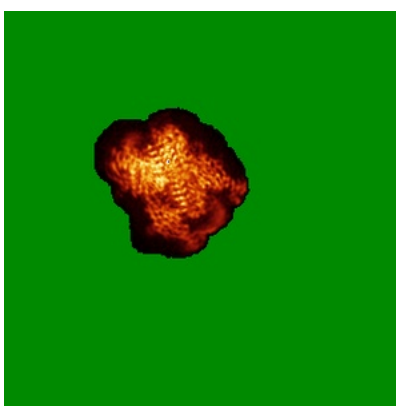
The images above show the largest variance slices of the map in three orthogonal directions.

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

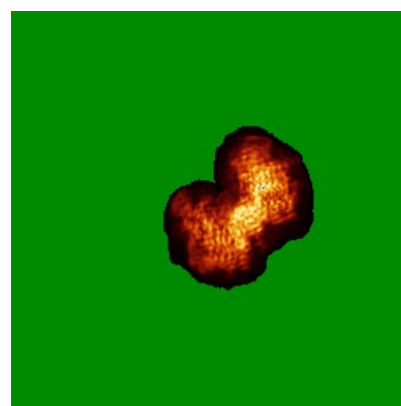
6.4.1 Primary map



X



Y

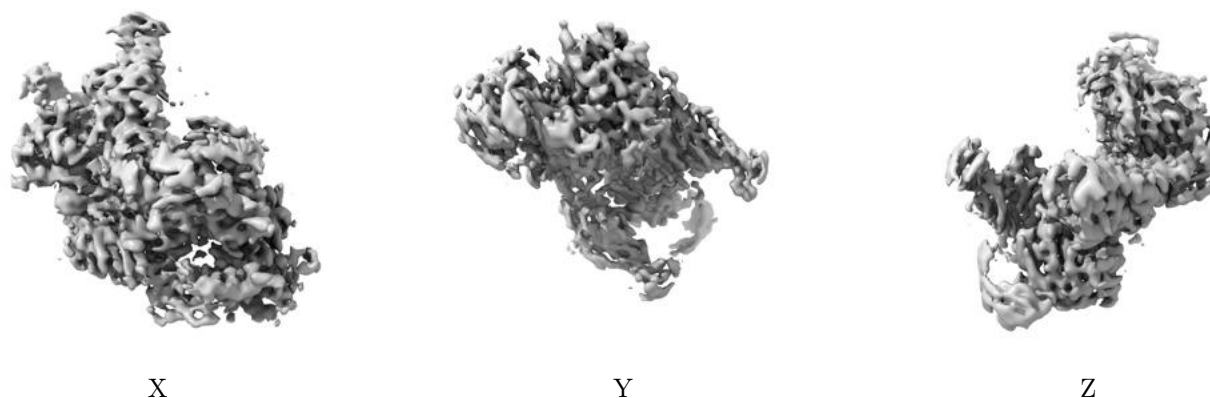


Z

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

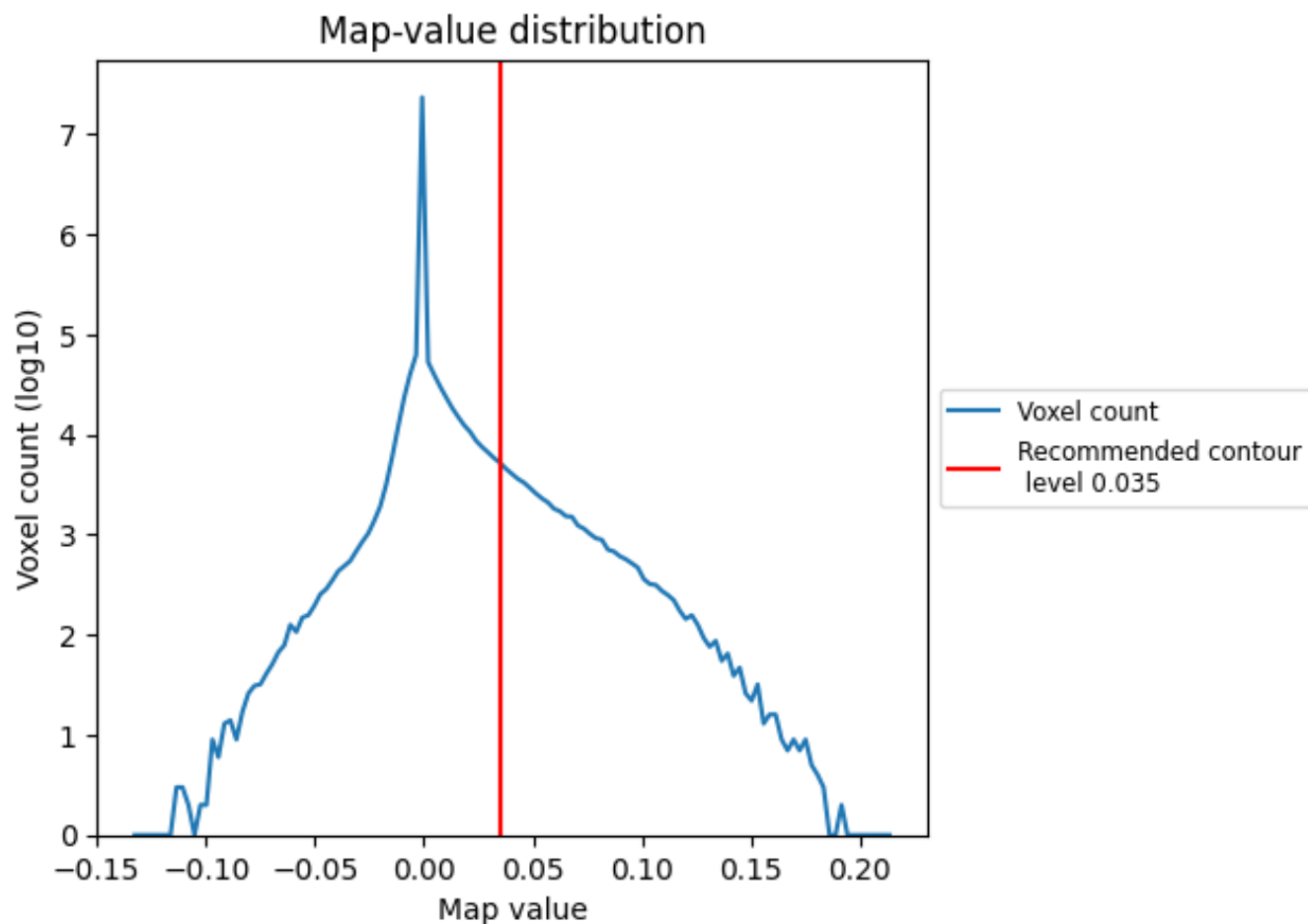
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

