



Full wwPDB EM Validation Report ⓘ

Sep 6, 2026 – 07:09 am BST

PDB ID : 9T7Q / pdb_00009t7q
EMDB ID : EMD-55651
Title : Cryo-EM structure of EA-Ri-112-bound D3 dopamine receptor with mini-Go
Authors : Yardeni, E.H.; Kiss, D.J.; Keseru, G.M.; Shalev-Benami, M.
Deposited on : 2025-11-11
Resolution : 3.03 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

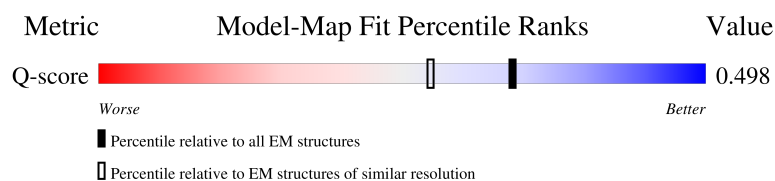
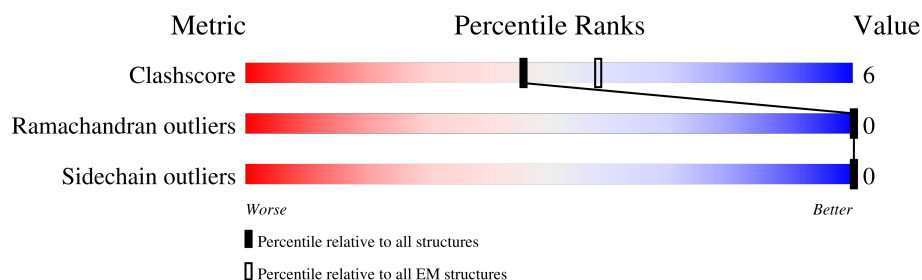
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.03 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	13929 (2.53 - 3.53)

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	B	366	
2	C	71	
3	R	573	
4	A	226	

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Mol	Chain	Length	Quality of chain
5	S	256	6% 78% 13% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8628 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	342	Total	C	N	O	S	0	0
			2607	1606	465	515	21		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLY	-	expression tag	UNP P62873
B	341	SER	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	GLY	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	SER	-	expression tag	UNP P62873
B	348	GLY	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	VAL	-	expression tag	UNP P62873
B	356	SER	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	TRP	-	expression tag	UNP P62873
B	359	ARG	-	expression tag	UNP P62873
B	360	LEU	-	expression tag	UNP P62873
B	361	PHE	-	expression tag	UNP P62873
B	362	LYS	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	ILE	-	expression tag	UNP P62873
B	365	SER	-	expression tag	UNP P62873

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	58	Total	C	N	O	S	0	0
			447	280	79	85	3		

- Molecule 3 is a protein called D(3) dopamine receptor,Dopamine 3 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	278	Total	C	N	O	S	0	0
			2064	1353	335	357	19		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(o) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	221	Total	C	N	O	S	0	0
			1731	1097	292	329	13		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P09471
A	3	VAL	LEU	engineered mutation	UNP P09471
A	7	ASP	GLU	engineered mutation	UNP P09471
A	8	LYS	ARG	engineered mutation	UNP P09471
A	11	ALA	LEU	engineered mutation	UNP P09471
A	16	MET	ALA	engineered mutation	UNP P09471
A	40	ASP	GLY	engineered mutation	UNP P09471
A	41	ASN	GLU	engineered mutation	UNP P09471
A	56	GLY	-	linker	UNP P09471
A	57	GLY	-	linker	UNP P09471
A	58	SER	-	linker	UNP P09471
A	59	GLY	-	linker	UNP P09471
A	60	GLY	-	linker	UNP P09471
A	61	SER	-	linker	UNP P09471
A	62	GLY	-	linker	UNP P09471
A	63	GLY	-	linker	UNP P09471
A	109	ASP	ALA	engineered mutation	UNP P09471
A	112	ASP	GLY	engineered mutation	UNP P09471
A	?	-	ASP	deletion	UNP P09471
A	?	-	GLN	deletion	UNP P09471
A	?	-	VAL	deletion	UNP P09471
A	?	-	LEU	deletion	UNP P09471

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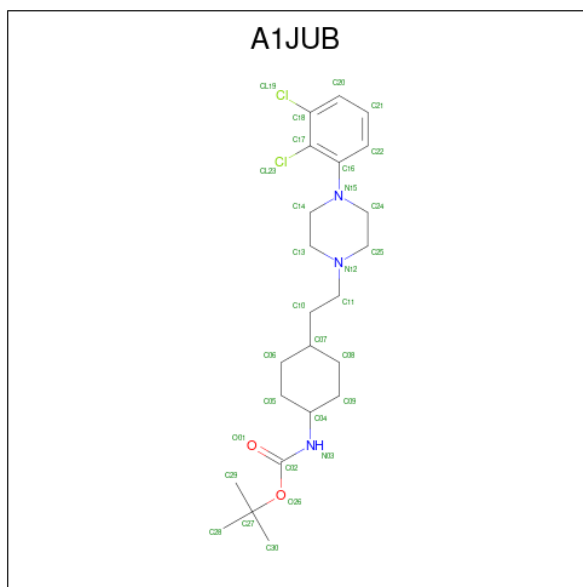
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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P09471
A	?	-	GLU	deletion	UNP P09471
A	?	-	ASP	deletion	UNP P09471
A	?	-	GLU	deletion	UNP P09471
A	?	-	THR	deletion	UNP P09471
A	?	-	THR	deletion	UNP P09471
A	204	ALA	ILE	engineered mutation	UNP P09471
A	207	ILE	VAL	engineered mutation	UNP P09471

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	232	Total	C	N	O	S	0	0
			1749	1115	294	330	10		

- Molecule 6 is {tert}-butyl {N}-[4-[2-[4-[2,3-bis(chloranyl)phenyl]piperazin-1-yl]ethyl]cyclohexyl]carbamate (CCD ID: A1JUB) (formula: C₂₃H₃₅Cl₂N₃O₂) (labeled as "Ligand of Interest" by depositor).

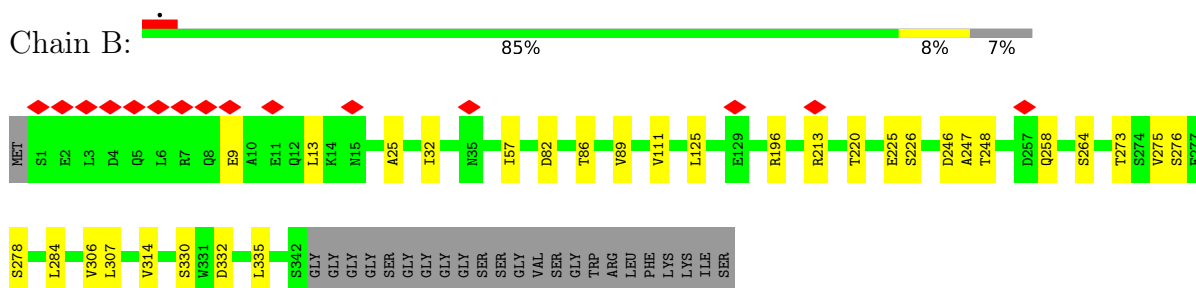


Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	Cl	N	O	0
			30	23	2	3	2	

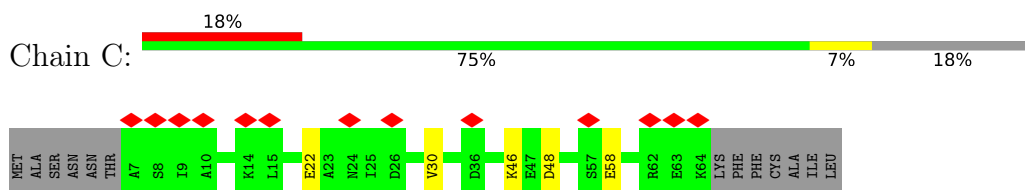
3 Residue-property plots

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.

