Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 04:16 PM JST

PDB ID	:	7C7Q
EMDB ID	:	EMD-30300
Title	:	Cryo-EM structure of the baclofen/BHFF-bound human GABA(B) receptor in active state
Authors	:	Mao, C.; Shen, C.; Li, C.; Shen, D.; Xu, C.; Zhang, S.; Zhou, R.; Shen, Q.; Chen, L.; Jiang, Z.; Liu, J.; Zhang, Y.
Deposited on	:	2020-05-26
Resolution	:	3.00 Å(reported)
Based on initial model	:	7C7S

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 (i) 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 (1)) were used in the production of this report:

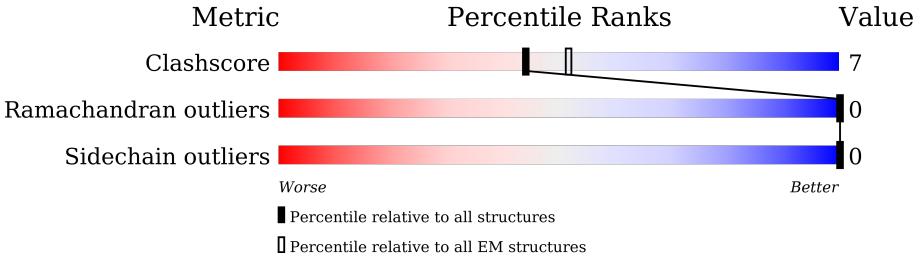
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	879	5% 65% 13% 23%
2	B	769	6% 73% 15% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10894 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	678	5406	3503	897	981	25	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q9UBS5
A	0	LYS	-	expression tag	UNP Q9UBS5
A	1	THR	-	expression tag	UNP Q9UBS5
A	2	ILE	-	expression tag	UNP Q9UBS5
A	3	ILE	-	expression tag	UNP Q9UBS5
A	4	ALA	-	expression tag	UNP Q9UBS5
A	5	LEU	-	expression tag	UNP Q9UBS5
A	6	SER	-	expression tag	UNP Q9UBS5
A	7	TYR	-	expression tag	UNP Q9UBS5
A	8	ILE	-	expression tag	UNP Q9UBS5
A	9	PHE	-	expression tag	UNP Q9UBS5
A	10	CYS	-	expression tag	UNP Q9UBS5
A	11	LEU	-	expression tag	UNP Q9UBS5
A	12	VAL	-	expression tag	UNP Q9UBS5
A	13	PHE	-	expression tag	UNP Q9UBS5
A	14	ALA	-	expression tag	UNP Q9UBS5
A	863	GLU	-	expression tag	UNP Q9UBS5
A	864	VAL	-	expression tag	UNP Q9UBS5
A	865	LEU	-	expression tag	UNP Q9UBS5
A	866	PHE	-	expression tag	UNP Q9UBS5
A	867	GLN	-	expression tag	UNP Q9UBS5
A	868	GLY	-	expression tag	UNP Q9UBS5
A	869	PRO	-	expression tag	UNP Q9UBS5
A	870	HIS	-	expression tag	UNP Q9UBS5
A	871	HIS	-	expression tag	UNP Q9UBS5
A	872	HIS	-	expression tag	UNP Q9UBS5
A	873	HIS	-	expression tag	UNP Q9UBS5
A	874	HIS	-	expression tag	UNP Q9UBS5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	875	HIS	-	expression tag	UNP Q9UBS5
A	876	HIS	-	expression tag	UNP Q9UBS5
A	877	HIS	-	expression tag	UNP Q9UBS5

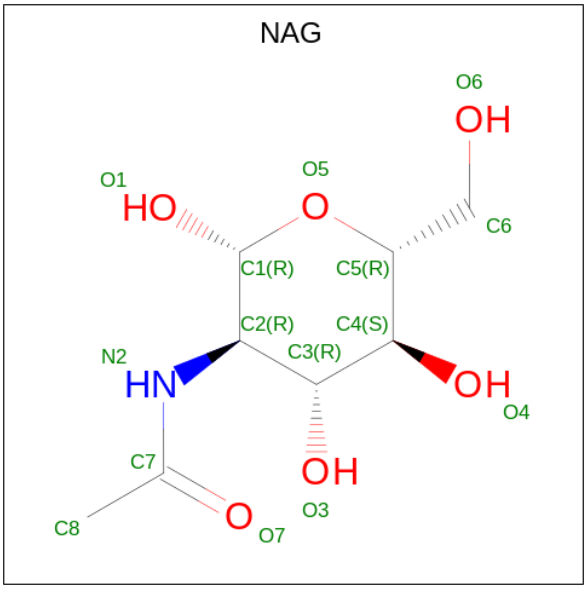
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	670	5339	3463	883	957	36	1	0

There are 29 discrepancies between the modelled and reference sequences:

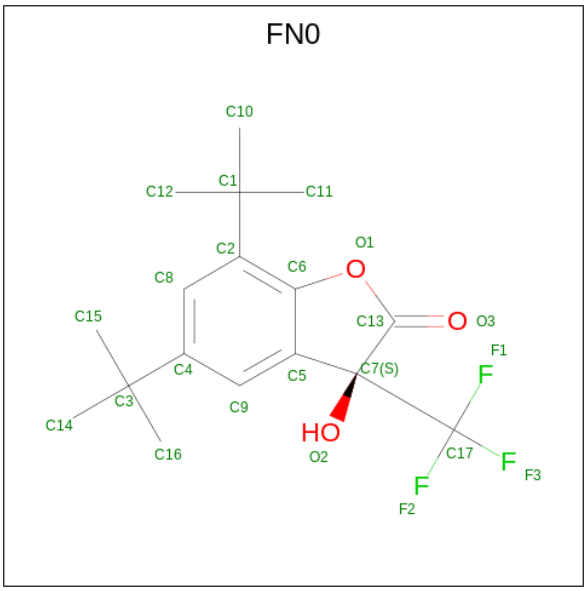
Chain	Residue	Modelled	Actual	Comment	Reference
B	12	MET	-	expression tag	UNP O75899
B	13	LYS	-	expression tag	UNP O75899
B	14	THR	-	expression tag	UNP O75899
B	15	ILE	-	expression tag	UNP O75899
B	16	ILE	-	expression tag	UNP O75899
B	17	ALA	-	expression tag	UNP O75899
B	18	LEU	-	expression tag	UNP O75899
B	19	SER	-	expression tag	UNP O75899
B	20	TYR	-	expression tag	UNP O75899
B	21	ILE	-	expression tag	UNP O75899
B	22	PHE	-	expression tag	UNP O75899
B	23	CYS	-	expression tag	UNP O75899
B	24	LEU	-	expression tag	UNP O75899
B	25	VAL	-	expression tag	UNP O75899
B	26	PHE	-	expression tag	UNP O75899
B	27	ALA	-	expression tag	UNP O75899
B	28	ASP	-	expression tag	UNP O75899
B	29	TYR	-	expression tag	UNP O75899
B	30	LYS	-	expression tag	UNP O75899
B	31	ASP	-	expression tag	UNP O75899
B	32	ASP	-	expression tag	UNP O75899
B	33	ASP	-	expression tag	UNP O75899
B	34	ASP	-	expression tag	UNP O75899
B	35	LYS	-	expression tag	UNP O75899
B	36	GLY	-	expression tag	UNP O75899
B	37	SER	-	expression tag	UNP O75899
B	38	GLY	-	expression tag	UNP O75899
B	39	GLY	-	expression tag	UNP O75899
B	40	SER	-	expression tag	UNP O75899