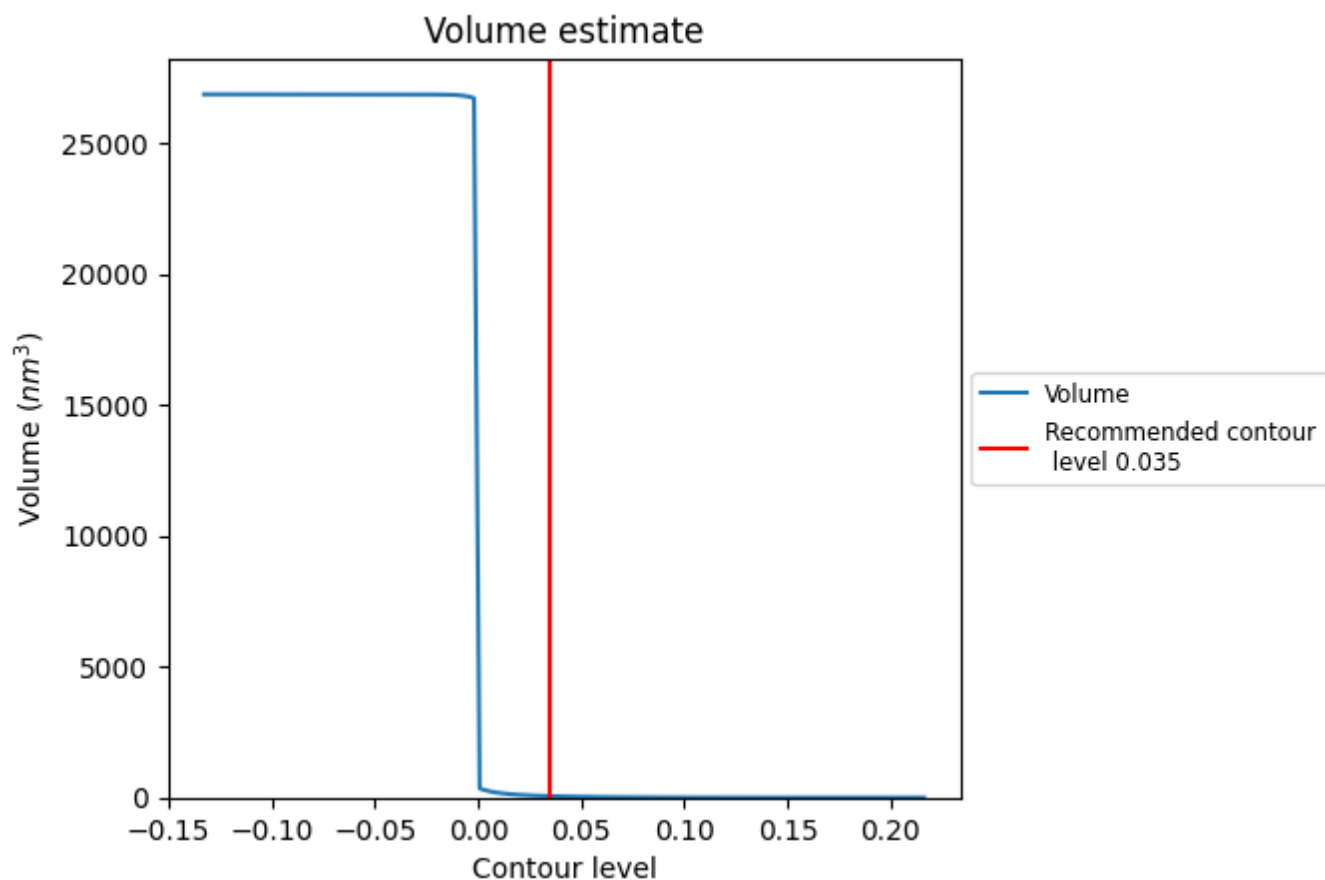
This section contains the results of statistical analysis of the map.

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.

