



Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 11:23 PM JST

PDB ID : 8WVY / pdb_00008wvy
EMDB ID : EMD-37876
Title : Cryo-EM structure of LGR4 in complex with Norrin
Authors : Lin, C.; Chang, Z.
Deposited on : 2023-10-24
Resolution : 3.29 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

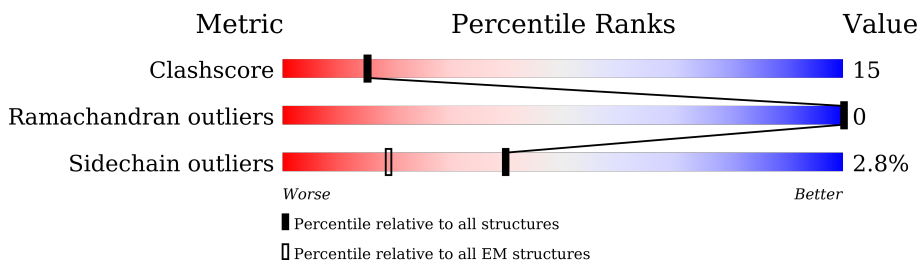
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	832	<div> <div>11%</div> <div>68%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
2	E	103	<div> <div>19%</div> <div>64%</div> <div>29%</div> <div>•</div> <div>•</div> </div>
2	F	103	<div> <div>23%</div> <div>35%</div> <div>48%</div> <div>14%</div> <div>•</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7241 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 Leucine-rich repeat-containing G-protein coupled receptor 4.

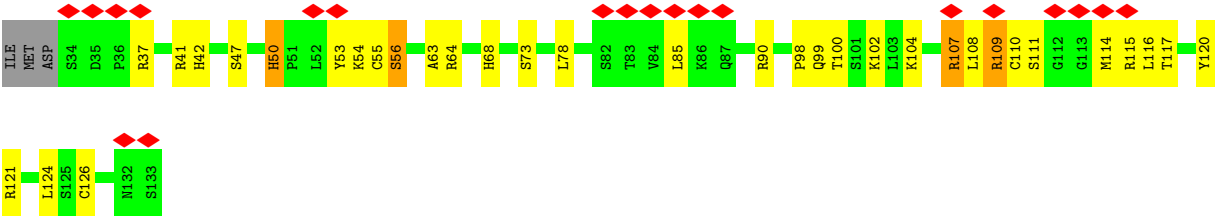
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	731	5671	3685	930	1027	29	0	0

There are 23 discrepancies between the modelled and reference sequences:

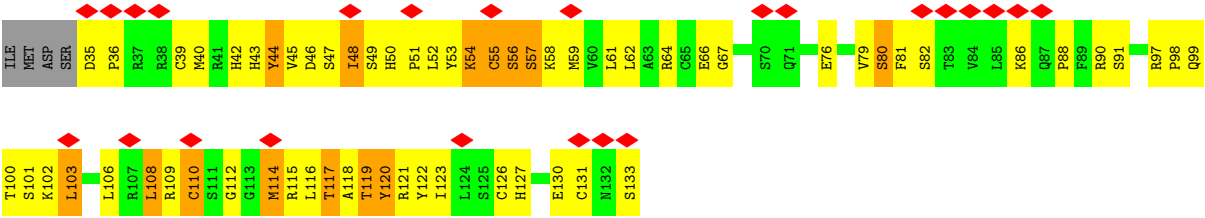
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9BXB1
A	2	LYS	-	expression tag	UNP Q9BXB1
A	3	THR	-	expression tag	UNP Q9BXB1
A	4	ILE	-	expression tag	UNP Q9BXB1
A	5	ILE	-	expression tag	UNP Q9BXB1
A	6	ALA	-	expression tag	UNP Q9BXB1
A	7	LEU	-	expression tag	UNP Q9BXB1
A	8	SER	-	expression tag	UNP Q9BXB1
A	9	TYR	-	expression tag	UNP Q9BXB1
A	10	ILE	-	expression tag	UNP Q9BXB1
A	11	PHE	-	expression tag	UNP Q9BXB1
A	12	CYS	-	expression tag	UNP Q9BXB1
A	13	LEU	-	expression tag	UNP Q9BXB1
A	14	VAL	-	expression tag	UNP Q9BXB1
A	15	PHE	-	expression tag	UNP Q9BXB1
A	16	ALA	-	expression tag	UNP Q9BXB1
A	17	ASP	-	expression tag	UNP Q9BXB1
A	18	TYR	-	expression tag	UNP Q9BXB1
A	19	LYS	-	expression tag	UNP Q9BXB1
A	20	ASP	-	expression tag	UNP Q9BXB1
A	21	ASP	-	expression tag	UNP Q9BXB1
A	22	ASP	-	expression tag	UNP Q9BXB1
A	23	ASP	-	expression tag	UNP Q9BXB1

- Molecule 2 is a protein called Norrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	100	Total	C	N	O	S	0	0
			788	480	154	140	14		
2	F	99	Total	C	N	O	S	0	0
			782	477	153	138	14		