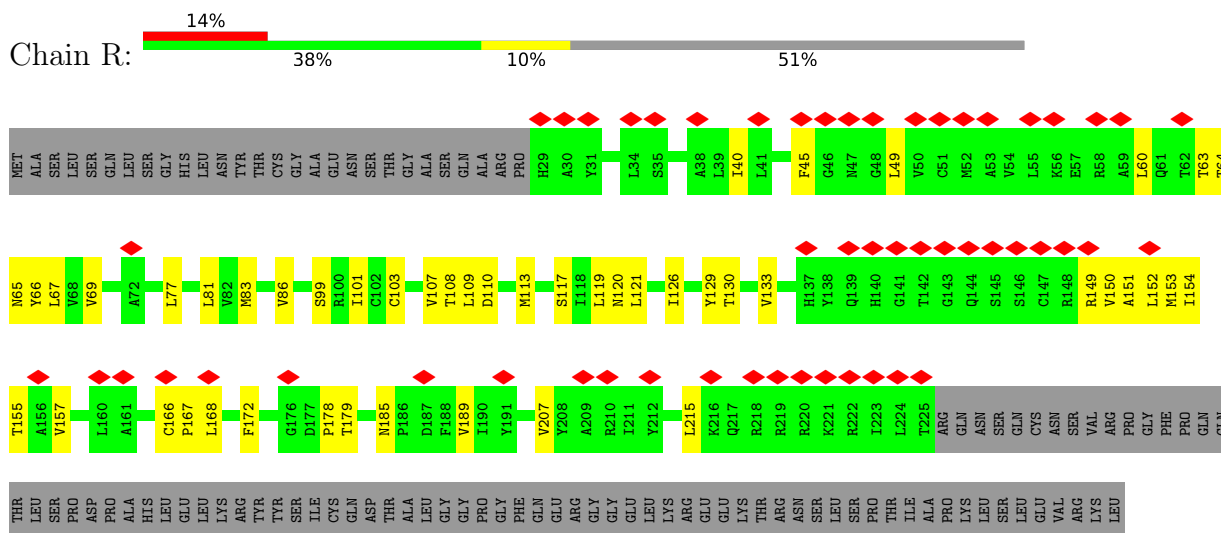
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

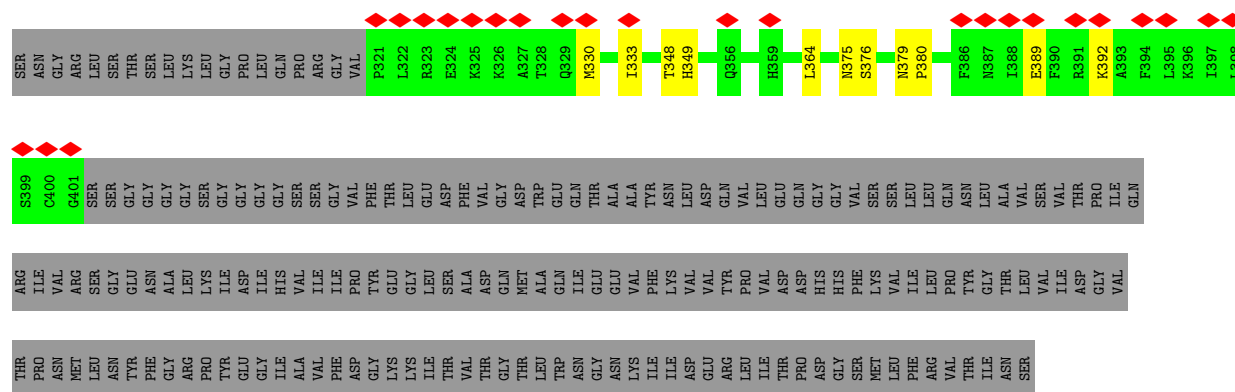


- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

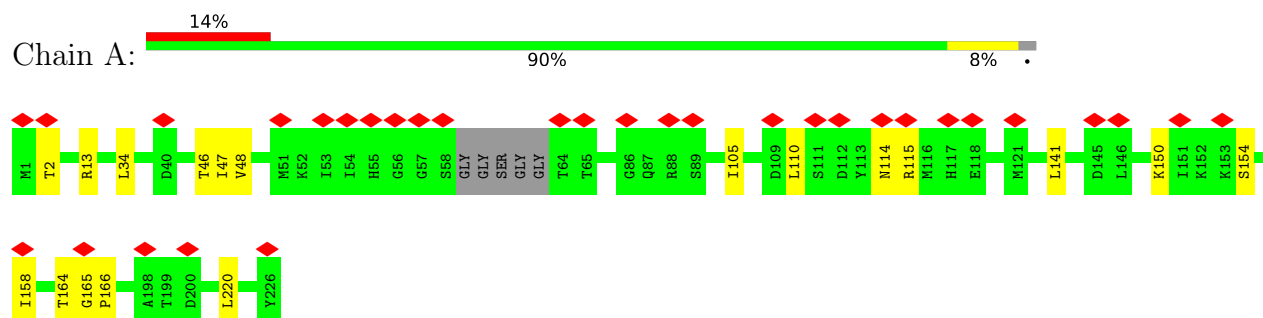


- Molecule 3: D(3) dopamine receptor,Dopamine 3 receptor

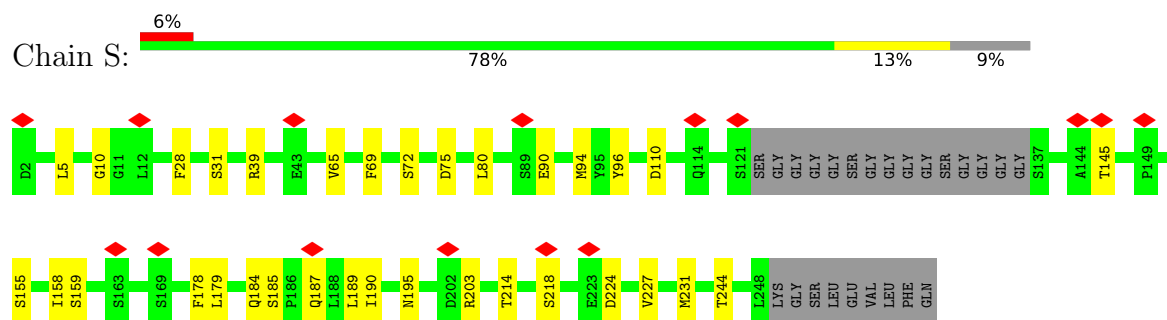




• Molecule 4: Guanine nucleotide-binding protein G(o) subunit alpha



• Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175447	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 ($e^-/\text{\AA}^2$)	38.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.895	Depositor
Minimum map value	-1.211	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.293	Depositor
Map size (Å)	303.228, 303.228, 303.228	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8423, 0.8423, 0.8423	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: A1JUB

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	B	0.11	0/2654	0.25	0/3600
2	C	0.11	0/453	0.30	0/610
3	R	0.23	0/2112	0.38	0/2899
4	A	0.25	0/1761	0.37	1/2371 (0.0%)
5	S	0.12	0/1793	0.43	2/2435 (0.1%)
All	All	0.18	0/8773	0.35	3/11915 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	10	GLY	CA-C-N	11.21	143.37	121.41
5	S	10	GLY	C-N-CA	11.21	143.37	121.41
4	A	158	ILE	CG1-CB-CG2	5.04	125.81	110.70

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	B	2607	0	2495	24	0
2	C	447	0	460	6	0
3	R	2064	0	2015	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1731	0	1703	15	0
5	S	1749	0	1665	19	0
6	R	30	0	0	2	0
All	All	8628	0	8338	105	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 6.