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



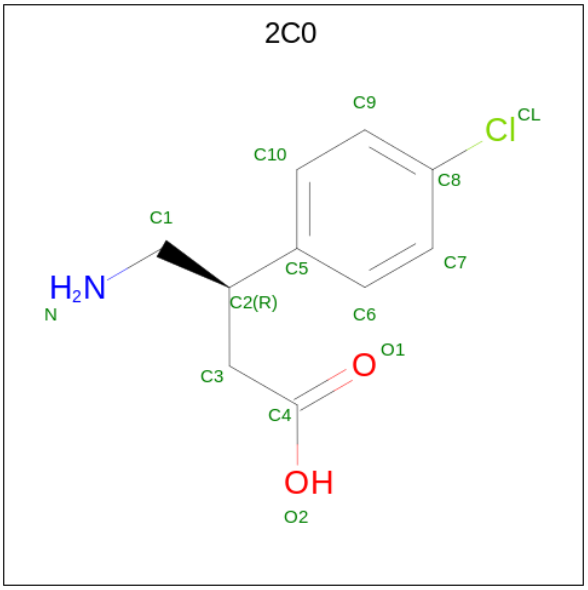
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	A	1	70	40	5	25	0
			Total	C	N	O	
3	B	1	42	24	3	15	0
			Total	C	N	O	
3	B	1	42	24	3	15	0
			Total	C	N	O	
3	B	1	42	24	3	15	0

- Molecule 4 is (3S)-5,7-ditert-butyl-3-oxidanyl-3-(trifluoromethyl)-1-benzofuran-2-one (three-letter code: FN0) (formula: $C_{17}H_{21}F_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	F	O	
4	A	1	23	17	3	3	0

- Molecule 5 is baclofen (three-letter code: 2C0) (formula: $C_{10}H_{12}ClNO_2$).



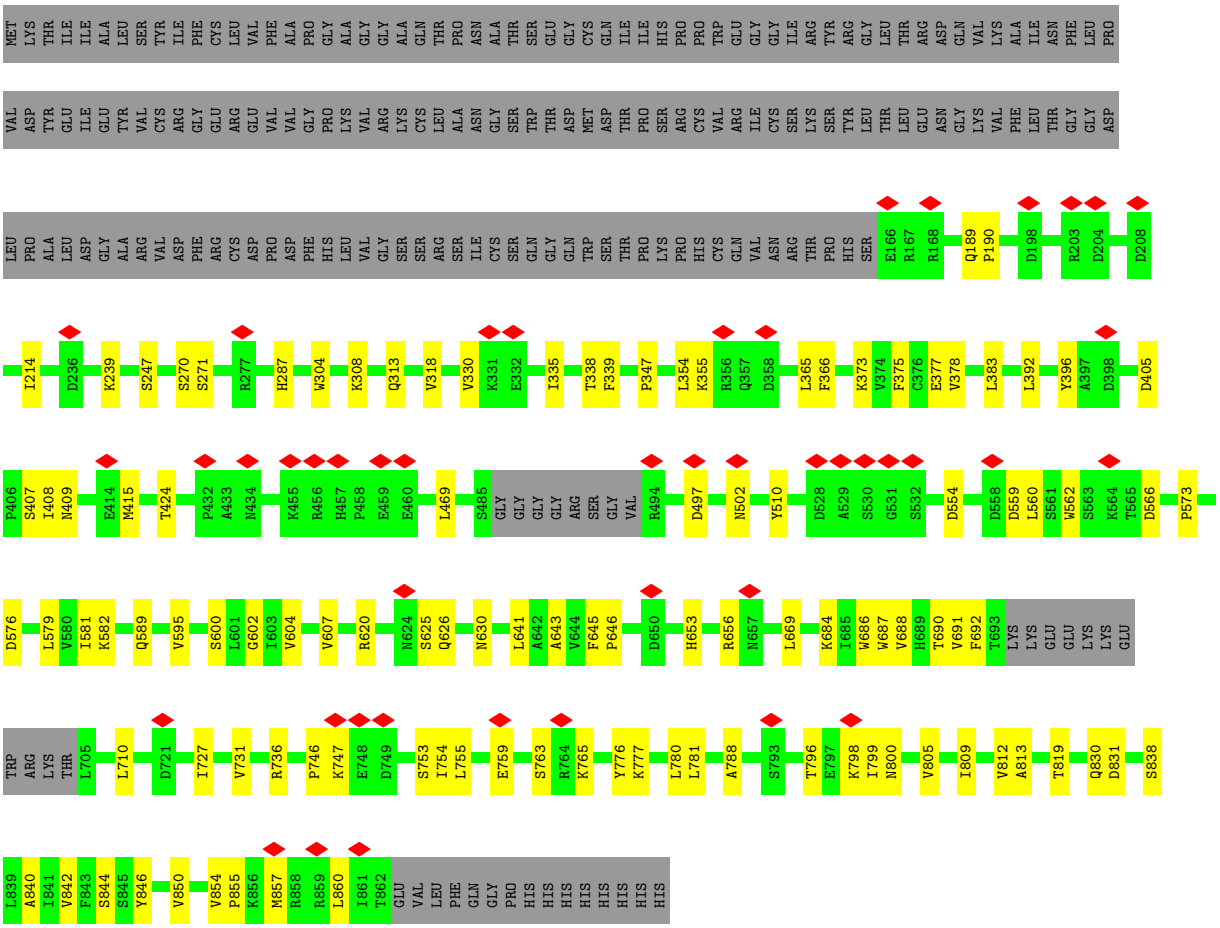
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
5	A	1	14	10	1	1	2	0

3 Residue-property plots (i)

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

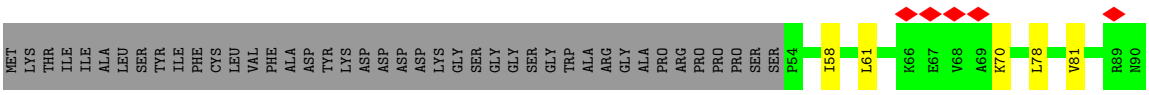
• Molecule 1: Gamma-aminobutyric acid type B receptor subunit 1

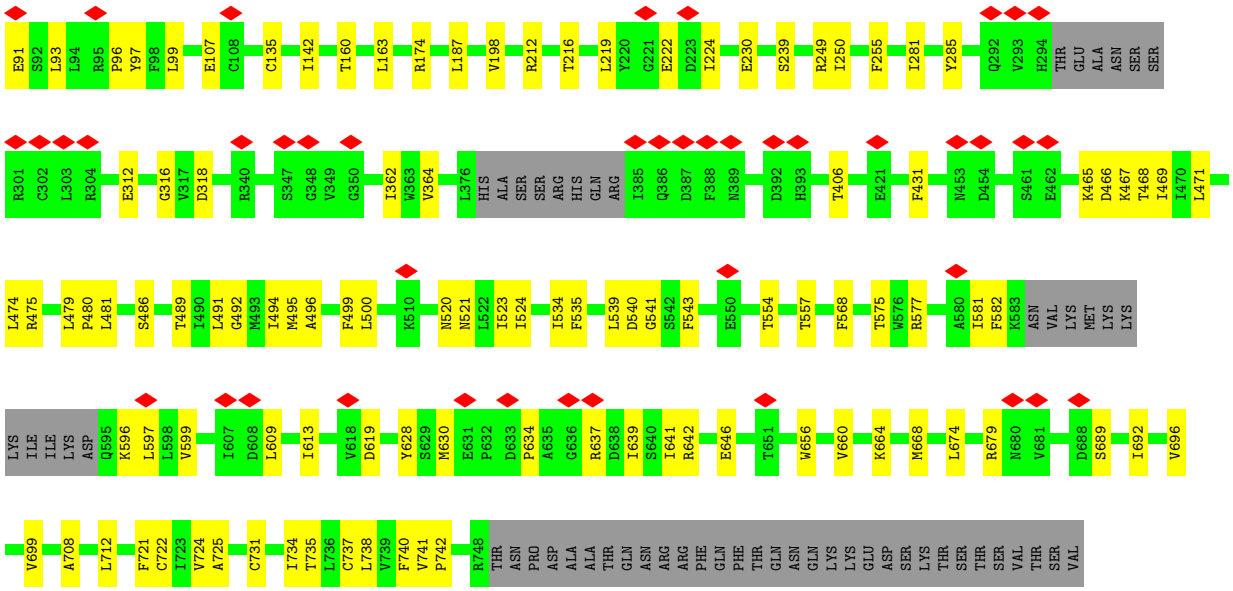
Chain A:



• Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2

Chain B:




E91 S92 L93 L94 R95 P96 Y97 F98 L99 E107 C108 C135 I142 T160 L163 R174 L187 V198 R212 T216 L219 Y220 G221 E222 D223 I224 E230 S239 R249 I250 F255 I281 Y285 Q292 V293 H294 THR GLU ALA ASN SER SER
R301 C302 L303 R304 E312 G316 V317 D318 R340 S347 G348 V349 G350 I362 W363 V364 L376 HIS ALA SER SER ARG HIS GLN ARG I385 Q386 D387 F388 N389 D392 H393 T406 E421 F431 N453 D454 S461 E462 K465 D466 K467 T468 I469 I470 L471
L474 R475 L479 P480 L481 S486 T489 I490 L491 G492 M493 I494 M495 A496 F499 L500 K510 N520 N521 L522 I523 I524 I534 F535 L539 D540 G541 S542 F543 E550 T554 T557 F568 T575 W576 R577 A580 I581 F582 K583 ASN VAL LYS MET LYS LYS
LYS ILE ILE LYS ASP Q595 K596 L597 L598 V599 I607 D608 L609 I613 V618 D619 Y628 S629 M630 E631 P632 D633 P634 A635 G636 R637 D638 I639 S640 I641 R642 E646 T651 W656 V660 K664 M668 L674 R679 N680 V681 D688 S689 I692 V696
V699 A708 L712 F721 C722 I723 V724 A725 C731 I734 T735 L736 C737 L738 V739 F740 V741 P742 R748 THR ASN PRO ASP ALA ALA THR GLN ASN ARG ARG PHE GLN PHE THR GLN ASN GLN LYS LYS GLU ASP SER LYS THR SER THR SER VAL THR SER VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	49310	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.442	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	324.48, 324.48, 324.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: FN0, 2C0, 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	0.27	0/5541	0.45	0/7527
2	B	0.28	0/5458	0.46	0/7391
All	All	0.27	0/10999	0.45	0/14918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	5406	0	5399	75	0
2	B	5339	0	5401	73	0
3	A	70	0	65	7	0
3	B	42	0	39	0	0
4	A	23	0	0	0	0
5	A	14	0	11	2	0
All	All	10894	0	10915	150	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 7.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HG2	1:A:408:ILE:HG22	1.68	0.75
1:A:287:HIS:NE2	5:A:1007:2C0:N	2.37	0.71
2:B:81:VAL:HG23	2:B:362:ILE:HG13	1.69	0.71
2:B:577:ARG:HD2	2:B:597:LEU:HD11	1.71	0.71
2:B:212:ARG:NH1	2:B:216:THR:OG1	2.24	0.70
1:A:408:ILE:HG13	1:A:408:ILE:O	1.93	0.68
2:B:160:THR:O	2:B:174:ARG:NH2	2.28	0.66
2:B:475:ARG:NH1	2:B:628:TYR:OH	2.29	0.65
1:A:502:ASN:ND2	3:A:1004:NAG:H83	2.12	0.65
3:A:1003:NAG:O3	3:A:1003:NAG:O7	2.14	0.64
1:A:746:PRO:HG3	1:A:754:ILE:HG23	1.80	0.63
2:B:78:LEU:HA	2:B:81:VAL:HG12	1.80	0.63
2:B:249:ARG:NH1	2:B:468:THR:OG1	2.32	0.63
1:A:510:TYR:HE1	3:A:1005:NAG:H82	1.64	0.62
2:B:500:LEU:HD13	2:B:524:ILE:HG21	1.80	0.62
1:A:581:ILE:HB	1:A:754:ILE:HG22	1.83	0.61
1:A:620:ARG:HB2	1:A:860:LEU:HD11	1.83	0.60
2:B:534:ILE:CD1	2:B:725:ALA:HA	2.32	0.60
1:A:510:TYR:CE1	3:A:1005:NAG:H82	2.36	0.59
2:B:539:LEU:HD22	2:B:543:PHE:HE2	1.68	0.59
2:B:465:LYS:NZ	2:B:466:ASP:O	2.33	0.59
2:B:521:ASN:HA	2:B:524:ILE:HG22	1.85	0.59
2:B:679:ARG:HB2	2:B:689:SER:HB3	1.84	0.59
1:A:409:ASN:OD1	1:A:409:ASN:O	2.22	0.58
2:B:475:ARG:HH22	2:B:628:TYR:HE2	1.51	0.57
1:A:579:LEU:H	1:A:579:LEU:HD23	1.68	0.57
1:A:270:SER:HB3	1:A:287:HIS:CE1	2.41	0.56
2:B:734:ILE:HG23	2:B:738:LEU:HD13	1.87	0.56
2:B:637:ARG:O	2:B:637:ARG:HG2	2.06	0.56
1:A:656:ARG:HG3	1:A:736:ARG:HH11	1.70	0.56
2:B:581:ILE:HG13	2:B:582:PHE:HD1	1.72	0.55
2:B:646:GLU:N	2:B:646:GLU:OE1	2.39	0.55
1:A:602:GLY:HA2	1:A:846:TYR:HE1	1.69	0.55
2:B:107:GLU:N	2:B:107:GLU:OE2	2.40	0.55
1:A:854:VAL:HA	1:A:857:MET:HG2	1.88	0.54
1:A:408:ILE:HD11	1:A:415:MET:HE1	1.90	0.54
2:B:634:PRO:HG3	2:B:639:ILE:H	1.70	0.54
1:A:560:LEU:HD21	1:A:562:TRP:HE3	1.73	0.54
1:A:625:SER:HB2	1:A:800:ASN:HB3	1.90	0.54
1:A:582:LYS:HG2	1:A:755:LEU:HD21	1.90	0.54
1:A:796:THR:HG22	1:A:798:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ILE:HD11	2:B:99:LEU:HD11	1.90	0.53
2:B:534:ILE:HD12	2:B:725:ALA:CB	2.38	0.53
1:A:595:VAL:HG11	1:A:838:SER:HB2	1.90	0.52
2:B:61:LEU:HD13	2:B:142:ILE:HD13	1.91	0.52
1:A:687:TRP:O	1:A:691:VAL:HG12	2.09	0.52
2:B:70:LYS:HD3	2:B:135:CYS:SG	2.49	0.52
2:B:539:LEU:HD22	2:B:543:PHE:CE2	2.43	0.52
1:A:308:LYS:HE3	1:A:338:THR:HG21	1.92	0.52
1:A:850:VAL:O	1:A:854:VAL:HG12	2.09	0.52
2:B:737:CYS:O	2:B:741:VAL:HG12	2.10	0.51
2:B:187:LEU:HD12	2:B:219:LEU:HD23	1.92	0.51
1:A:643:ALA:HB2	1:A:669:LEU:HB3	1.92	0.51
2:B:492:GLY:O	2:B:495:MET:HG3	2.11	0.51
2:B:534:ILE:HD12	2:B:725:ALA:HA	1.92	0.51
2:B:486:SER:HG	2:B:535:PHE:HE1	1.56	0.51
1:A:330:VAL:HB	1:A:335:ILE:HB	1.93	0.50
1:A:788:ALA:HB2	1:A:809:ILE:HD11	1.92	0.50
2:B:568:PHE:HZ	2:B:699:VAL:HG21	1.76	0.50
2:B:198:VAL:HG12	2:B:250:ILE:HB	1.92	0.50
2:B:577:ARG:HB2	2:B:597:LEU:HD21	1.93	0.50
1:A:366:PHE:O	1:A:396:TYR:OH	2.18	0.50
1:A:405:ASP:OD2	1:A:407:SER:OG	2.26	0.50
1:A:641:LEU:HD11	1:A:842:VAL:HG22	1.92	0.50
1:A:355:LYS:HD3	1:A:383:LEU:HD13	1.93	0.50
2:B:230:GLU:HB3	2:B:239:SER:OG	2.11	0.50
2:B:312:GLU:HA	2:B:431:PHE:HD2	1.77	0.49
1:A:812:VAL:HG22	1:A:844:SER:OG	2.12	0.49
1:A:686:TRP:O	1:A:690:THR:HG22	2.13	0.49
2:B:496:ALA:HB1	2:B:524:ILE:HD11	1.95	0.49
2:B:679:ARG:HB2	2:B:689:SER:CB	2.42	0.49
2:B:708:ALA:O	2:B:712:LEU:HD13	2.13	0.49
1:A:759:GLU:N	1:A:759:GLU:OE1	2.46	0.48
2:B:255:PHE:O	2:B:285:TYR:OH	2.24	0.48
2:B:318:ASP:N	2:B:318:ASP:OD1	2.46	0.48
2:B:619:ASP:OD2	2:B:656:TRP:NE1	2.46	0.48
1:A:247:SER:OG	5:A:1007:2C0:O1	2.31	0.48
1:A:645:PHE:HB2	1:A:646:PRO:HD3	1.96	0.48
2:B:575:THR:HG22	2:B:674:LEU:HD23	1.95	0.48
1:A:497:ASP:HB2	3:A:1004:NAG:O7	2.13	0.48
1:A:746:PRO:HG3	1:A:754:ILE:HG12	1.96	0.48