• Molecule 2: Norrin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	584272	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 ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.615	Depositor
Minimum map value	-0.563	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.283	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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	0.85	42/5806 (0.7%)	0.84	36/7902 (0.5%)
2	E	0.76	4/804 (0.5%)	0.71	4/1078 (0.4%)
2	F	1.49	18/798 (2.3%)	1.67	28/1070 (2.6%)
All	All	0.93	64/7408 (0.9%)	0.95	68/10050 (0.7%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	100	THR	C-N	17.56	1.56	1.33
1	A	770	PRO	C-N	13.90	1.52	1.33
1	A	815	LEU	C-N	12.06	1.49	1.33
1	A	706	PHE	C-N	11.54	1.48	1.33
1	A	819	VAL	C-N	9.85	1.47	1.33
1	A	728	LEU	C-N	9.83	1.46	1.33
2	F	47	SER	C-N	9.55	1.45	1.33
2	F	40	MET	C-N	9.44	1.46	1.33
1	A	746	ILE	C-N	-9.32	1.21	1.33
2	F	64	ARG	C-N	-9.27	1.20	1.33
2	F	35	ASP	C-N	9.09	1.44	1.34
1	A	534	TYR	C-N	-8.74	1.22	1.33
1	A	726	THR	C-N	8.45	1.45	1.33
1	A	801	TYR	C-N	8.27	1.43	1.33
1	A	818	ARG	C-N	8.20	1.43	1.33
1	A	32	PRO	N-CD	-8.13	1.36	1.47
2	F	48	ILE	C-N	-8.12	1.23	1.33
1	A	709	THR	C-N	-8.09	1.23	1.33
2	F	57	SER	C-N	8.08	1.44	1.33
2	E	47	SER	C-N	8.00	1.43	1.33
2	F	90	ARG	C-N	7.90	1.43	1.33
2	E	120	TYR	C-N	-7.87	1.22	1.33
1	A	742	GLN	C-N	-7.82	1.23	1.33
2	F	110	CYS	C-N	-7.75	1.23	1.33
1	A	730	CYS	C-N	7.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	740	ASN	C-N	7.72	1.43	1.33
2	F	39	CYS	C-N	7.69	1.44	1.33
2	F	56	SER	C-N	-7.56	1.21	1.33
1	A	556	ASN	C-N	-7.32	1.24	1.33
1	A	526	THR	C-N	6.70	1.43	1.33
2	F	82	SER	C-N	6.67	1.43	1.33
2	F	67	GLY	C-N	6.58	1.42	1.33
1	A	535	LEU	C-N	-6.47	1.25	1.33
1	A	540	MET	C-N	6.38	1.42	1.33
1	A	699	GLY	C-N	-6.34	1.24	1.33
1	A	537	GLY	C-N	-6.34	1.24	1.33
1	A	704	LEU	C-N	-6.34	1.24	1.33
1	A	744	SER	C-N	6.32	1.42	1.33
1	A	782	MET	C-N	6.23	1.42	1.33
1	A	759	PHE	C-O	6.22	1.31	1.24
1	A	707	THR	C-N	6.22	1.41	1.33
1	A	764	ALA	C-O	6.13	1.31	1.24
2	F	59	MET	C-N	6.13	1.42	1.33
1	A	543	LEU	C-N	6.00	1.41	1.33
1	A	573	SER	C-N	-5.99	1.25	1.33
1	A	572	SER	C-N	5.91	1.41	1.33
1	A	713	LEU	C-N	-5.91	1.26	1.33
2	E	50	HIS	C-N	-5.81	1.26	1.34
2	F	46	ASP	C-N	-5.77	1.25	1.33
1	A	642	GLU	C-N	5.70	1.41	1.33
1	A	745	MET	C-N	-5.68	1.26	1.33
1	A	527	GLY	C-N	5.66	1.41	1.33
2	E	56	SER	C-N	5.63	1.40	1.33
1	A	727	LYS	C-N	5.59	1.42	1.33
1	A	536	LEU	C-N	5.54	1.41	1.33
1	A	544	THR	C-N	5.53	1.40	1.33
1	A	800	LEU	C-N	5.52	1.42	1.33
2	F	79	VAL	C-N	-5.49	1.26	1.33
1	A	774	ALA	C-N	5.43	1.41	1.33
2	F	44	TYR	C-N	-5.42	1.27	1.33
2	F	36	PRO	C-N	-5.37	1.25	1.33
1	A	561	LEU	C-N	5.31	1.41	1.34
1	A	777	ILE	C-N	5.22	1.41	1.33
1	A	710	LEU	C-N	-5.02	1.27	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	56	SER	O-C-N	-15.47	101.48	121.74
2	F	42	HIS	O-C-N	-12.88	106.20	122.43
2	F	56	SER	CA-C-N	12.21	142.51	122.73
2	F	56	SER	C-N-CA	12.21	142.51	122.73
1	A	726	THR	O-C-N	11.65	135.44	122.15
1	A	726	THR	CA-C-N	-10.24	106.55	120.28
1	A	726	THR	C-N-CA	-10.24	106.55	120.28
2	F	80	SER	O-C-N	-9.81	111.37	123.44
2	F	42	HIS	CA-C-N	9.63	138.18	122.29
2	F	42	HIS	C-N-CA	9.63	138.18	122.29
1	A	729	TYR	O-C-N	9.26	131.61	122.07
1	A	813	LYS	O-C-N	8.90	131.56	122.12
2	F	102	LYS	O-C-N	8.88	133.70	123.31
2	F	110	CYS	O-C-N	8.66	133.46	122.37
2	F	45	VAL	O-C-N	8.64	132.05	122.97
1	A	727	LYS	O-C-N	8.45	131.08	122.12
1	A	817	ARG	O-C-N	8.26	130.87	122.12
1	A	697	PRO	N-CA-C	-7.82	101.92	112.48
1	A	814	LEU	O-C-N	7.74	130.36	122.08
2	F	110	CYS	CA-C-N	-7.17	112.17	122.36
2	F	110	CYS	C-N-CA	-7.17	112.17	122.36
2	F	103	LEU	O-C-N	6.94	131.55	123.02
1	A	730	CYS	O-C-N	6.92	130.79	122.27
2	E	107	ARG	O-C-N	6.79	131.08	122.93
2	F	102	LYS	CA-C-N	-6.73	111.95	121.72
2	F	102	LYS	C-N-CA	-6.73	111.95	121.72
1	A	760	PHE	N-CA-C	-6.59	103.36	111.33
2	F	45	VAL	CA-C-N	-6.57	108.98	121.54
2	F	45	VAL	C-N-CA	-6.57	108.98	121.54
2	F	57	SER	O-C-N	6.49	131.19	123.27
1	A	811	ASP	O-C-N	6.29	128.79	122.12
1	A	762	PRO	CA-N-CD	-6.15	103.39	112.00
1	A	729	TYR	CA-C-N	-6.14	110.98	120.31
1	A	729	TYR	C-N-CA	-6.14	110.98	120.31
1	A	812	TRP	O-C-N	6.09	128.34	122.07
2	F	54	LYS	CA-C-O	-5.98	114.61	121.07
2	F	80	SER	CA-C-N	5.96	133.86	121.94
2	F	80	SER	C-N-CA	5.96	133.86	121.94
1	A	809	LYS	O-C-N	5.96	128.43	122.12
1	A	810	GLU	O-C-N	5.87	128.12	122.07
1	A	818	ARG	O-C-N	5.81	129.02	122.22
1	A	580	ILE	N-CA-C	-5.77	104.74	110.62
2	E	107	ARG	CA-C-N	-5.70	114.86	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	107	ARG	C-N-CA	-5.70	114.86	122.72
2	F	91	SER	O-C-N	-5.68	116.58	123.29
1	A	814	LEU	CA-C-N	-5.63	113.12	120.44
1	A	814	LEU	C-N-CA	-5.63	113.12	120.44
1	A	32	PRO	N-CA-CB	-5.60	97.36	103.25
1	A	704	LEU	O-C-N	5.59	129.35	122.20
1	A	32	PRO	CA-N-CD	5.58	119.82	112.00
1	A	716	LEU	O-C-N	-5.53	115.84	122.15
1	A	816	LYS	O-C-N	5.47	127.70	122.07
1	A	727	LYS	CA-C-N	-5.27	111.92	121.14
1	A	727	LYS	C-N-CA	-5.27	111.92	121.14
1	A	757	CYS	N-CA-C	5.24	120.01	111.37
2	F	76	GLU	O-C-N	-5.24	116.74	121.66
1	A	819	VAL	O-C-N	5.18	127.48	121.94
1	A	717	ALA	O-C-N	-5.17	116.64	122.12
1	A	728	LEU	CA-C-N	-5.10	113.81	120.44
1	A	728	LEU	C-N-CA	-5.10	113.81	120.44
2	E	47	SER	O-C-N	-5.10	117.41	123.22
2	F	103	LEU	CA-C-N	-5.05	114.33	122.82
2	F	103	LEU	C-N-CA	-5.05	114.33	122.82
1	A	817	ARG	CA-C-N	-5.05	113.01	120.28
1	A	817	ARG	C-N-CA	-5.05	113.01	120.28
2	F	47	SER	O-C-N	5.05	129.02	122.81
2	F	76	GLU	CA-C-N	5.04	125.02	120.03
2	F	76	GLU	C-N-CA	5.04	125.02	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5671	0	5682	123	0
2	E	788	0	776	30	0
2	F	782	0	774	65	0
All	All	7241	0	7232	210	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 15.