All (105) 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:B:330:SER:OG	1:B:332:ASP:OD1	2.03	0.77
1:B:196:ARG:HG3	1:B:213:ARG:NH1	2.00	0.76
5:S:155:SER:OG	5:S:218:SER:O	2.03	0.74
4:A:164:THR:HG22	4:A:165:GLY:H	1.53	0.74
3:R:129:TYR:O	3:R:133:VAL:HG22	1.91	0.71
1:B:258:GLN:OE1	2:C:30:VAL:HG11	1.90	0.71
3:R:107:VAL:HG12	3:R:168:LEU:HD21	1.73	0.69
1:B:258:GLN:OE1	2:C:30:VAL:CG1	2.41	0.69
1:B:226:SER:OG	1:B:246:ASP:OD1	2.12	0.67
3:R:63:THR:HG22	3:R:150:VAL:HG21	1.76	0.66
3:R:151:ALA:O	3:R:155:THR:HG23	1.96	0.66
3:R:45:PHE:O	3:R:49:LEU:HD23	1.96	0.65
3:R:126:ILE:O	3:R:130:THR:HG23	1.97	0.64
3:R:120:ASN:OD1	3:R:157:VAL:HG21	1.97	0.64
5:S:185:SER:O	5:S:187:GLN:NE2	2.33	0.62
3:R:172:PHE:O	3:R:185:ASN:OD1	2.19	0.61
1:B:220:THR:N	2:C:22:GLU:OE1	2.34	0.60
3:R:376:SER:HA	3:R:379:ASN:HD22	1.67	0.59
3:R:185:ASN:O	3:R:189:VAL:HG23	2.02	0.59
3:R:389:GLU:OE1	3:R:392:LYS:HE2	2.03	0.59
1:B:273:THR:OG1	1:B:314:VAL:O	2.19	0.58
4:A:165:GLY:N	4:A:166:PRO:CD	2.66	0.58
3:R:119:LEU:CB	3:R:157:VAL:HG23	2.34	0.58
3:R:178:PRO:O	3:R:179:THR:OG1	2.23	0.57
2:C:46:LYS:O	2:C:46:LYS:HG3	2.05	0.57
1:B:89:VAL:O	4:A:13:ARG:NH1	2.38	0.56
1:B:9:GLU:O	1:B:13:LEU:HD23	2.06	0.56
3:R:152:LEU:O	3:R:155:THR:OG1	2.23	0.55
3:R:389:GLU:OE1	3:R:392:LYS:CE	2.55	0.55
3:R:117:SER:O	3:R:121:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:OG	2:C:48:ASP:OD1	2.23	0.55
3:R:108:THR:HA	3:R:168:LEU:HD23	1.88	0.55
3:R:60:LEU:HD21	3:R:389:GLU:HB3	1.90	0.54
4:A:150:LYS:O	4:A:154:SER:N	2.37	0.54
1:B:275:VAL:HG13	1:B:284:LEU:HD11	1.89	0.54
3:R:60:LEU:HD21	3:R:389:GLU:CB	2.38	0.54
3:R:330:MET:HA	3:R:330:MET:HE2	1.90	0.53
3:R:129:TYR:HB2	3:R:207:VAL:HG13	1.91	0.53
5:S:158:ILE:CG2	5:S:244:THR:HG21	2.39	0.53
1:B:111:VAL:HG13	1:B:125:LEU:HD11	1.91	0.52
5:S:185:SER:O	5:S:187:GLN:CD	2.54	0.50
3:R:215:LEU:HD11	4:A:220:LEU:HD11	1.93	0.49
1:B:25:ALA:HB2	1:B:258:GLN:HE22	1.77	0.49
4:A:165:GLY:N	4:A:166:PRO:HD3	2.27	0.49
1:B:196:ARG:HG3	1:B:213:ARG:HH12	1.75	0.49
5:S:227:VAL:HG13	5:S:244:THR:O	2.13	0.49
4:A:164:THR:C	4:A:166:PRO:HD2	2.37	0.48
5:S:110:ASP:OD1	5:S:110:ASP:C	2.56	0.48
3:R:348:THR:HG21	3:R:364:LEU:HD21	1.95	0.48
1:B:82:ASP:O	1:B:86:THR:N	2.45	0.48
3:R:119:LEU:HB3	3:R:157:VAL:HG23	1.94	0.48
3:R:119:LEU:HB2	3:R:157:VAL:HG23	1.96	0.47
5:S:145:THR:O	5:S:244:THR:HG22	2.14	0.47
3:R:349:HIS:CE1	6:R:601:A1JUB:CL23	3.04	0.47
3:R:66:TYR:O	3:R:69:VAL:HG12	2.15	0.47
5:S:203:ARG:NE	5:S:224:ASP:OD2	2.48	0.47
1:B:32:ILE:HG22	1:B:32:ILE:O	2.15	0.46
4:A:110:LEU:HD21	4:A:141:LEU:HD23	1.97	0.46
4:A:114:ASN:OD1	4:A:115:ARG:N	2.49	0.46
4:A:46:THR:O	4:A:46:THR:HG23	2.14	0.46
1:B:225:GLU:N	1:B:246:ASP:OD2	2.41	0.46
4:A:34:LEU:HD13	4:A:105:ILE:HD11	1.97	0.46
3:R:149:ARG:CG	3:R:153:MET:HE3	2.46	0.45
4:A:164:THR:C	4:A:166:PRO:CD	2.90	0.45
1:B:306:VAL:O	1:B:306:VAL:HG23	2.17	0.45
1:B:276:SER:O	1:B:284:LEU:HD12	2.17	0.45
3:R:99:SER:OG	3:R:101:ILE:HG12	2.17	0.45
5:S:72:SER:O	5:S:80:LEU:HD12	2.17	0.45
4:A:47:ILE:O	4:A:48:VAL:HB	2.17	0.45
3:R:64:THR:HG23	3:R:65:ASN:N	2.32	0.44
3:R:110:ASP:OD2	6:R:601:A1JUB:N12	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:40:ILE:CG1	3:R:83:MET:SD	3.05	0.44
3:R:63:THR:HG22	3:R:150:VAL:CG2	2.46	0.44
3:R:215:LEU:HD11	4:A:220:LEU:CD1	2.46	0.44
3:R:330:MET:HE2	3:R:330:MET:CA	2.47	0.43
1:B:196:ARG:HG3	1:B:213:ARG:HH11	1.77	0.43
3:R:103:CYS:O	3:R:107:VAL:HG23	2.19	0.43
5:S:31:SER:HG	5:S:75:ASP:CG	2.25	0.43
3:R:189:VAL:HG13	3:R:349:HIS:CD2	2.55	0.42
3:R:40:ILE:HG13	3:R:83:MET:SD	2.60	0.42
5:S:5:LEU:HD21	5:S:28:PHE:CE2	2.54	0.42
5:S:190:ILE:HG23	5:S:195:ASN:O	2.20	0.42
1:B:307:LEU:HD12	1:B:307:LEU:N	2.34	0.42
3:R:166:CYS:N	3:R:167:PRO:CD	2.83	0.42
3:R:379:ASN:N	3:R:380:PRO:HD2	2.35	0.42
3:R:375:ASN:O	3:R:379:ASN:ND2	2.53	0.42
5:S:39:ARG:NH2	5:S:90:GLU:O	2.53	0.42
5:S:184:GLN:HE21	5:S:187:GLN:NE2	2.18	0.41
4:A:2:THR:HG22	4:A:2:THR:O	2.20	0.41
5:S:94:MET:HE3	5:S:96:TYR:CZ	2.55	0.41
1:B:57:ILE:HD13	1:B:335:LEU:CD1	2.50	0.41
1:B:246:ASP:O	1:B:247:ALA:HB3	2.20	0.41
3:R:67:LEU:HD23	3:R:154:ILE:HD13	2.02	0.41
5:S:159:SER:OG	5:S:214:THR:HG22	2.20	0.41
2:C:58:GLU:OE2	2:C:58:GLU:HA	2.20	0.41
3:R:77:LEU:HB3	3:R:113:MET:SD	2.61	0.41
3:R:330:MET:O	3:R:333:ILE:HG22	2.20	0.41
1:B:248:THR:HG22	1:B:264:SER:HB3	2.02	0.41
3:R:153:MET:O	3:R:157:VAL:HG12	2.21	0.41
5:S:65:VAL:HG12	5:S:69:PHE:CE2	2.56	0.41
3:R:40:ILE:HG12	3:R:83:MET:SD	2.61	0.40
3:R:83:MET:O	3:R:86:VAL:N	2.53	0.40
3:R:81:LEU:HD23	3:R:109:LEU:HD22	2.04	0.40
5:S:178:PHE:CZ	5:S:231:MET:HE2	2.57	0.40
5:S:179:LEU:HB2	5:S:189:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/366 (93%)	335 (98%)	5 (2%)	0	100	100
2	C	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
3	R	274/573 (48%)	265 (97%)	9 (3%)	0	100	100
4	A	217/226 (96%)	210 (97%)	7 (3%)	0	100	100
5	S	228/256 (89%)	217 (95%)	11 (5%)	0	100	100
All	All	1115/1492 (75%)	1082 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	281/298 (94%)	281 (100%)	0	100	100
2	C	47/58 (81%)	47 (100%)	0	100	100
3	R	213/490 (44%)	213 (100%)	0	100	100
4	A	188/194 (97%)	188 (100%)	0	100	100
5	S	185/208 (89%)	185 (100%)	0	100	100
All	All	914/1248 (73%)	914 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	109	ASN
1	B	175	GLN
1	B	267	ASN
2	C	24	ASN
3	R	29	HIS
3	R	65	ASN
3	R	349	HIS
3	R	379	ASN
4	A	87	GLN
4	A	194	HIS
4	A	205	GLN
5	S	184	GLN
5	S	233	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1JUB	R	601	-	32,32,32	3.52	11 (34%)	44,45,45	1.82	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1JUB	R	601	-	-	11/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	A1JUB	C16-C17	13.10	1.53	1.40
6	R	601	A1JUB	C20-C18	6.89	1.53	1.38
6	R	601	A1JUB	C21-C22	6.74	1.53	1.38
6	R	601	A1JUB	C18-C17	-5.35	1.32	1.39
6	R	601	A1JUB	C22-C16	-4.72	1.31	1.39
6	R	601	A1JUB	C02-N03	4.47	1.45	1.34
6	R	601	A1JUB	O26-C27	-4.40	1.40	1.48
6	R	601	A1JUB	C21-C20	-3.33	1.31	1.38
6	R	601	A1JUB	O26-C02	2.77	1.40	1.34
6	R	601	A1JUB	C17-CL23	2.76	1.78	1.72
6	R	601	A1JUB	C18-CL19	2.20	1.78	1.73