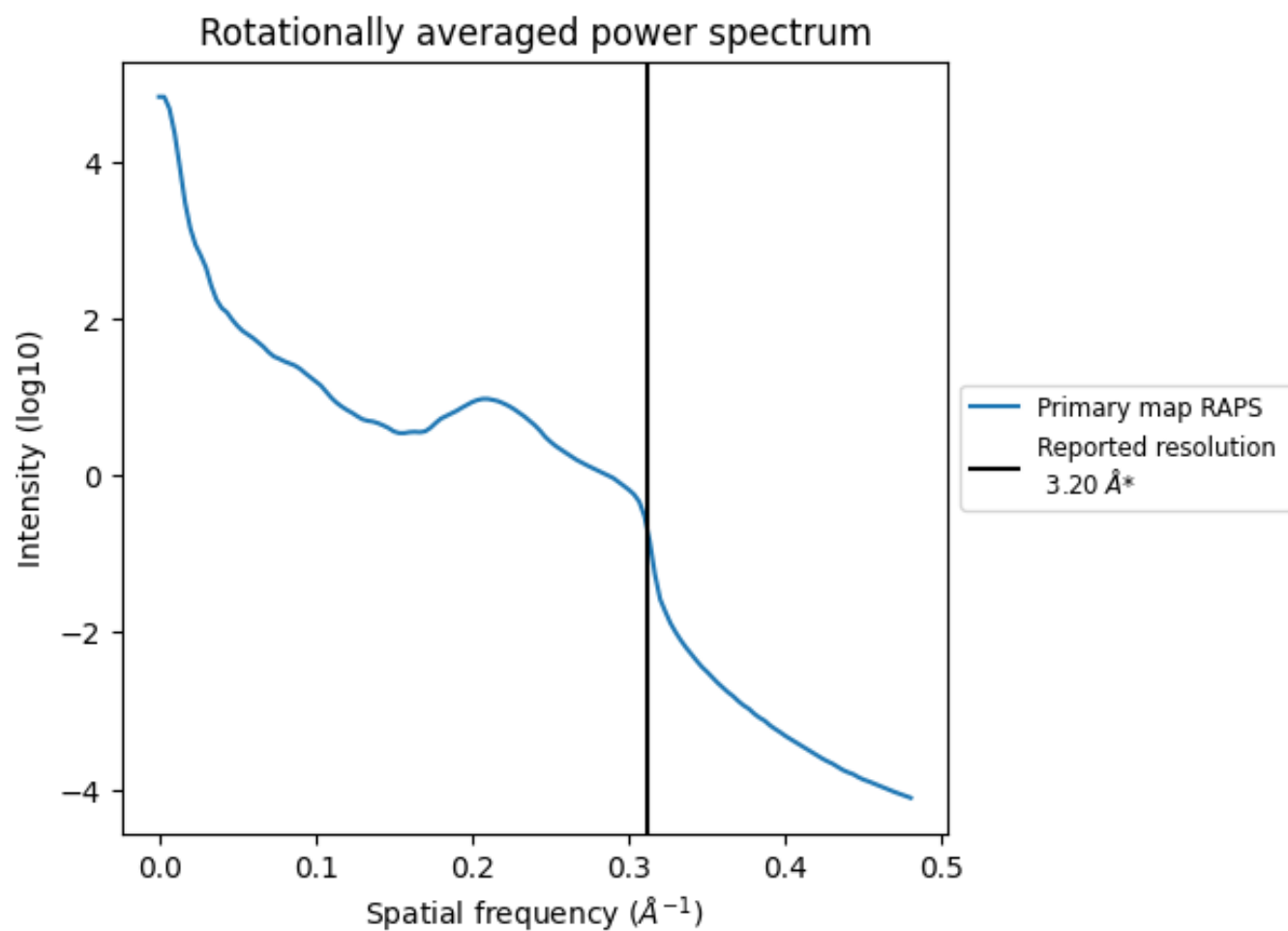
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm^3 ; this corresponds to an approximate mass of 50 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 0.312 Å⁻¹

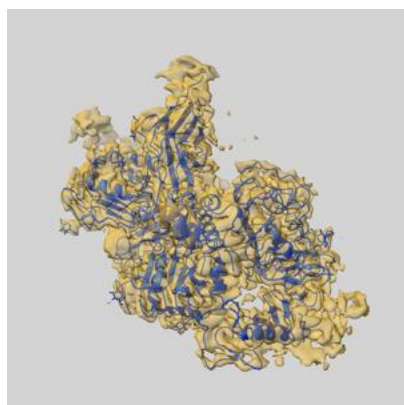
8 Fourier-Shell correlation ⓘ

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

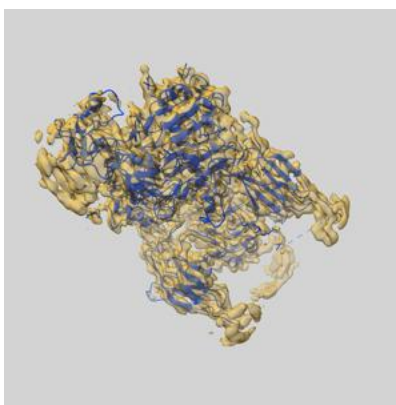
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0247 and PDB model 6HN5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