All (210) 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:758:ILE:O	1:A:762:PRO:HD3	1.37	1.22
1:A:412:LEU:HD12	1:A:412:LEU:O	1.44	1.17
2:F:80:SER:HB2	2:F:86:LYS:HE2	1.35	1.07
2:F:55:CYS:SG	2:F:109:ARG:C	2.42	1.03
2:F:55:CYS:SG	2:F:110:CYS:CA	2.48	1.02
1:A:759:PHE:O	1:A:762:PRO:HD2	1.58	1.01
2:F:55:CYS:SG	2:F:110:CYS:N	2.37	0.97
2:F:48:ILE:O	2:F:57:SER:HA	1.63	0.97
2:F:101:SER:HB2	2:F:121:ARG:HB3	1.46	0.95
2:F:55:CYS:SG	2:F:110:CYS:HA	2.07	0.95
1:A:801:TYR:CE2	1:A:812:TRP:HZ3	1.85	0.93
2:F:43:HIS:HB3	2:F:61:LEU:HD11	1.51	0.91
1:A:801:TYR:CE2	1:A:812:TRP:CZ3	2.59	0.91
1:A:728:LEU:HA	1:A:731:ASN:HB3	1.53	0.89
2:E:50:HIS:CD2	2:E:116:LEU:HD13	2.09	0.87
1:A:31:ALA:HB3	1:A:32:PRO:HD3	1.55	0.87
1:A:758:ILE:O	1:A:761:CYS:HB2	1.74	0.87
2:F:52:LEU:HD12	2:F:52:LEU:H	1.39	0.86
2:F:101:SER:OG	2:F:121:ARG:HD3	1.76	0.86
2:E:102:LYS:NZ	2:E:104:LYS:HE3	1.93	0.84
1:A:801:TYR:CD2	1:A:812:TRP:HZ3	1.95	0.84
1:A:812:TRP:CD1	1:A:813:LYS:N	2.49	0.81
1:A:809:LYS:HA	1:A:812:TRP:CE3	2.16	0.81
2:F:130:GLU:HB2	2:F:133:SER:HB3	1.65	0.79
2:F:114:MET:HE2	2:F:115:ARG:O	1.82	0.78
1:A:412:LEU:CD1	1:A:415:ILE:HG21	2.14	0.77
2:F:80:SER:HB2	2:F:86:LYS:CE	2.14	0.77
2:E:55:CYS:HA	2:E:110:CYS:HA	1.68	0.75
2:F:109:ARG:HA	2:F:115:ARG:HD2	1.66	0.75
2:F:55:CYS:SG	2:F:109:ARG:O	2.43	0.75
2:F:55:CYS:HA	2:F:110:CYS:HA	1.70	0.73
1:A:725:TYR:O	1:A:729:TYR:N	2.23	0.72
1:A:801:TYR:CD2	1:A:812:TRP:CZ3	2.79	0.71
2:E:102:LYS:NZ	2:E:104:LYS:CE	2.54	0.70
1:A:759:PHE:C	1:A:762:PRO:HD2	2.17	0.69
2:F:50:HIS:CB	2:F:110:CYS:SG	2.81	0.68
1:A:750:ALA:HA	1:A:753:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:SER:CB	2:F:86:LYS:HE2	2.21	0.67
1:A:412:LEU:O	1:A:412:LEU:CD1	2.33	0.67
1:A:686:GLU:OE1	1:A:703:SER:OG	2.05	0.67
1:A:696:PHE:HZ	1:A:790:PHE:CD1	2.14	0.66
1:A:759:PHE:CE1	1:A:792:LEU:HD23	2.32	0.65
2:E:121:ARG:HD2	2:F:88:PRO:HB3	1.79	0.65
2:F:50:HIS:HB3	2:F:110:CYS:SG	2.37	0.65
1:A:391:LEU:HD23	1:A:412:LEU:HD22	1.78	0.64
2:E:54:LYS:O	2:E:111:SER:N	2.25	0.63
1:A:815:LEU:O	1:A:819:VAL:HG23	1.98	0.63
1:A:70:THR:HG22	1:A:92:ASP:HB3	1.82	0.62
1:A:749:VAL:O	1:A:753:ILE:HG23	1.99	0.62
2:E:102:LYS:HZ2	2:E:104:LYS:HE3	1.65	0.62
2:E:110:CYS:HB2	2:E:114:MET:HB3	1.81	0.62
2:F:101:SER:CB	2:F:121:ARG:HD3	2.29	0.62
1:A:644:SER:HA	1:A:728:LEU:HD21	1.81	0.60
2:F:51:PRO:HG2	2:F:52:LEU:HD12	1.83	0.60
1:A:816:LYS:O	1:A:819:VAL:HB	2.02	0.60
1:A:528:ALA:O	1:A:783:LYS:NZ	2.31	0.60
2:F:56:SER:N	2:F:109:ARG:O	2.33	0.60
2:F:55:CYS:SG	2:F:110:CYS:CB	2.89	0.59
1:A:812:TRP:HD1	1:A:813:LYS:N	1.95	0.59
1:A:684:ARG:HA	1:A:684:ARG:HH11	1.68	0.59
2:E:53:TYR:CD1	2:E:114:MET:HE1	2.37	0.59
2:F:55:CYS:HG	2:F:110:CYS:HG	0.62	0.59
1:A:766:PHE:HE2	1:A:782:MET:HA	1.68	0.58
1:A:766:PHE:CE2	1:A:782:MET:HA	2.39	0.57
1:A:417:ASN:HD22	1:A:438:GLN:HB3	1.70	0.56
1:A:32:PRO:O	1:A:46:LYS:HD3	2.04	0.56
1:A:467:ALA:HB1	1:A:526:THR:HG22	1.87	0.56
1:A:802:VAL:HA	1:A:812:TRP:HH2	1.70	0.56
1:A:536:LEU:HD13	1:A:545:VAL:HG21	1.87	0.56
1:A:704:LEU:HD12	1:A:708:VAL:HG23	1.86	0.55
1:A:802:VAL:HA	1:A:812:TRP:CH2	2.40	0.55
1:A:32:PRO:CB	1:A:46:LYS:HE2	2.36	0.55
2:F:43:HIS:HB3	2:F:61:LEU:CD1	2.33	0.55
1:A:530:LYS:NZ	1:A:613:GLU:OE2	2.40	0.55
1:A:726:THR:HA	1:A:729:TYR:HB3	1.88	0.55
1:A:373:GLN:OE1	1:A:398:ARG:NH2	2.39	0.55
1:A:809:LYS:HA	1:A:812:TRP:CD2	2.41	0.55