2:B:471:LEU:HD21	2:B:641:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:VAL:HG22	1:A:799:ILE:HG21	1.96	0.47
1:A:560:LEU:HD21	1:A:562:TRP:CE3	2.48	0.47
2:B:481:LEU:HD11	2:B:722:CYS:HB2	1.96	0.47
2:B:486:SER:OG	2:B:535:PHE:HE1	1.97	0.47
1:A:392:LEU:HB2	1:A:424:THR:HG22	1.95	0.47
1:A:746:PRO:HD2	1:A:753:SER:HA	1.95	0.47
2:B:660:VAL:HG12	2:B:664:LYS:HE2	1.96	0.47
2:B:741:VAL:N	2:B:742:PRO:HD2	2.30	0.47
1:A:692:PHE:CZ	1:A:796:THR:HG21	2.50	0.46
2:B:96:PRO:HG2	2:B:97:TYR:CD2	2.50	0.46
1:A:409:ASN:OD1	1:A:409:ASN:C	2.54	0.46
2:B:554:THR:HA	2:B:557:THR:HG22	1.96	0.46
1:A:776:TYR:HE2	1:A:777:LYS:HZ3	1.64	0.46
2:B:731:CYS:O	2:B:735:THR:HG23	2.16	0.46
1:A:339:PHE:HD2	1:A:354:LEU:HD23	1.81	0.46
1:A:554:ASP:HB2	1:A:559:ASP:OD1	2.15	0.46
2:B:596:LYS:O	2:B:599:VAL:HG12	2.16	0.45
1:A:375:PHE:HA	1:A:378:VAL:HB	1.98	0.45
2:B:609:LEU:O	2:B:613:ILE:HG12	2.16	0.45
2:B:465:LYS:NZ	2:B:467:LYS:O	2.49	0.45
1:A:684:LYS:HD2	1:A:805:VAL:HG21	1.97	0.45
1:A:576:ASP:N	1:A:576:ASP:OD1	2.48	0.45
1:A:589:GLN:OE1	1:A:653:HIS:NE2	2.44	0.45
2:B:212:ARG:HH12	2:B:216:THR:HG1	1.63	0.45
1:A:620:ARG:NH1	1:A:860:LEU:O	2.51	0.45
1:A:747:LYS:HD3	1:A:747:LYS:HA	1.80	0.45
1:A:409:ASN:OD1	3:A:1001:NAG:O5	2.34	0.44
1:A:854:VAL:CG1	1:A:855:PRO:HD3	2.48	0.44
1:A:626:GLN:HE21	1:A:710:LEU:HD22	1.81	0.44
1:A:781:LEU:HD22	1:A:813:ALA:HA	2.00	0.44
2:B:281:ILE:O	2:B:316:GLY:HA2	2.17	0.44
1:A:780:LEU:HD23	1:A:780:LEU:HA	1.87	0.44
2:B:668:MET:SD	2:B:696:VAL:HG13	2.58	0.44
1:A:313:GLN:HB2	1:A:365:LEU:HB2	1.98	0.44
1:A:830:GLN:HG2	1:A:831:ASP:N	2.33	0.44
1:A:189:GLN:HB3	1:A:190:PRO:HD3	1.99	0.43
1:A:630:ASN:OD1	1:A:684:LYS:NZ	2.51	0.43
2:B:721:PHE:HA	2:B:724:VAL:HG12	2.00	0.43
1:A:271:SER:HA	1:A:318:VAL:HG23	1.99	0.43
2:B:486:SER:HA	2:B:489:THR:HG22	2.00	0.43
1:A:566:ASP:OD1	1:A:566:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ILE:H	2:B:469:ILE:HD12	1.83	0.43
2:B:499:PHE:HB3	2:B:740:PHE:HD2	1.82	0.43
1:A:727:ILE:O	1:A:731:VAL:HB	2.19	0.43
2:B:474:LEU:HD22	2:B:646:GLU:OE1	2.18	0.42
1:A:405:ASP:OD2	1:A:408:ILE:HG23	2.18	0.42
1:A:604:VAL:HA	1:A:607:VAL:HG12	2.01	0.42
1:A:763:SER:OG	1:A:765:LYS:O	2.25	0.42
2:B:524:ILE:HD12	2:B:524:ILE:HA	1.87	0.42
2:B:689:SER:HA	2:B:692:ILE:HD12	2.01	0.42
2:B:491:LEU:HA	2:B:494:ILE:HG12	2.00	0.42
1:A:304:TRP:CD1	1:A:573:PRO:HG3	2.54	0.42
1:A:214:ILE:HD12	1:A:239:LYS:HE3	2.02	0.41
1:A:600:SER:O	1:A:604:VAL:HG13	2.21	0.41
2:B:630:MET:HG3	2:B:642:ARG:HG3	2.02	0.41
1:A:347:PRO:HG2	1:A:377:GLU:OE1	2.20	0.41
1:A:688:VAL:O	1:A:692:PHE:HB2	2.20	0.41
2:B:222:GLU:HB3	2:B:224:ILE:HD12	2.01	0.41
2:B:479:LEU:N	2:B:480:PRO:HD2	2.35	0.41
1:A:287:HIS:HA	1:A:469:LEU:HD13	2.01	0.41
1:A:819:THR:HG21	1:A:840:ALA:HB2	2.02	0.41
2:B:91:GLU:OE2	2:B:93:LEU:HB2	2.19	0.41
2:B:163:LEU:HB2	2:B:174:ARG:NH2	2.35	0.41
2:B:520:ASN:O	2:B:523:ILE:HG12	2.21	0.41
3:A:1001:NAG:O7	3:A:1001:NAG:O3	2.35	0.41
2:B:465:LYS:HG2	2:B:466:ASP:O	2.21	0.41
2:B:540:ASP:OD1	2:B:541:GLY:N	2.55	0.40
2:B:364:VAL:HG22	2:B:406:THR:HG21	2.02	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	672/879 (76%)	651 (97%)	21 (3%)	0	100	100
2	B	663/769 (86%)	633 (96%)	30 (4%)	0	100	100
All	All	1335/1648 (81%)	1284 (96%)	51 (4%)	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	590/760 (78%)	590 (100%)	0	100	100
2	B	585/671 (87%)	585 (100%)	0	100	100
All	All	1175/1431 (82%)	1175 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	246	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
3	NAG	A	1002	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1005	1	14,14,15	0.21	0	17,19,21	0.42	0
4	FN0	A	1006	-	23,24,24	1.05	2 (8%)	35,42,42	2.07	5 (14%)
3	NAG	A	1003	1	14,14,15	0.28	0	17,19,21	0.55	0
3	NAG	B	1001	2	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	1002	2	14,14,15	0.27	0	17,19,21	0.60	0
5	2C0	A	1007	-	13,14,14	1.06	0	15,18,18	1.25	3 (20%)
3	NAG	A	1001	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	A	1004	1	14,14,15	0.28	0	17,19,21	0.59	0
3	NAG	B	1003	2	14,14,15	0.21	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
4	FN0	A	1006	-	-	10/21/37/37	0/2/2/2
3	NAG	A	1003	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
5	2C0	A	1007	-	-	2/10/10/10	0/1/1/1
3	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1004	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	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)
4	A	1006	FN0	O3-C13	2.41	1.26	1.20
4	A	1006	FN0	C6-C2	-2.07	1.37	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1006	FN0	C5-C7-C13	-7.78	98.07	101.75
4	A	1006	FN0	C17-C7-C5	5.68	121.99	112.72
4	A	1006	FN0	C4-C9-C5	-3.27	118.72	123.80
4	A	1006	FN0	C8-C2-C6	-2.74	113.19	117.11
4	A	1006	FN0	C7-C5-C6	-2.57	107.79	108.88
5	A	1007	2C0	O1-C4-C3	-2.14	115.94	122.80
5	A	1007	2C0	C2-C3-C4	2.08	115.73	113.50
5	A	1007	2C0	C7-C6-C5	2.07	123.28	121.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAG	C3-C2-N2-C7
3	A	1001	NAG	C8-C7-N2-C2
3	A	1001	NAG	O7-C7-N2-C2
3	A	1003	NAG	C3-C2-N2-C7
3	A	1004	NAG	C8-C7-N2-C2
3	A	1004	NAG	O7-C7-N2-C2
3	B	1002	NAG	C8-C7-N2-C2
4	A	1006	FN0	F1-C17-C7-C5
4	A	1006	FN0	F2-C17-C7-C5
4	A	1006	FN0	F3-C17-C7-C5
5	A	1007	2C0	N-C1-C2-C5
5	A	1007	2C0	N-C1-C2-C3
3	B	1002	NAG	O7-C7-N2-C2
3	A	1002	NAG	C4-C5-C6-O6
3	A	1005	NAG	C4-C5-C6-O6
3	A	1002	NAG	O5-C5-C6-O6
3	A	1005	NAG	O5-C5-C6-O6
3	B	1003	NAG	C4-C5-C6-O6
3	A	1003	NAG	C8-C7-N2-C2
4	A	1006	FN0	C10-C1-C2-C6
3	B	1003	NAG	O5-C5-C6-O6
4	A	1006	FN0	C11-C1-C2-C6
4	A	1006	FN0	C12-C1-C2-C6