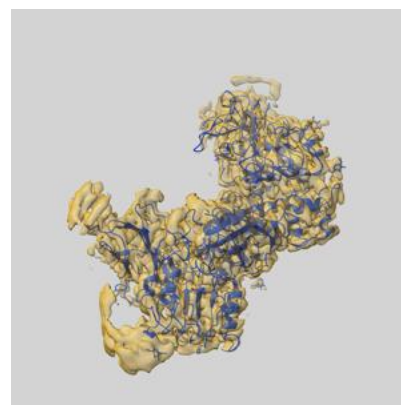
9.1 Map-model overlay [i](#)



X



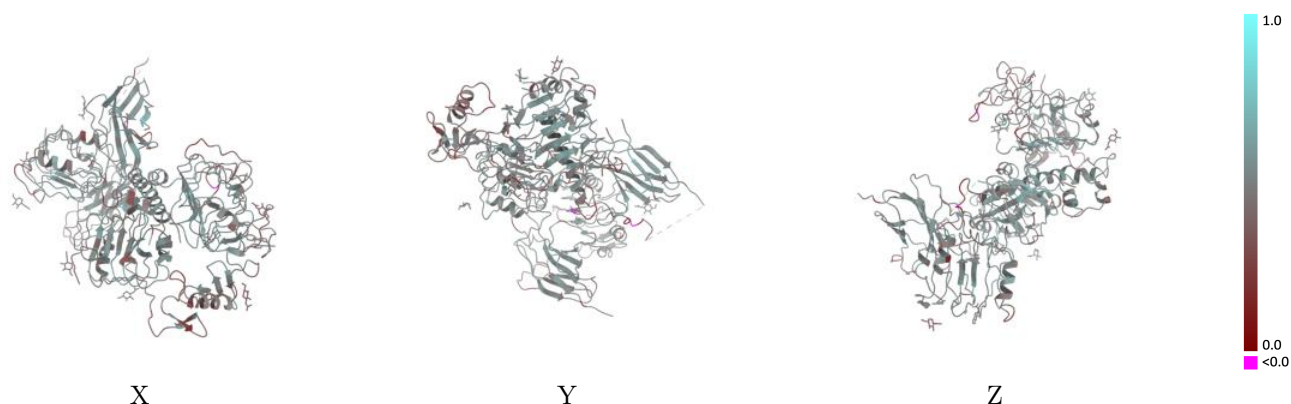
Y



Z

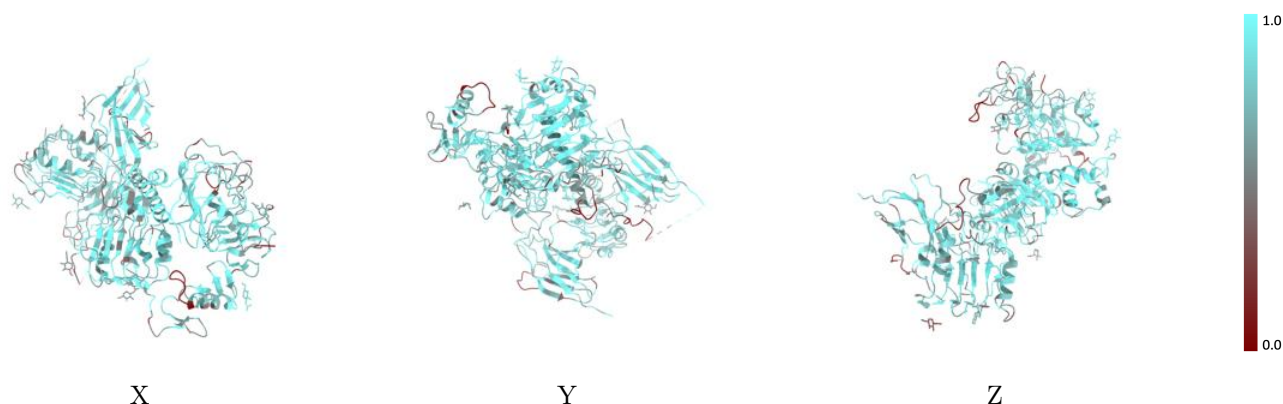
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