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	601	A1JUB	O26-C02-N03	5.70	119.60	110.02
6	R	601	A1JUB	C27-O26-C02	-4.13	114.63	120.99
6	R	601	A1JUB	C06-C05-C04	3.14	114.96	111.48
6	R	601	A1JUB	C24-N15-C14	3.13	118.42	111.52
6	R	601	A1JUB	O26-C02-O01	-2.97	120.20	125.62
6	R	601	A1JUB	O01-C02-N03	-2.84	120.20	124.85
6	R	601	A1JUB	C13-C14-N15	2.31	115.18	110.70
6	R	601	A1JUB	C08-C09-C04	2.30	114.03	111.48
6	R	601	A1JUB	C22-C16-C17	2.27	119.77	117.69
6	R	601	A1JUB	C24-N15-C16	2.22	121.54	116.27
6	R	601	A1JUB	C22-C16-N15	-2.04	119.05	122.30
6	R	601	A1JUB	C24-C25-N12	-2.02	106.50	110.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	A1JUB	N03-C02-O26-C27

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Continued from previous page...

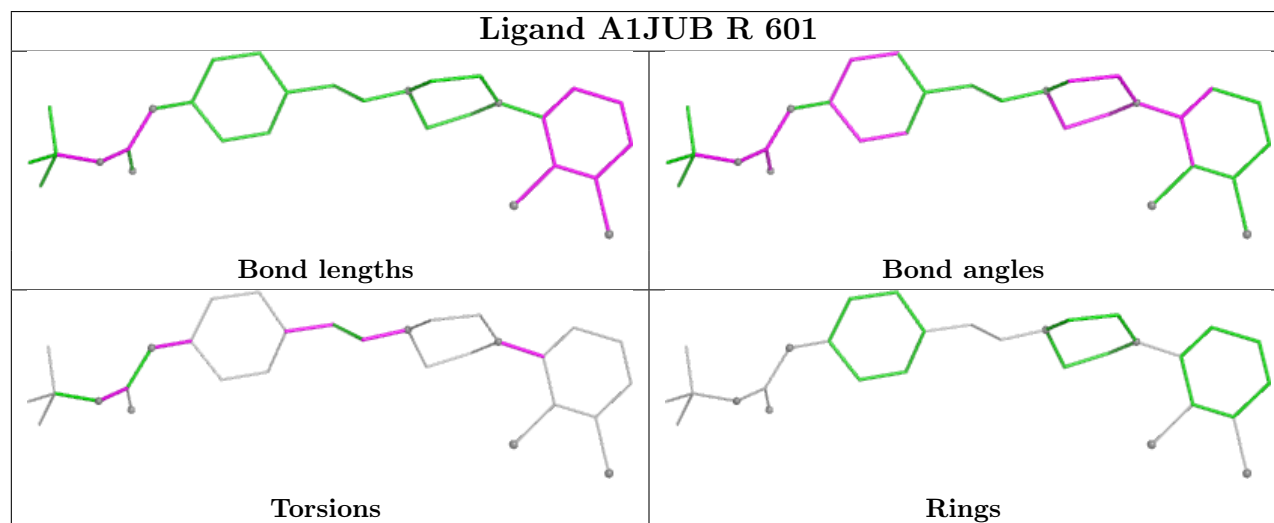
Mol	Chain	Res	Type	Atoms
6	R	601	A1JUB	C17-C16-N15-C14
6	R	601	A1JUB	O01-C02-O26-C27
6	R	601	A1JUB	C17-C16-N15-C24
6	R	601	A1JUB	C09-C04-N03-C02
6	R	601	A1JUB	C08-C07-C10-C11
6	R	601	A1JUB	C22-C16-N15-C14
6	R	601	A1JUB	C05-C04-N03-C02
6	R	601	A1JUB	C10-C11-N12-C25
6	R	601	A1JUB	C10-C11-N12-C13
6	R	601	A1JUB	C06-C07-C10-C11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	A1JUB	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 than 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.