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Mol	Chain	Res	Type	Atoms
3	A	1003	NAG	O7-C7-N2-C2
4	A	1006	FN0	C10-C1-C2-C8
4	A	1006	FN0	C12-C1-C2-C8
3	A	1004	NAG	O5-C5-C6-O6
4	A	1006	FN0	C11-C1-C2-C8
3	A	1003	NAG	C1-C2-N2-C7
3	A	1001	NAG	C1-C2-N2-C7
4	A	1006	FN0	F2-C17-C7-O2

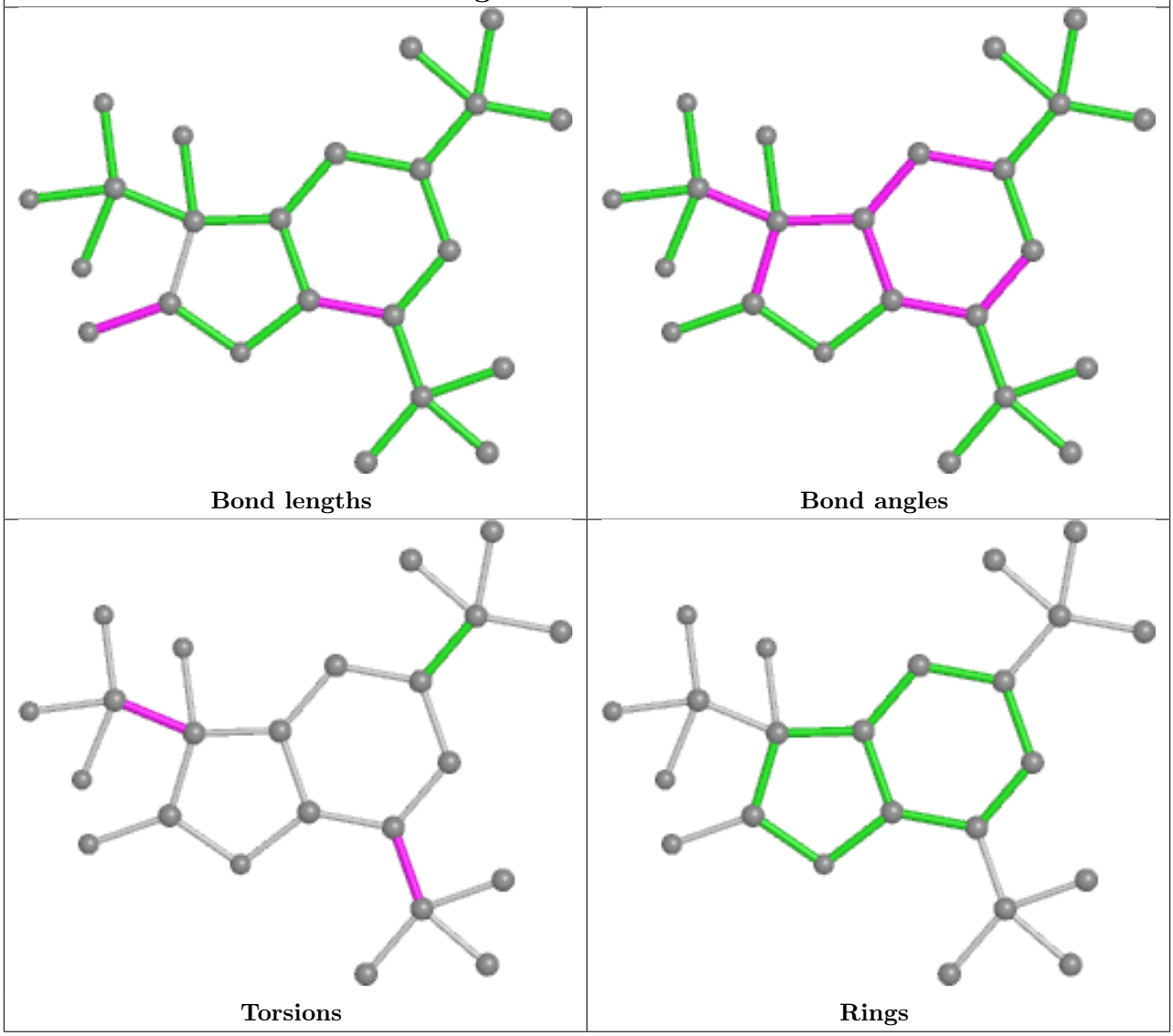
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	NAG	2	0
3	A	1003	NAG	1	0
5	A	1007	2C0	2	0
3	A	1001	NAG	2	0
3	A	1004	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FN0 A 1006



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.