2:F:116:LEU:N	2:F:116:LEU:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:LEU:HD22	2:F:81:PHE:HE1	1.72	0.54
1:A:758:ILE:O	1:A:762:PRO:CD	2.32	0.53
1:A:227:LEU:HD23	1:A:247:LEU:HD13	1.90	0.53
1:A:578:GLY:O	1:A:582:VAL:HG23	2.08	0.53
2:F:55:CYS:CA	2:F:110:CYS:HA	2.36	0.53
2:F:116:LEU:O	2:F:117:THR:HB	2.07	0.53
1:A:412:LEU:CD1	1:A:415:ILE:CG2	2.85	0.52
1:A:542:ARG:CZ	1:A:602:TRP:HZ3	2.22	0.52
1:A:531:PRO:O	1:A:605:PHE:HD2	1.94	0.51
1:A:536:LEU:HD13	1:A:545:VAL:CG2	2.41	0.51
2:E:56:SER:HB2	2:E:109:ARG:HH12	1.75	0.51
2:F:52:LEU:H	2:F:52:LEU:CD1	2.17	0.51
2:E:54:LYS:HD2	2:E:111:SER:HB3	1.93	0.51
2:F:55:CYS:HA	2:F:109:ARG:O	2.10	0.51
1:A:31:ALA:CB	1:A:32:PRO:HD3	2.29	0.50
1:A:696:PHE:C	1:A:698:THR:N	2.69	0.50
2:F:43:HIS:CD2	2:F:61:LEU:HD21	2.47	0.50
1:A:696:PHE:O	1:A:698:THR:N	2.43	0.50
1:A:759:PHE:C	1:A:762:PRO:CD	2.85	0.50
1:A:695:PRO:O	1:A:707:THR:OG1	2.30	0.50
2:F:44:TYR:CE2	2:F:62:LEU:HD12	2.46	0.50
1:A:681:LEU:HD23	1:A:681:LEU:O	2.12	0.49
1:A:161:ASP:O	1:A:163:ASN:ND2	2.46	0.49
1:A:747:LYS:O	1:A:750:ALA:HB3	2.13	0.49
2:F:98:PRO:HG3	2:F:123:ILE:HD13	1.95	0.49
1:A:765:PHE:O	1:A:766:PHE:C	2.54	0.49
1:A:34:SER:O	1:A:35:CYS:SG	2.71	0.49
1:A:32:PRO:O	1:A:46:LYS:CD	2.60	0.49
2:F:50:HIS:HB2	2:F:110:CYS:SG	2.53	0.48
2:F:55:CYS:CB	2:F:110:CYS:HA	2.42	0.48
1:A:811:ASP:O	1:A:814:LEU:HB3	2.13	0.48
2:F:54:LYS:O	2:F:110:CYS:CA	2.62	0.48
2:F:112:GLY:H	2:F:115:ARG:NH1	2.12	0.48
2:F:49:SER:OG	2:F:56:SER:O	2.31	0.48
2:F:54:LYS:O	2:F:110:CYS:HA	2.12	0.48
1:A:539:TRP:O	1:A:543:LEU:HG	2.14	0.48
1:A:135:ARG:HA	1:A:159:TRP:HB2	1.96	0.48
1:A:694:LEU:O	1:A:697:PRO:HD3	2.14	0.48
1:A:704:LEU:CD1	1:A:708:VAL:CG2	2.92	0.48
2:F:106:LEU:HG	2:F:108:LEU:HD23	1.95	0.48
1:A:723:VAL:O	1:A:727:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:PHE:HD2	1:A:782:MET:HG3	1.77	0.47
1:A:35:CYS:HA	1:A:41:VAL:HG22	1.97	0.47
2:F:122:TYR:O	2:F:123:ILE:C	2.58	0.47
2:E:102:LYS:HZ1	2:E:104:LYS:HE3	1.78	0.47
1:A:696:PHE:N	1:A:697:PRO:CD	2.78	0.47
1:A:726:THR:HA	1:A:729:TYR:CB	2.45	0.46
1:A:412:LEU:HD13	1:A:415:ILE:HG21	1.94	0.46
2:F:55:CYS:HG	2:F:110:CYS:CB	2.16	0.46
2:F:99:GLN:HB2	2:F:127:HIS:ND1	2.30	0.46
1:A:456:PHE:HB2	1:A:473:PHE:HE2	1.81	0.46
2:E:121:ARG:HD2	2:F:88:PRO:CB	2.44	0.46
1:A:135:ARG:HG2	1:A:159:TRP:CE3	2.50	0.46
1:A:138:ALA:H	1:A:162:ASP:HB2	1.81	0.46
1:A:459:LEU:HD21	1:A:462:LEU:HB2	1.97	0.46
1:A:740:ASN:OD1	1:A:740:ASN:N	2.48	0.46
2:F:43:HIS:HD2	2:F:61:LEU:HD21	1.80	0.46
2:F:97:ARG:NH2	2:F:131:CYS:SG	2.89	0.46
1:A:31:ALA:CB	1:A:32:PRO:CD	2.94	0.46
1:A:275:ARG:HG2	1:A:297:ASP:HB3	1.97	0.46
1:A:812:TRP:CD1	1:A:812:TRP:C	2.94	0.46
2:E:85:LEU:HD13	2:F:103:LEU:HD11	1.97	0.46
2:E:37:ARG:O	2:E:68:HIS:N	2.49	0.46
2:E:114:MET:HG2	2:E:116:LEU:HG	1.98	0.46
2:F:114:MET:HB2	2:F:114:MET:HE3	1.71	0.46
1:A:364:CYS:HB3	1:A:367:LEU:HB2	1.97	0.45
1:A:334:ILE:HD11	1:A:355:ILE:HD13	1.98	0.45
1:A:696:PHE:C	1:A:698:THR:H	2.25	0.45
1:A:536:LEU:HD12	1:A:542:ARG:HG3	1.98	0.45
2:F:52:LEU:HD12	2:F:52:LEU:N	2.19	0.45
1:A:216:LEU:HD12	1:A:241:PRO:HB3	1.98	0.45
1:A:171:HIS:HB3	1:A:172:PRO:HD3	1.99	0.45
1:A:704:LEU:HD12	1:A:708:VAL:CG2	2.46	0.45
2:F:54:LYS:O	2:F:110:CYS:O	2.35	0.45
1:A:74:GLU:HG3	1:A:99:LYS:HB2	1.98	0.45
2:F:50:HIS:CE1	2:F:52:LEU:HD13	2.51	0.45
2:F:43:HIS:CB	2:F:61:LEU:HD11	2.37	0.44
2:E:107:ARG:HB3	2:E:115:ARG:NH1	2.32	0.44
1:A:162:ASP:OD1	1:A:162:ASP:N	2.47	0.44
1:A:318:THR:O	1:A:342:GLN:NE2	2.51	0.44