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.

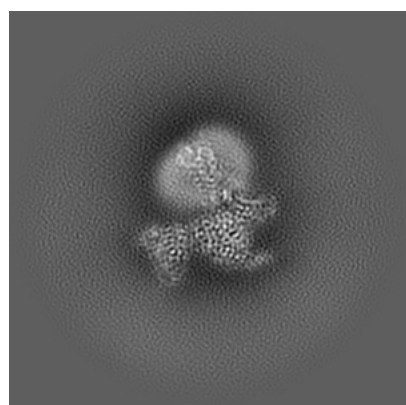
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55651. These allow visual inspection of the internal detail of the map and identification of artifacts.

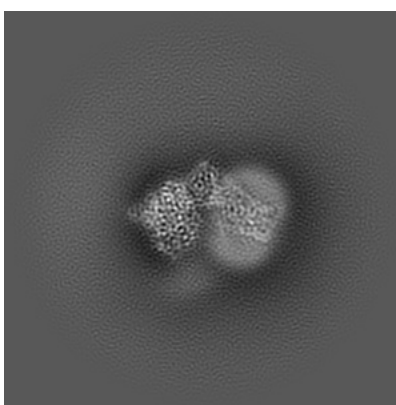
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

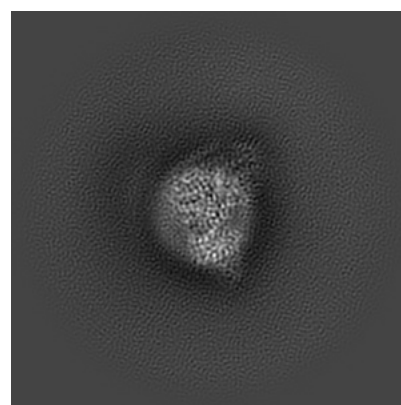
6.1.1 Primary map



X



Y

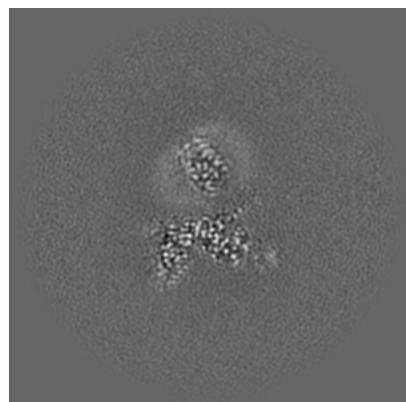


Z

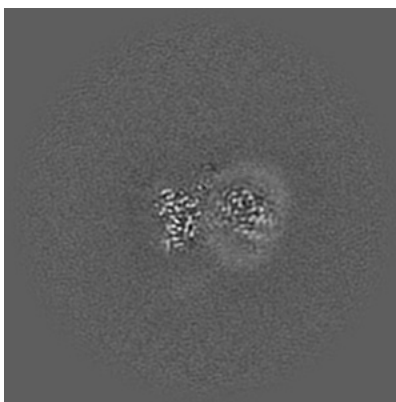
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

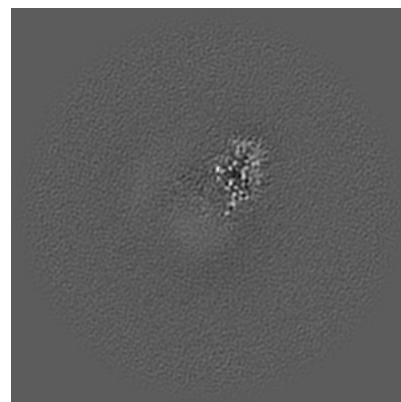
6.2.1 Primary map



X Index: 180



Y Index: 180

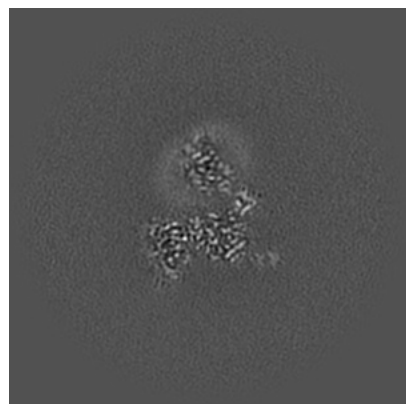


Z Index: 180

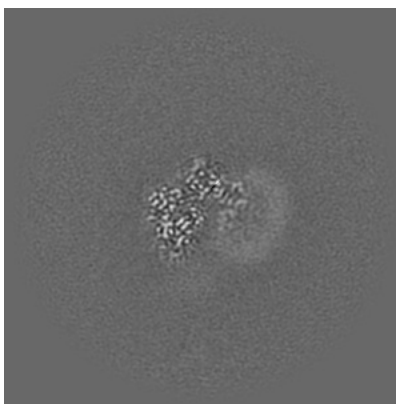
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

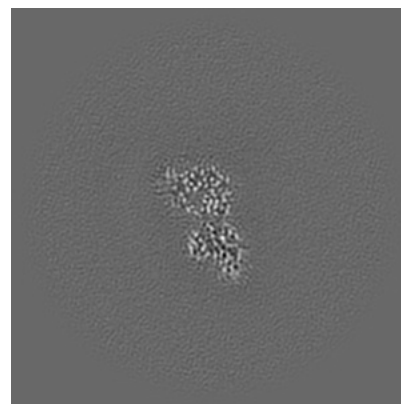
6.3.1 Primary map



X Index: 185



Y Index: 196

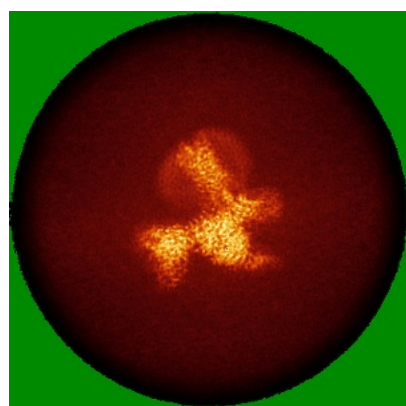


Z Index: 149

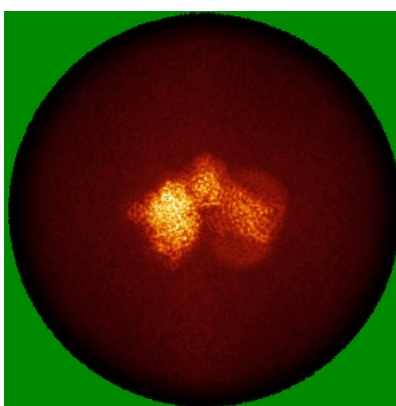
The images above show the largest variance slices of the map in three orthogonal directions.