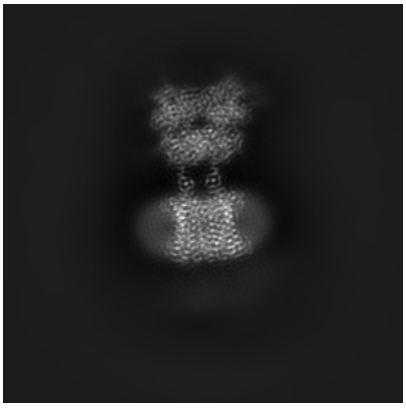
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30300. These allow visual inspection of the internal detail of the map and identification of artifacts.

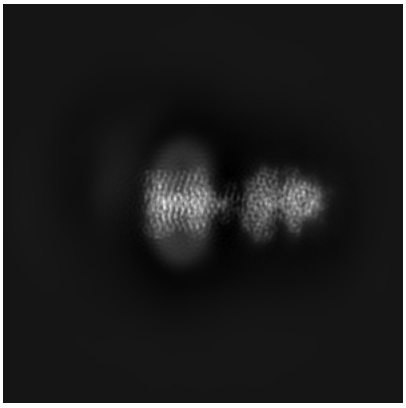
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

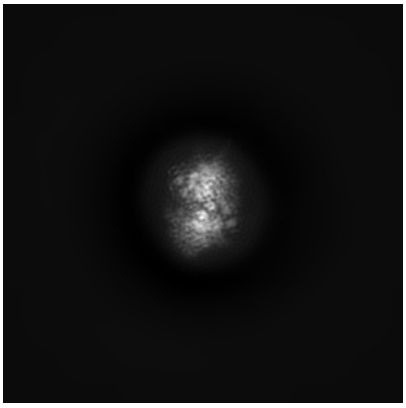
6.1.1 Primary map



X



Y

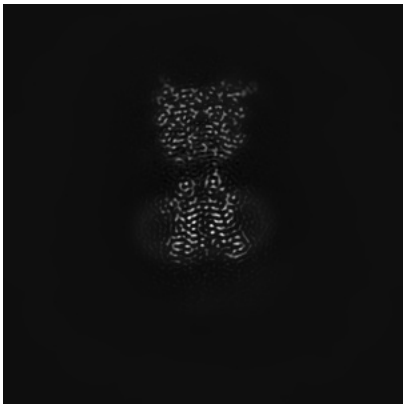


Z

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

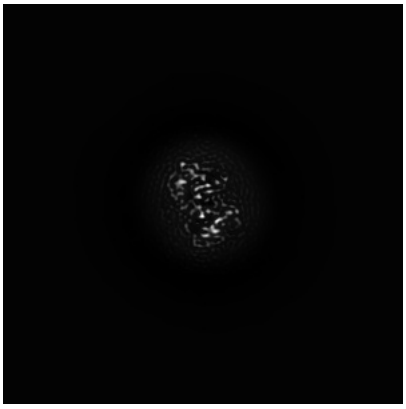
6.2 Central slices (i)

6.2.1 Primary map



X Index: 160

Y Index: 160

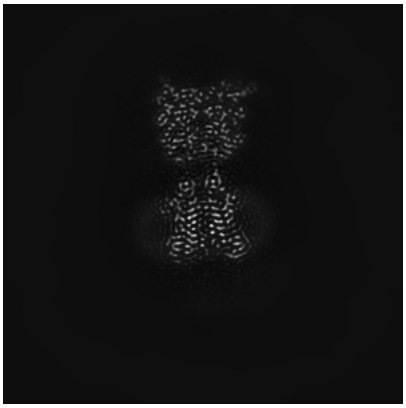


Z Index: 160

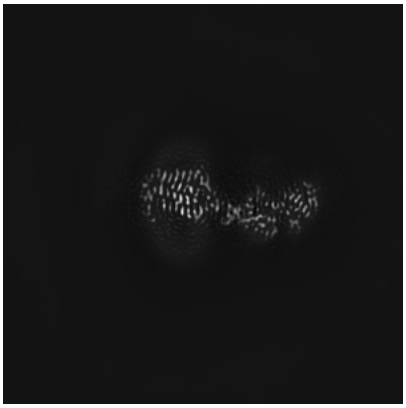
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

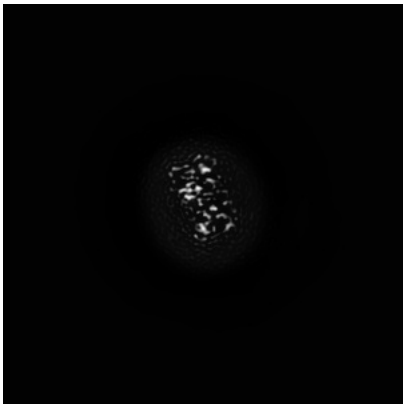
6.3.1 Primary map



X Index: 160



Y Index: 143



Z Index: 128

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

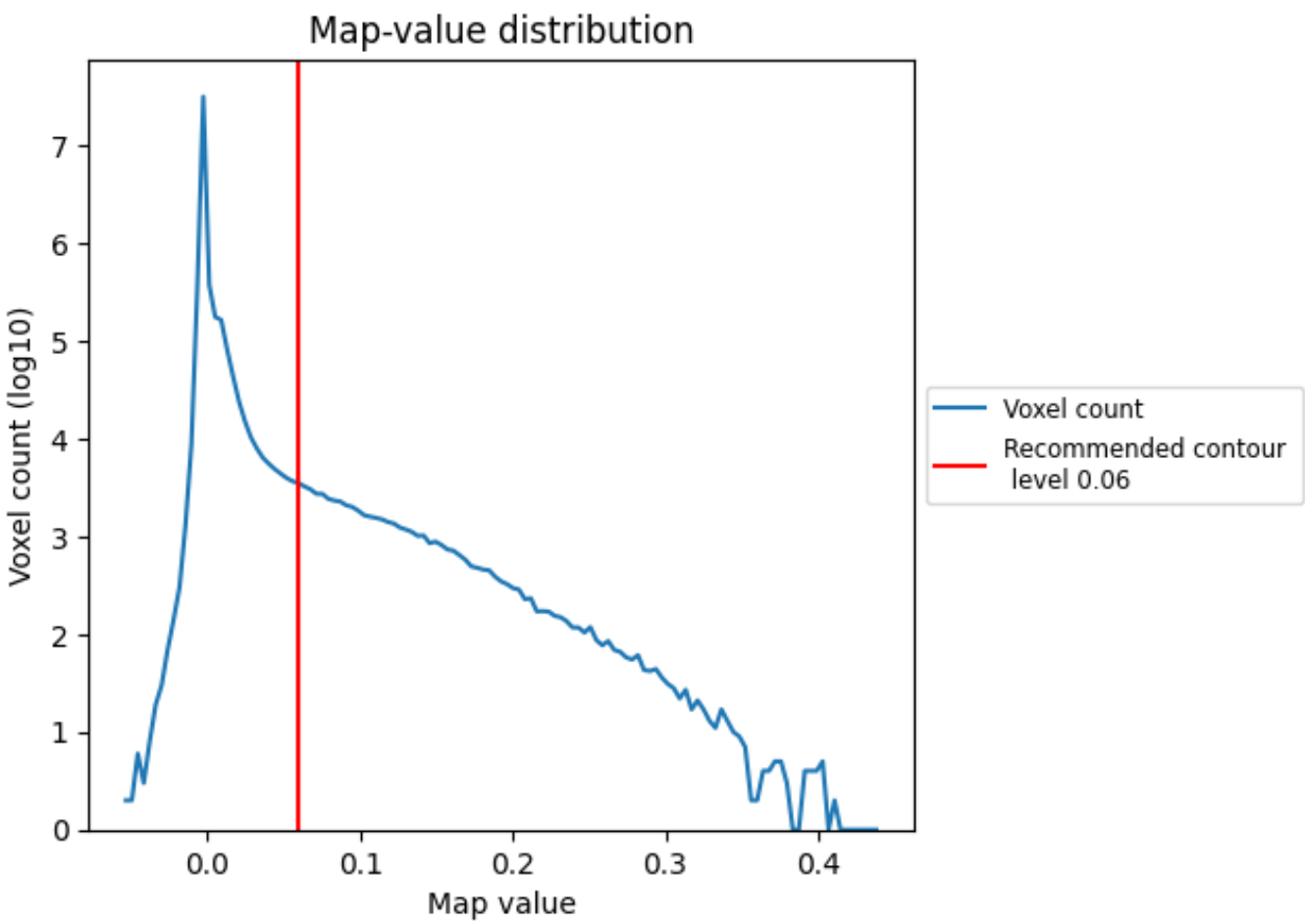
6.5 Mask visualisation (i)