1:A:38:ASP:OD1	1:A:40:ARG:HG3	2.18	0.44
1:A:759:PHE:HA	1:A:762:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:HIS:N	2:E:64:ARG:O	2.34	0.44
1:A:302:VAL:HA	1:A:325:THR:HB	1.99	0.44
1:A:714:ASN:HB2	1:A:760:PHE:CZ	2.52	0.44
2:F:114:MET:CE	2:F:115:ARG:O	2.61	0.44
1:A:552:ALA:O	1:A:556:ASN:ND2	2.51	0.44
1:A:686:GLU:OE1	1:A:686:GLU:HA	2.18	0.43
2:F:120:TYR:N	2:F:120:TYR:CD1	2.86	0.43
2:E:54:LYS:HB3	2:E:111:SER:OG	2.19	0.43
2:E:107:ARG:HE	2:E:115:ARG:NH2	2.16	0.43
1:A:537:GLY:HA3	1:A:541:ILE:HD11	1.99	0.43
1:A:696:PHE:N	1:A:697:PRO:HD3	2.34	0.43
1:A:772:ILE:C	1:A:774:ALA:H	2.27	0.43
2:E:41:ARG:HD2	2:E:63:ALA:HB1	2.00	0.43
2:F:53:TYR:O	2:F:54:LYS:C	2.62	0.43
1:A:40:ARG:NH2	2:E:124:LEU:HD22	2.34	0.43
1:A:185:ALA:O	1:A:187:ASN:ND2	2.51	0.43
1:A:587:MET:HB2	1:A:628:SER:OG	2.18	0.42
2:E:85:LEU:HD11	2:F:119:THR:HG21	2.01	0.42
1:A:704:LEU:HD12	1:A:704:LEU:HA	1.88	0.42
1:A:724:ILE:O	1:A:728:LEU:HD13	2.19	0.42
1:A:137:ASP:OD1	1:A:137:ASP:N	2.50	0.42
2:F:119:THR:C	2:F:120:TYR:HD1	2.27	0.42
1:A:704:LEU:HG	1:A:708:VAL:HG21	2.00	0.42
2:E:73:SER:O	2:F:66:GLU:HA	2.19	0.42
2:E:50:HIS:NE2	2:E:116:LEU:HD13	2.35	0.42
2:F:44:TYR:CZ	2:F:62:LEU:HD12	2.55	0.42
1:A:31:ALA:HB3	1:A:32:PRO:CD	2.36	0.41
1:A:555:PHE:HB3	1:A:798:PRO:HB2	2.01	0.41
1:A:814:LEU:C	1:A:814:LEU:HD13	2.45	0.41
2:F:55:CYS:CA	2:F:109:ARG:O	2.68	0.41
1:A:694:LEU:HD21	1:A:790:PHE:CE2	2.54	0.41
1:A:697:PRO:C	1:A:699:GLY:H	2.28	0.41
1:A:541:ILE:H	1:A:541:ILE:HG12	1.71	0.41
1:A:307:SER:O	1:A:330:LYS:NZ	2.39	0.41
1:A:692:LEU:HD13	1:A:787:LEU:HD21	2.01	0.41
1:A:696:PHE:O	1:A:696:PHE:HD1	2.04	0.41
2:E:78:LEU:HD21	2:E:90:ARG:HB2	2.01	0.41
1:A:41:VAL:HG11	1:A:55:LEU:HD13	2.02	0.41
1:A:319:VAL:HA	1:A:342:GLN:HG2	2.03	0.41
1:A:812:TRP:CD1	1:A:813:LYS:HG2	2.55	0.41
2:F:58:LYS:HD2	2:F:106:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:PHE:O	1:A:710:LEU:HB2	2.21	0.41
2:F:117:THR:HG23	2:F:118:ALA:N	2.35	0.41
1:A:574:LYS:NZ	1:A:745:MET:HE1	2.36	0.40
2:E:99:GLN:HG2	2:E:100:THR:HG23	2.02	0.40
2:E:117:THR:O	2:F:81:PHE:HA	2.20	0.40
1:A:644:SER:CA	1:A:728:LEU:HD21	2.50	0.40
2:E:98:PRO:HA	2:E:126:CYS:SG	2.61	0.40
1:A:812:TRP:NE1	1:A:813:LYS:HG2	2.36	0.40
1:A:816:LYS:O	1:A:820:THR:N	2.43	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	721/832 (87%)	680 (94%)	41 (6%)	0	100	100
2	E	98/103 (95%)	97 (99%)	1 (1%)	0	100	100
2	F	97/103 (94%)	85 (88%)	12 (12%)	0	100	100
All	All	916/1038 (88%)	862 (94%)	54 (6%)	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	635/730 (87%)	620 (98%)	15 (2%)	44	68
2	E	93/96 (97%)	92 (99%)	1 (1%)	70	82
2	F	92/96 (96%)	85 (92%)	7 (8%)	11	34
All	All	820/922 (89%)	797 (97%)	23 (3%)	40	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	162	ASP
1	A	279	LEU
1	A	442	VAL
1	A	541	ILE
1	A	568	THR
1	A	577	ILE
1	A	580	ILE
1	A	610	ILE
1	A	660	LYS
1	A	693	CYS
1	A	725	TYR
1	A	753	ILE
1	A	812	TRP
1	A	813	LYS
2	E	109	ARG
2	F	55	CYS
2	F	108	LEU
2	F	114	MET
2	F	117	THR
2	F	119	THR
2	F	120	TYR
2	F	126	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	71	GLN
1	A	163	ASN
1	A	226	ASN
1	A	233	ASN
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	278	HIS
1	A	311	GLN
1	A	342	GLN
1	A	379	GLN
1	A	386	GLN
1	A	417	ASN
1	A	444	ASN
1	A	556	ASN
1	A	740	ASN
2	E	87	GLN
2	E	127	HIS
2	F	43	HIS
2	F	50	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](#)