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

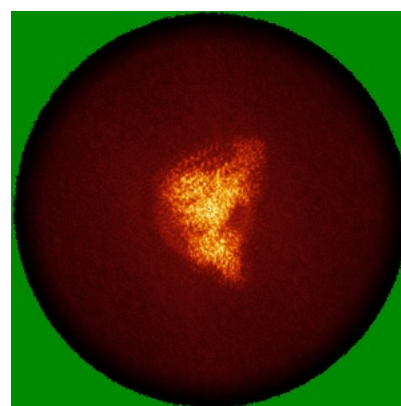
6.4.1 Primary map



X



Y

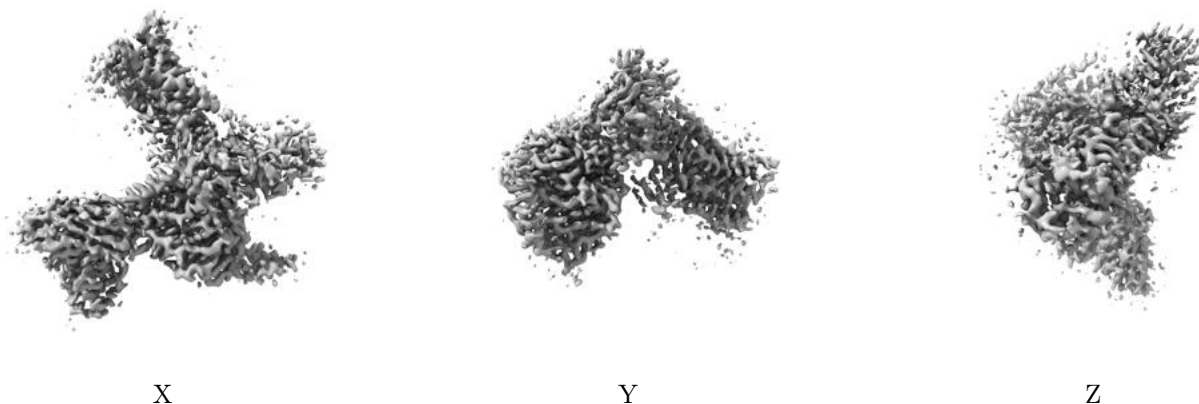


Z

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

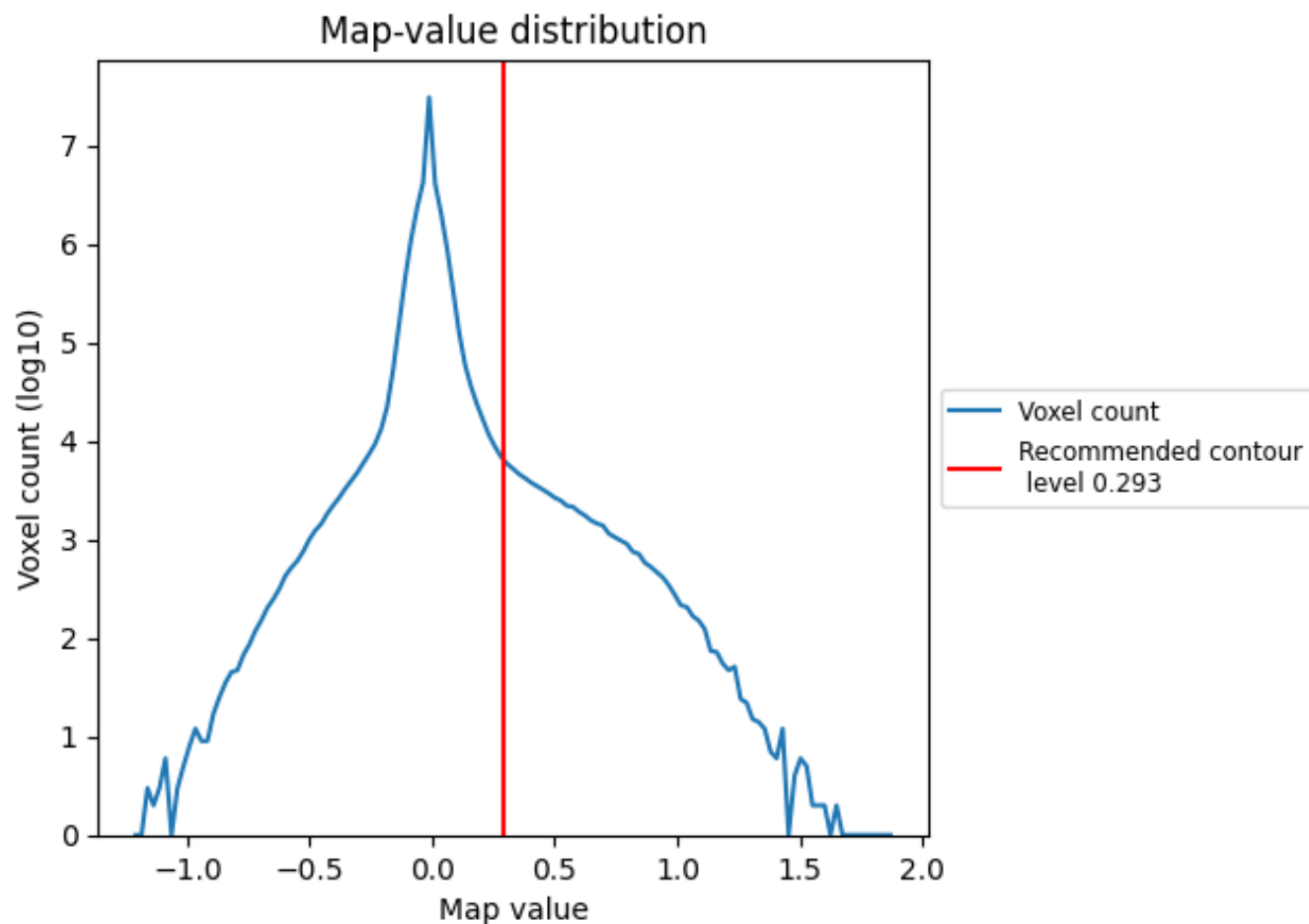
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

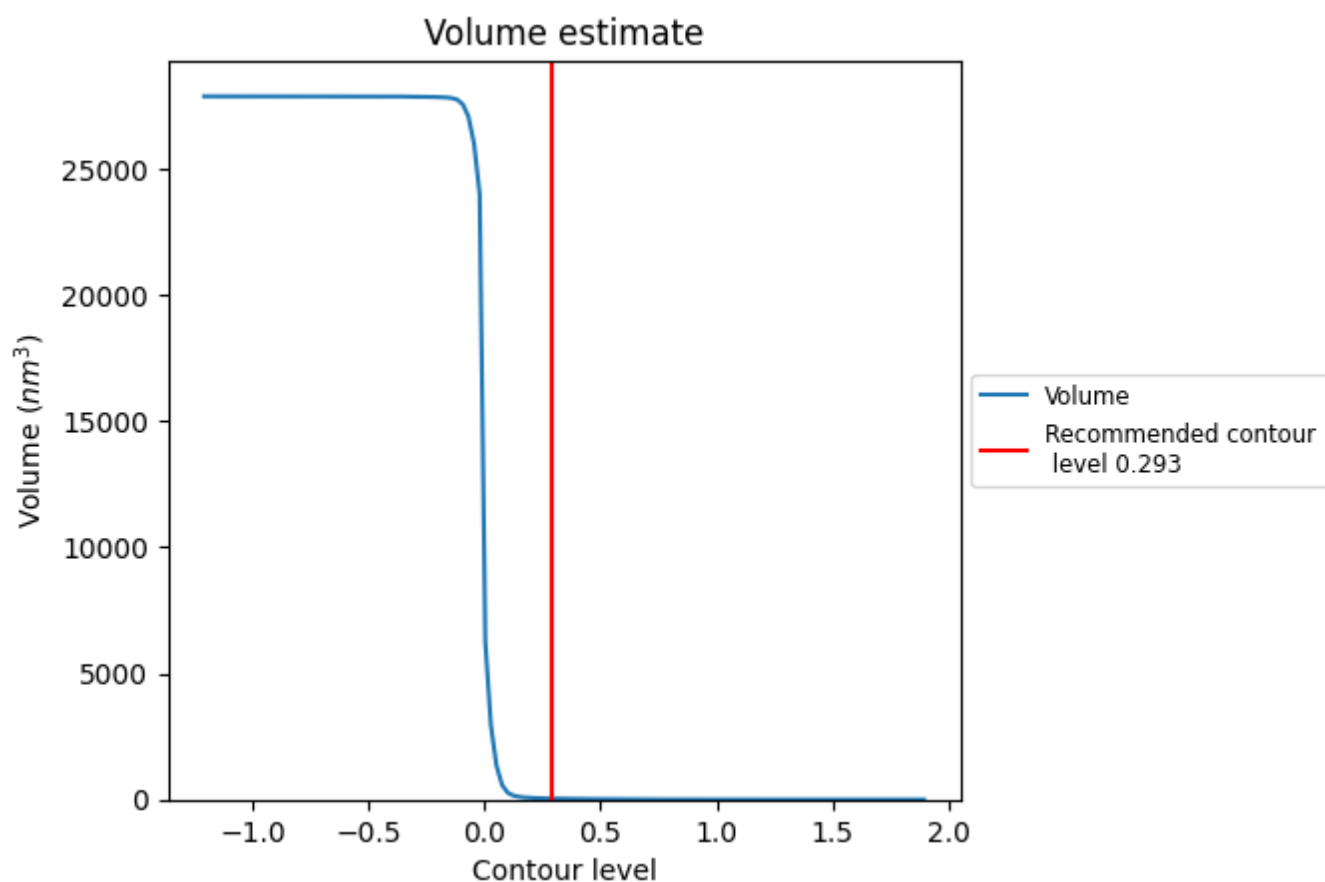
This section contains the results of statistical analysis of the map.