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

7 Map analysis (i)

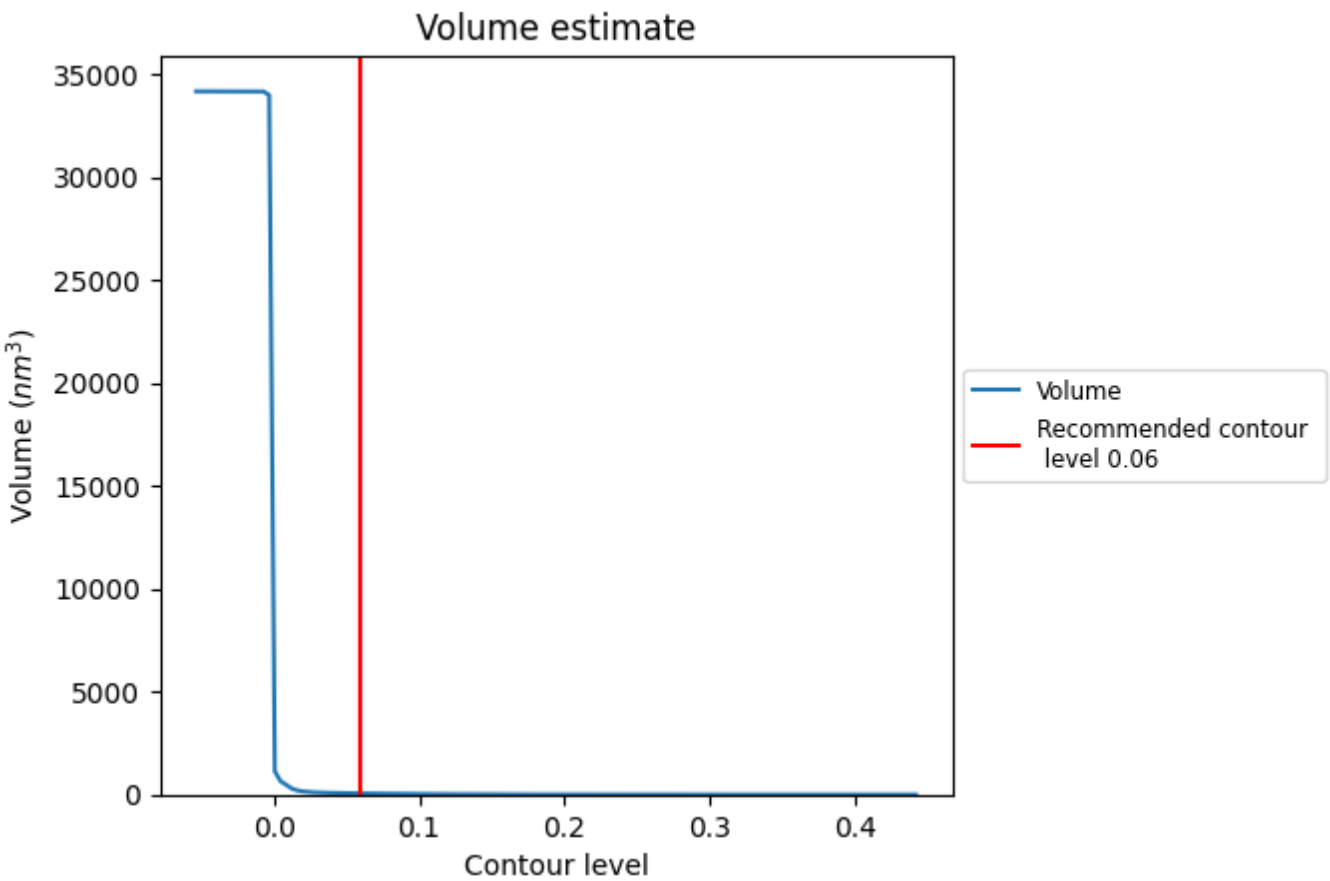
This section contains the results of statistical analysis of the map.

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.

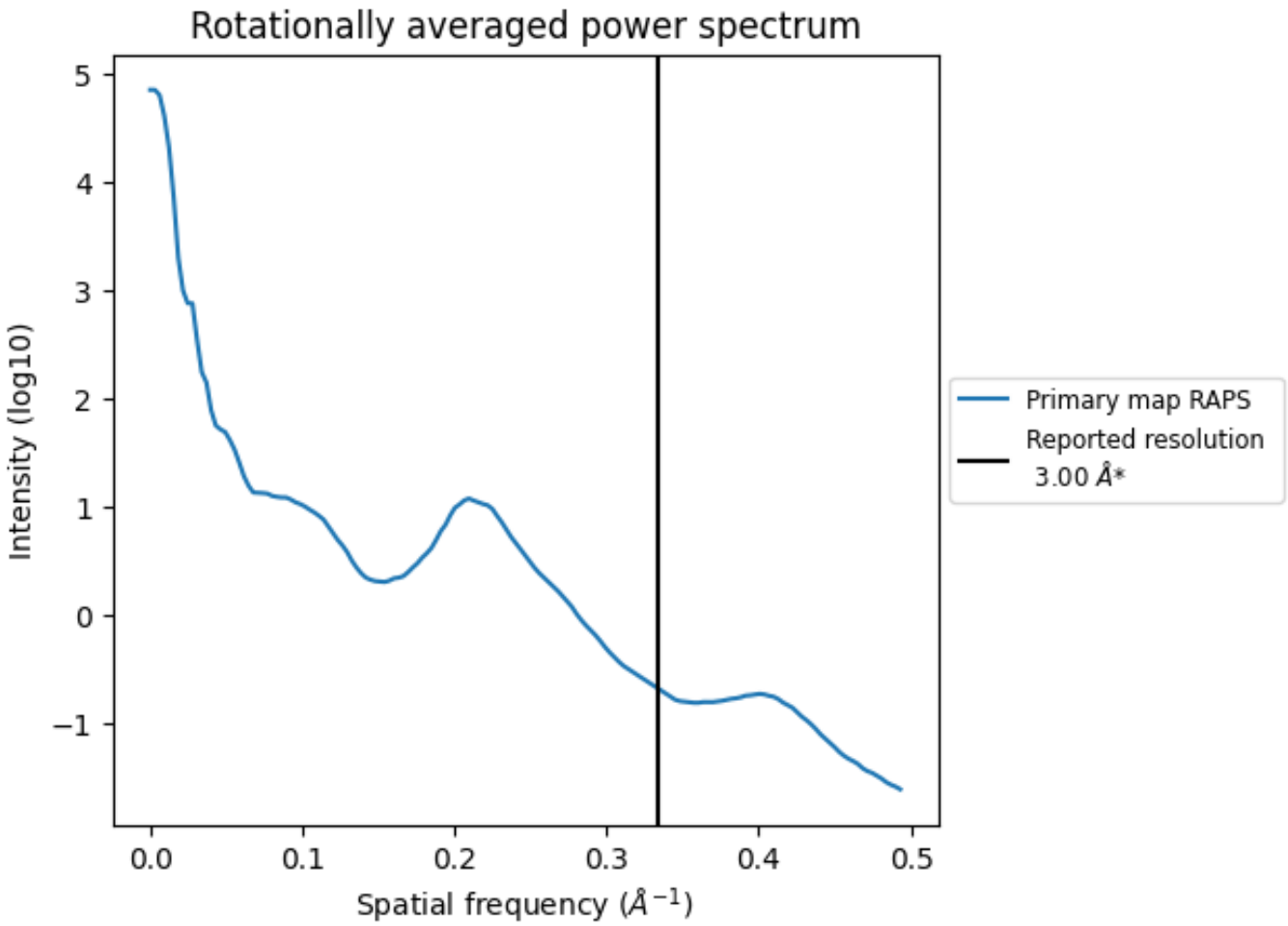
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