There are no ligands in this entry.

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.

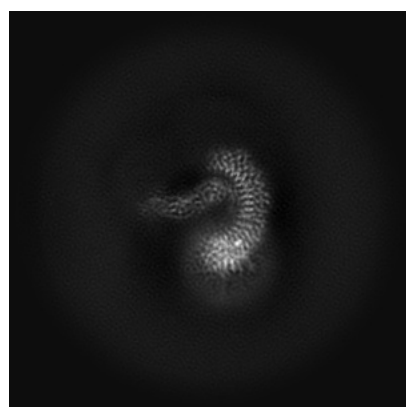
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37876. These allow visual inspection of the internal detail of the map and identification of artifacts.

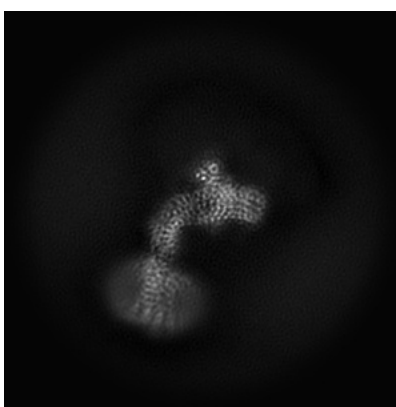
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

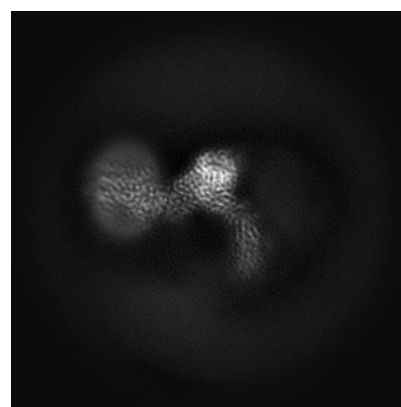
6.1.1 Primary map



X



Y

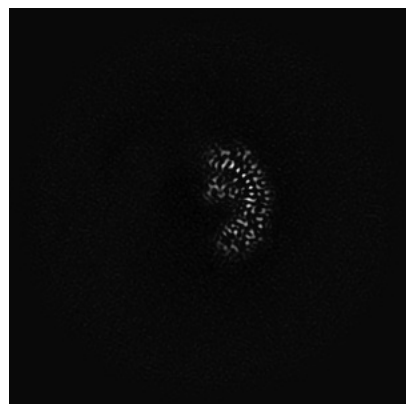


Z

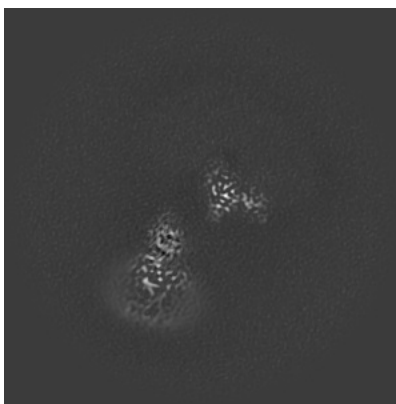
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