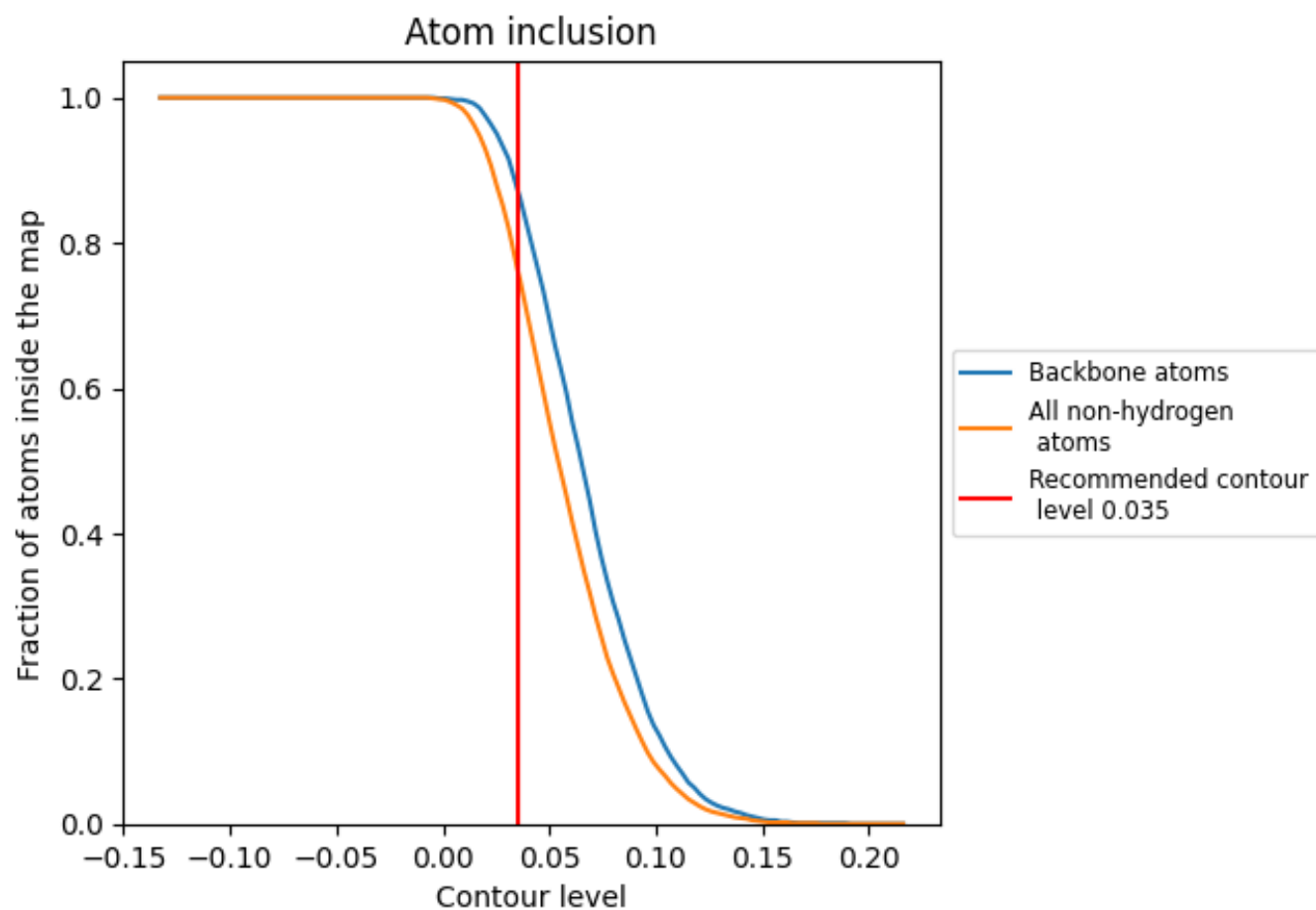
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.4840
A	0.7830	0.4660
B	0.8670	0.5020
C	0.7140	0.4860
E	0.7530	0.4780
F	0.7770	0.4960