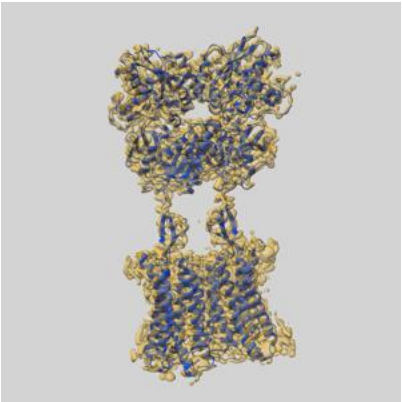
8 Fourier-Shell correlation (i)

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

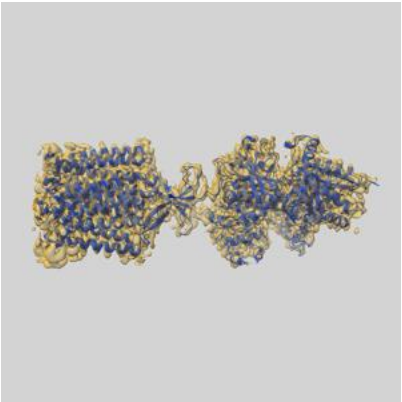
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30300 and PDB model 7C7Q. Per-residue inclusion information can be found in section 3 on page 7.

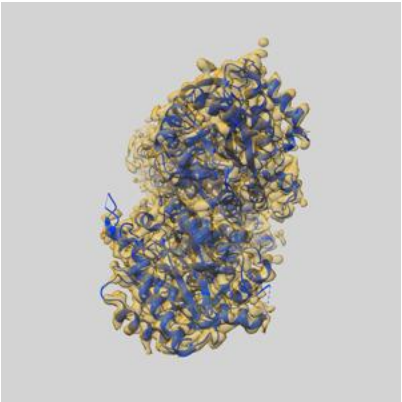
9.1 Map-model overlay (i)



X



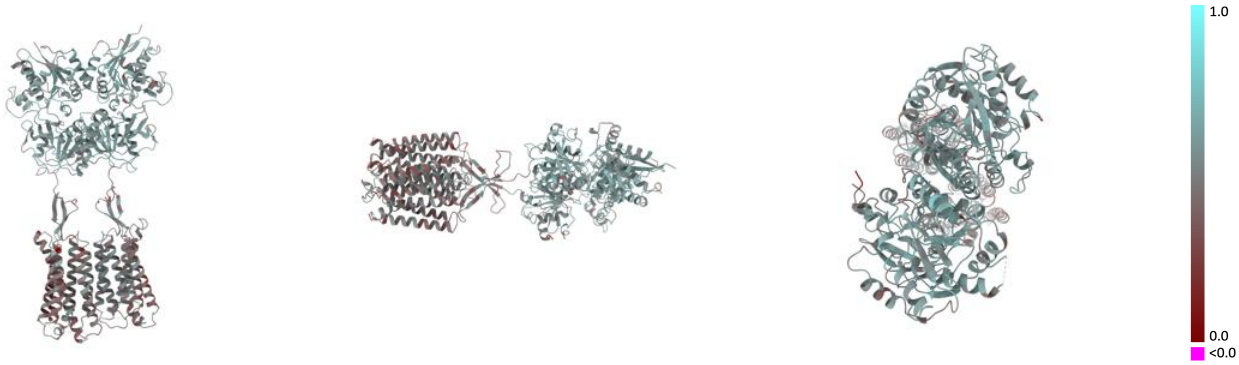
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



X Y Z

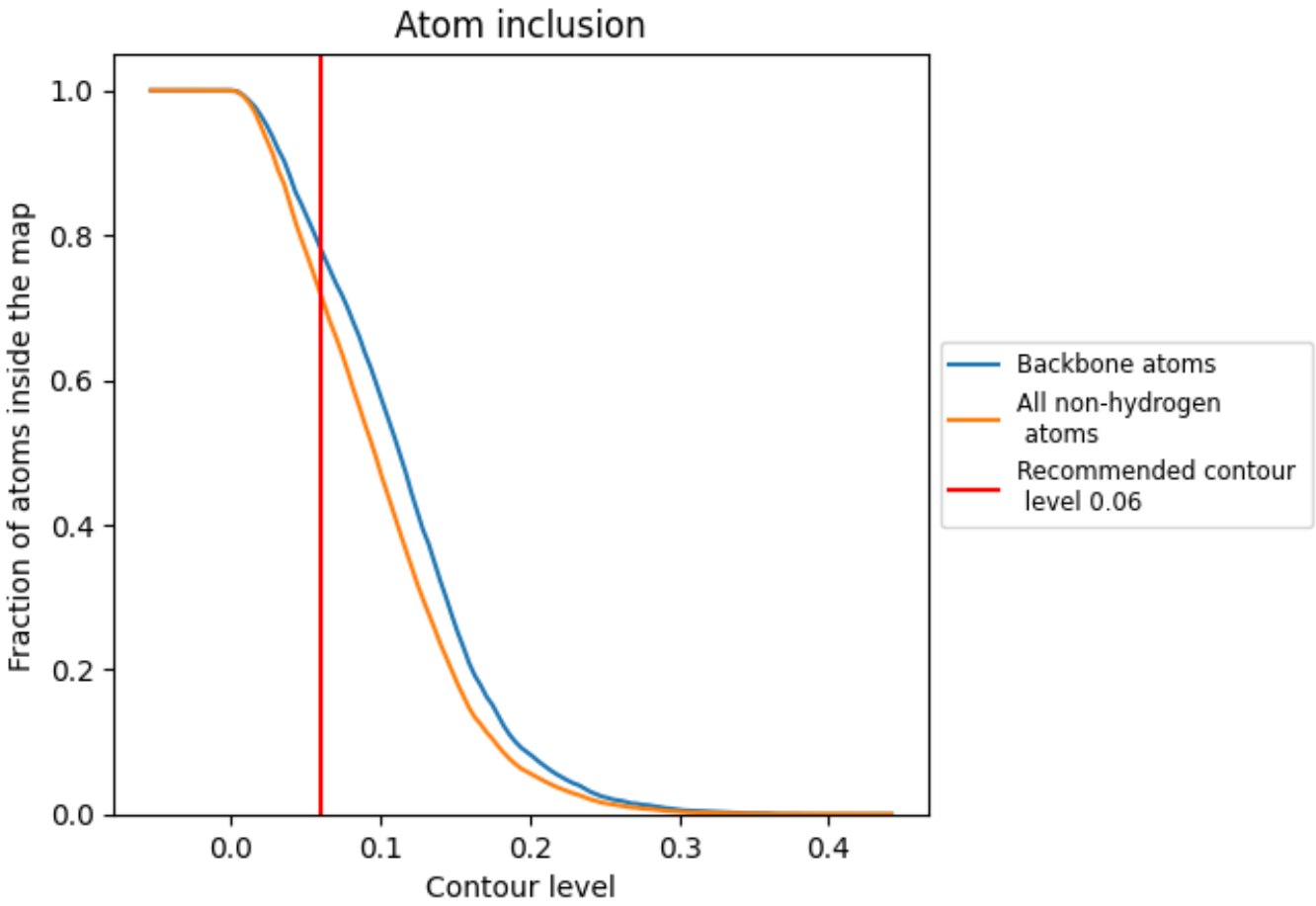
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7186	0.5090
A	0.7269	0.5150
B	0.7101	0.5030