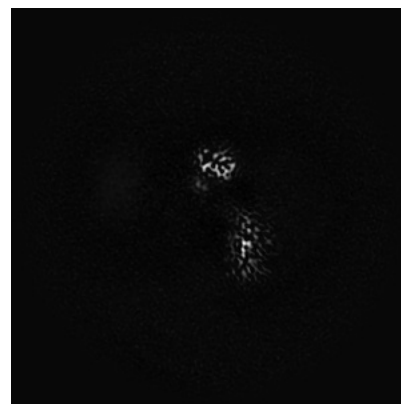
6.2.1 Primary map



X Index: 180



Y Index: 180

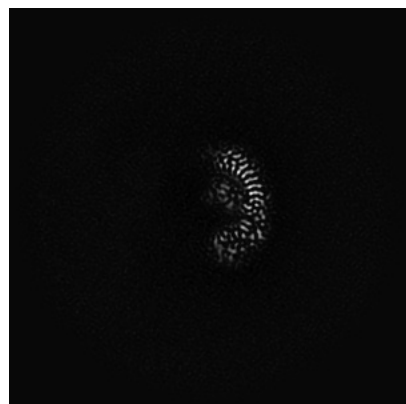


Z Index: 180

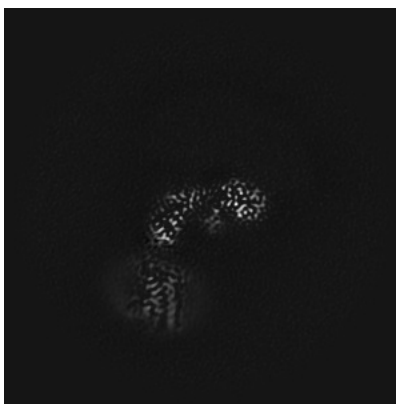
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