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.

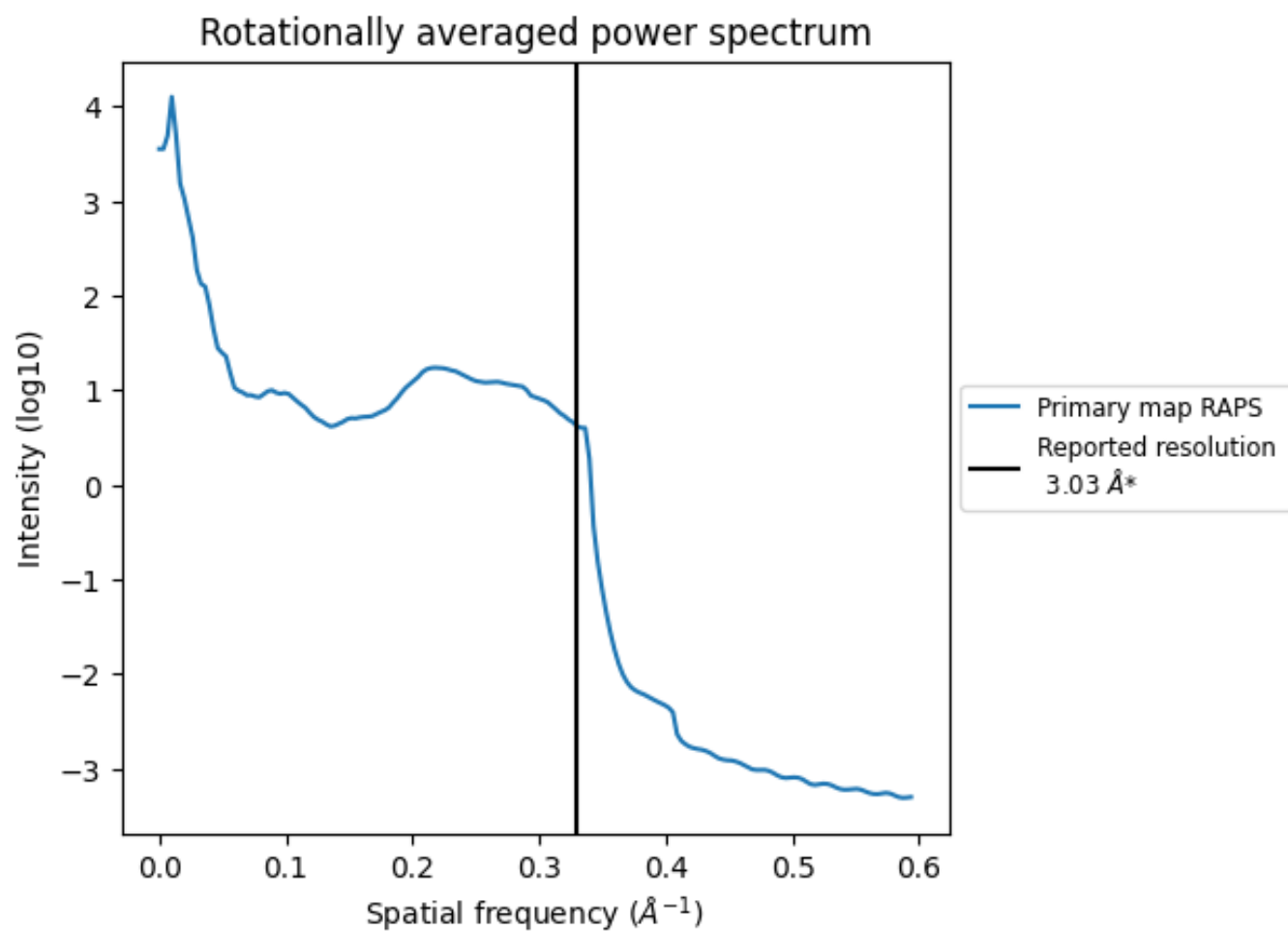
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm³; this corresponds to an approximate mass of 34 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 0.330 Å⁻¹

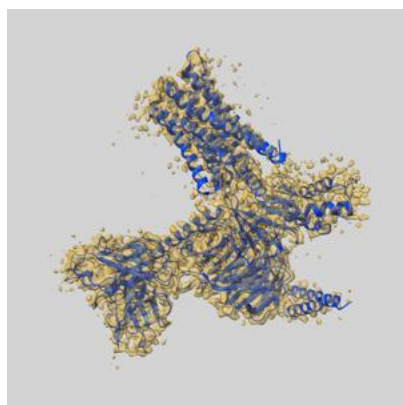
8 Fourier-Shell correlation

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

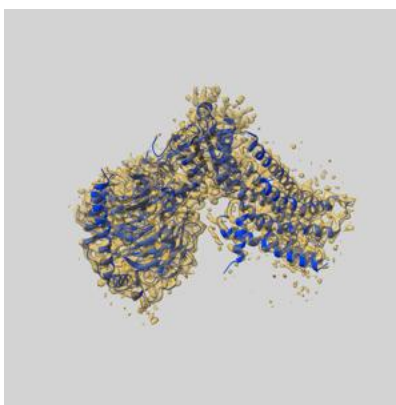
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55651 and PDB model 9T7Q. Per-residue inclusion information can be found in section [3](#) on page [7](#).

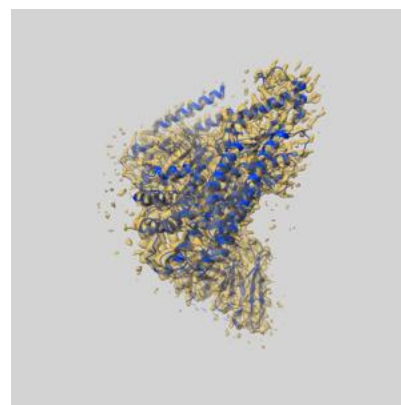
9.1 Map-model overlay [i](#)



X



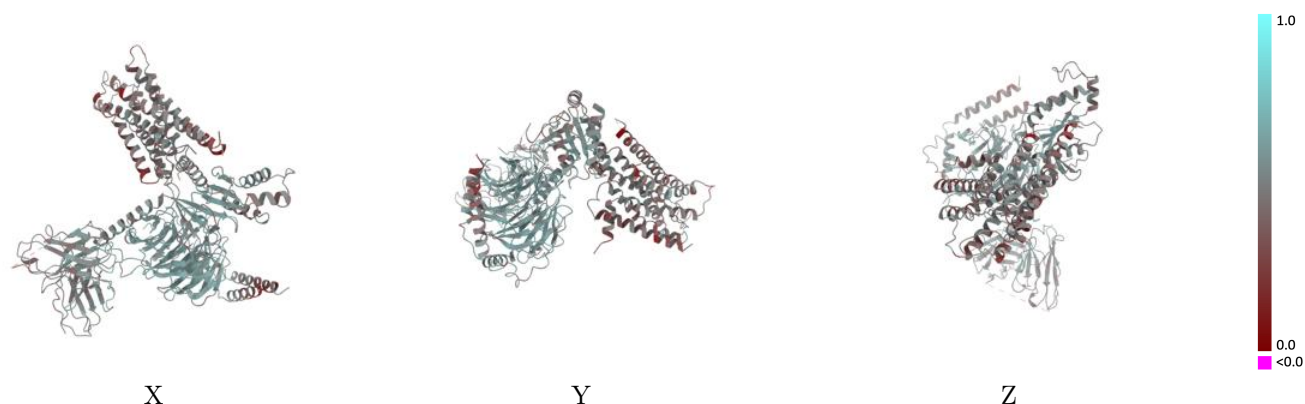
Y



Z

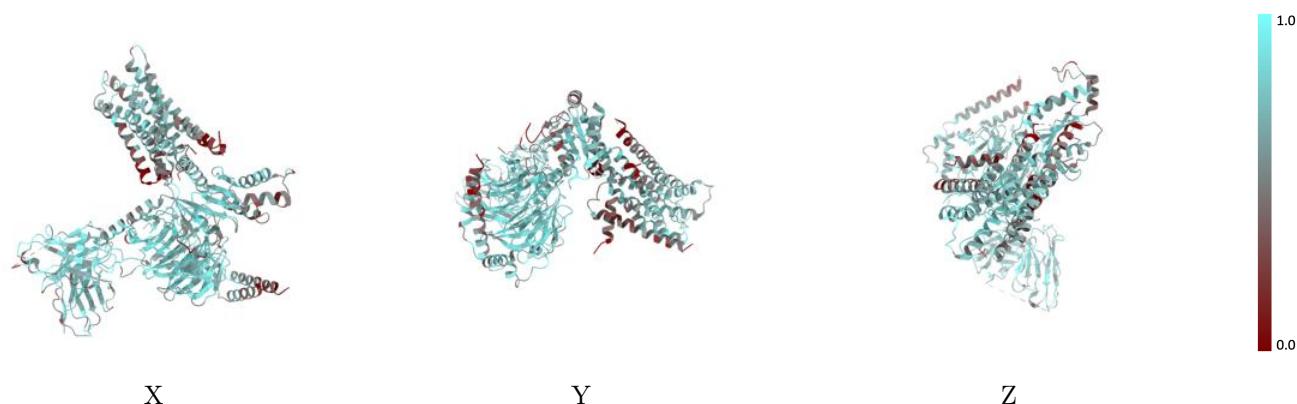
The images above show the 3D surface view of the map at the recommended contour level 0.293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



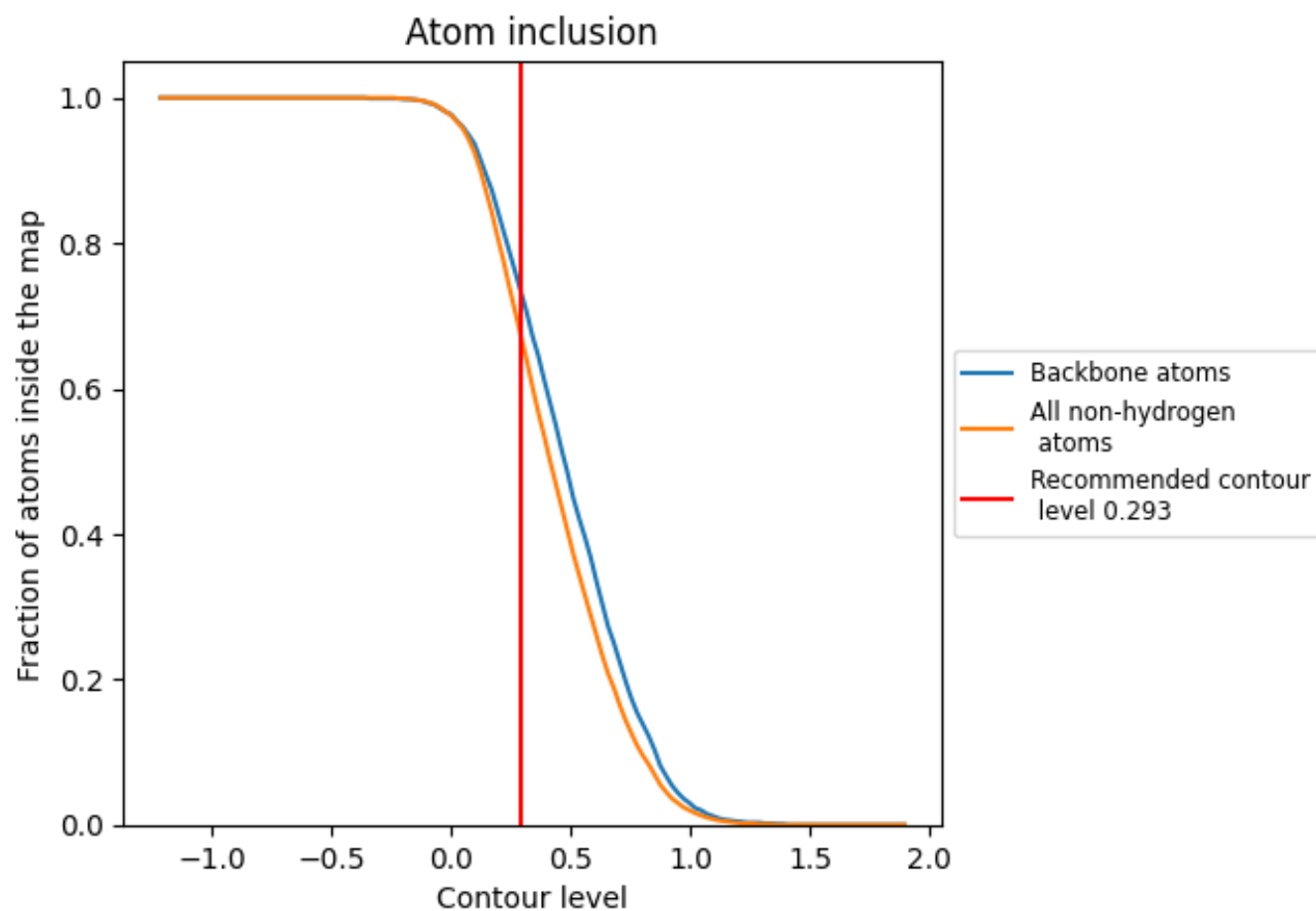
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.293).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.4980
A	0.6320	0.5000
B	0.7720	0.5650
C	0.6020	0.4830
R	0.5540	0.4150
S	0.7260	0.4970