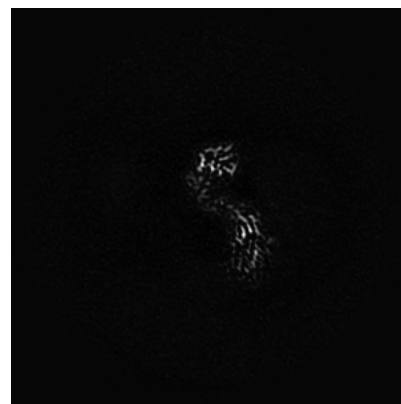
6.3.1 Primary map



X Index: 173



Y Index: 206

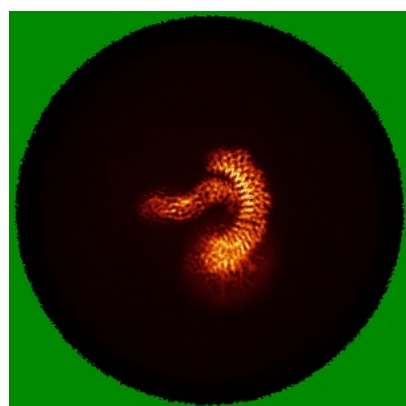


Z Index: 187

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

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

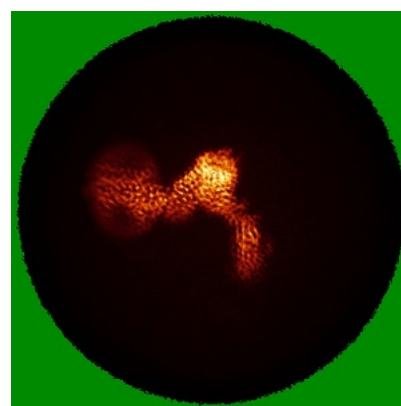
6.4.1 Primary map



X



Y

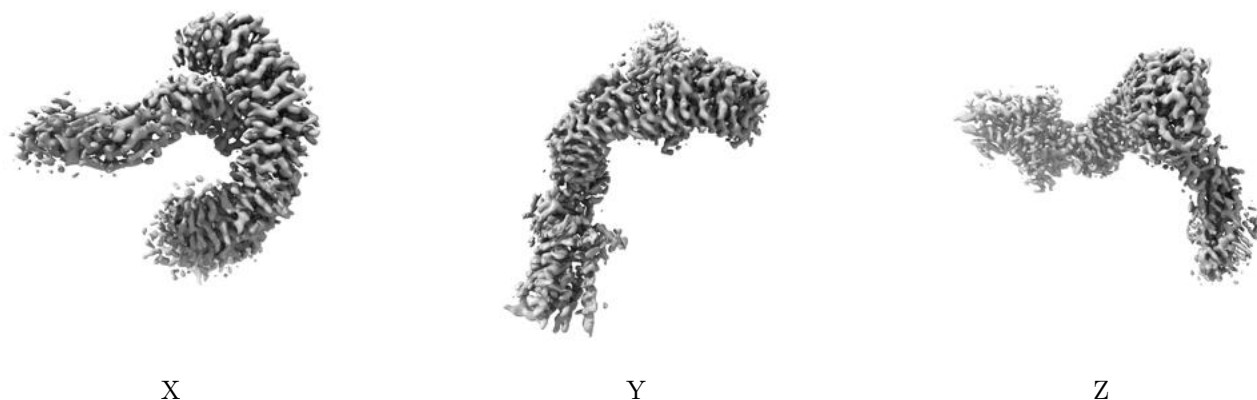


Z

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

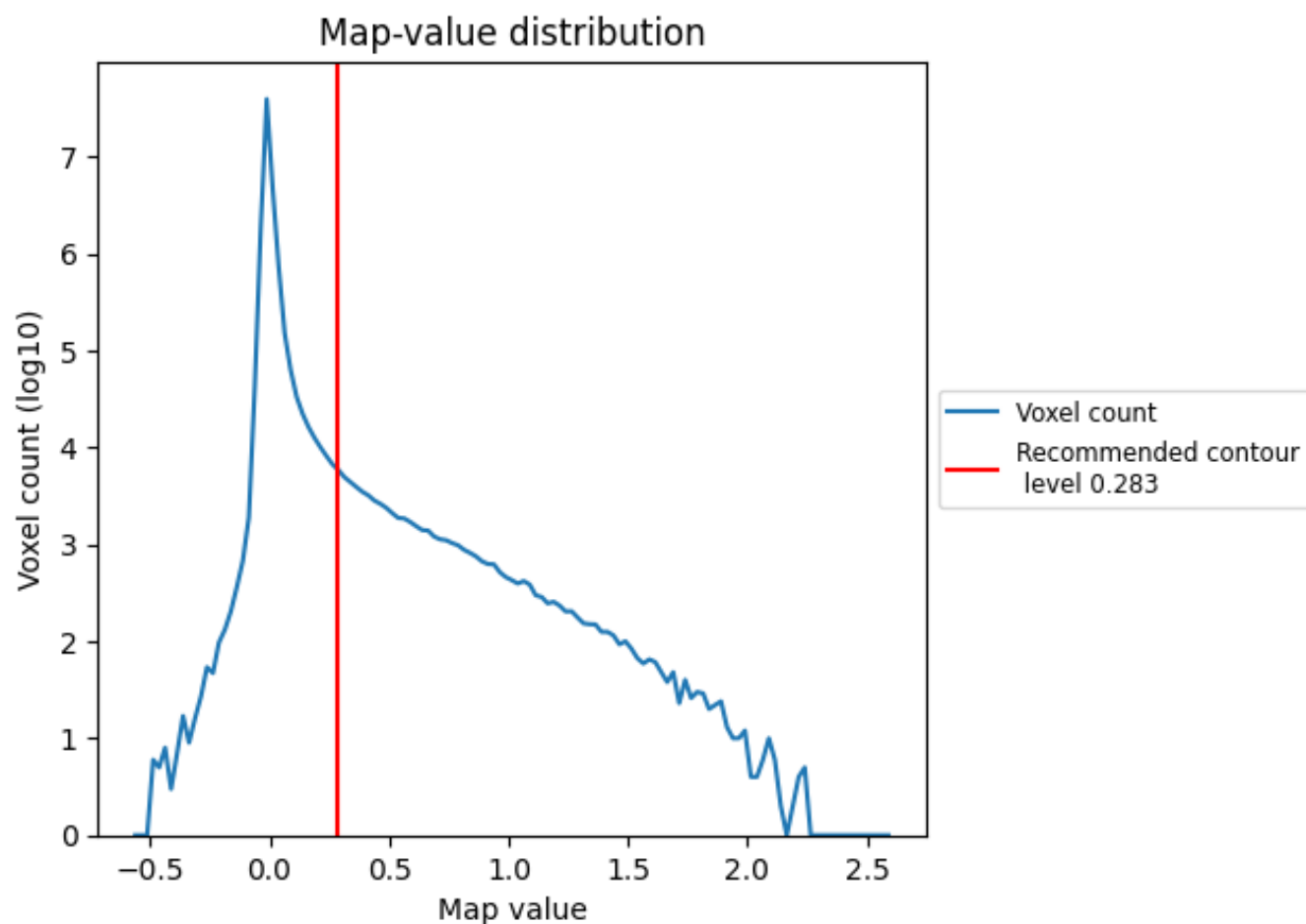
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

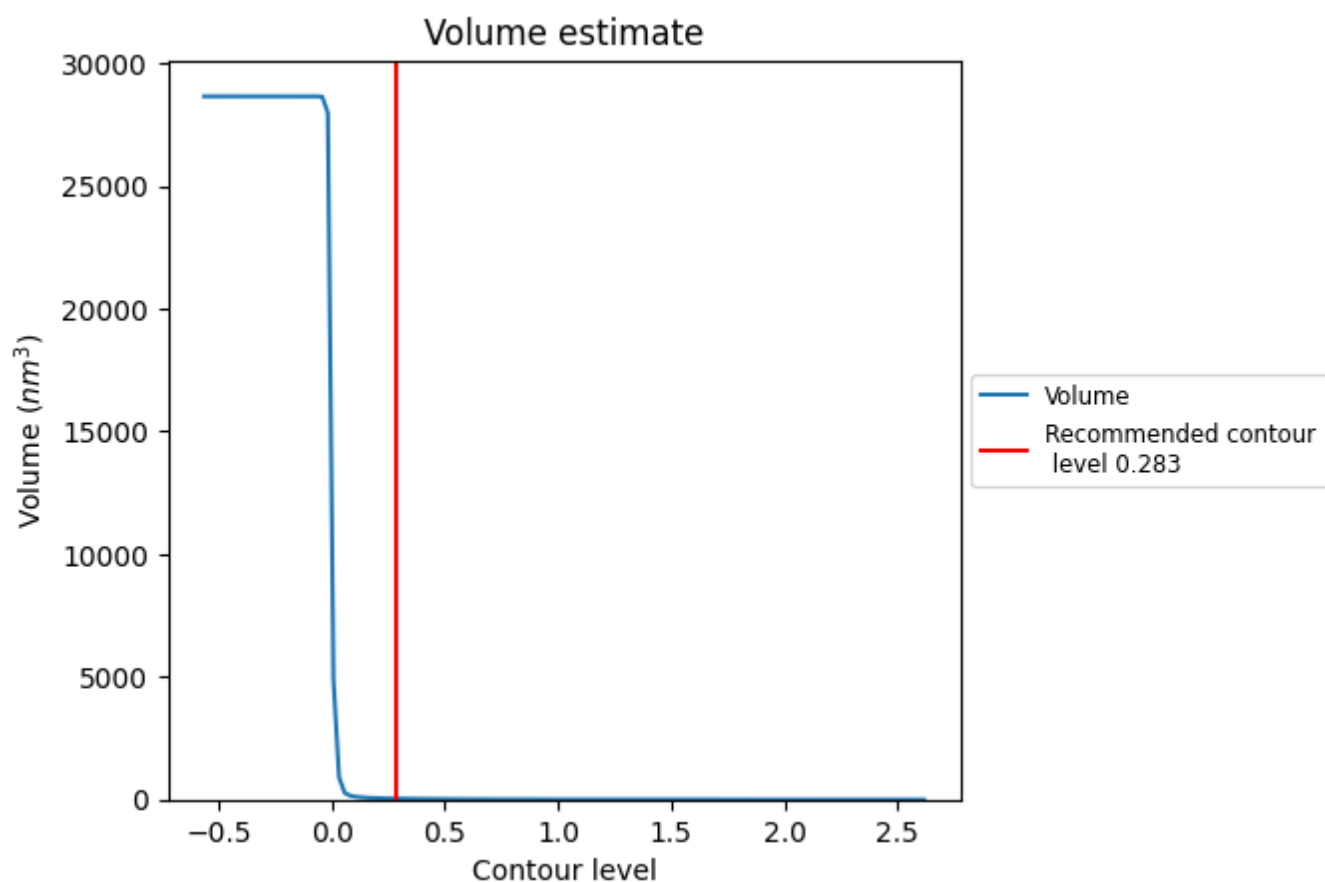
This section contains the results of statistical analysis of the map.

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.

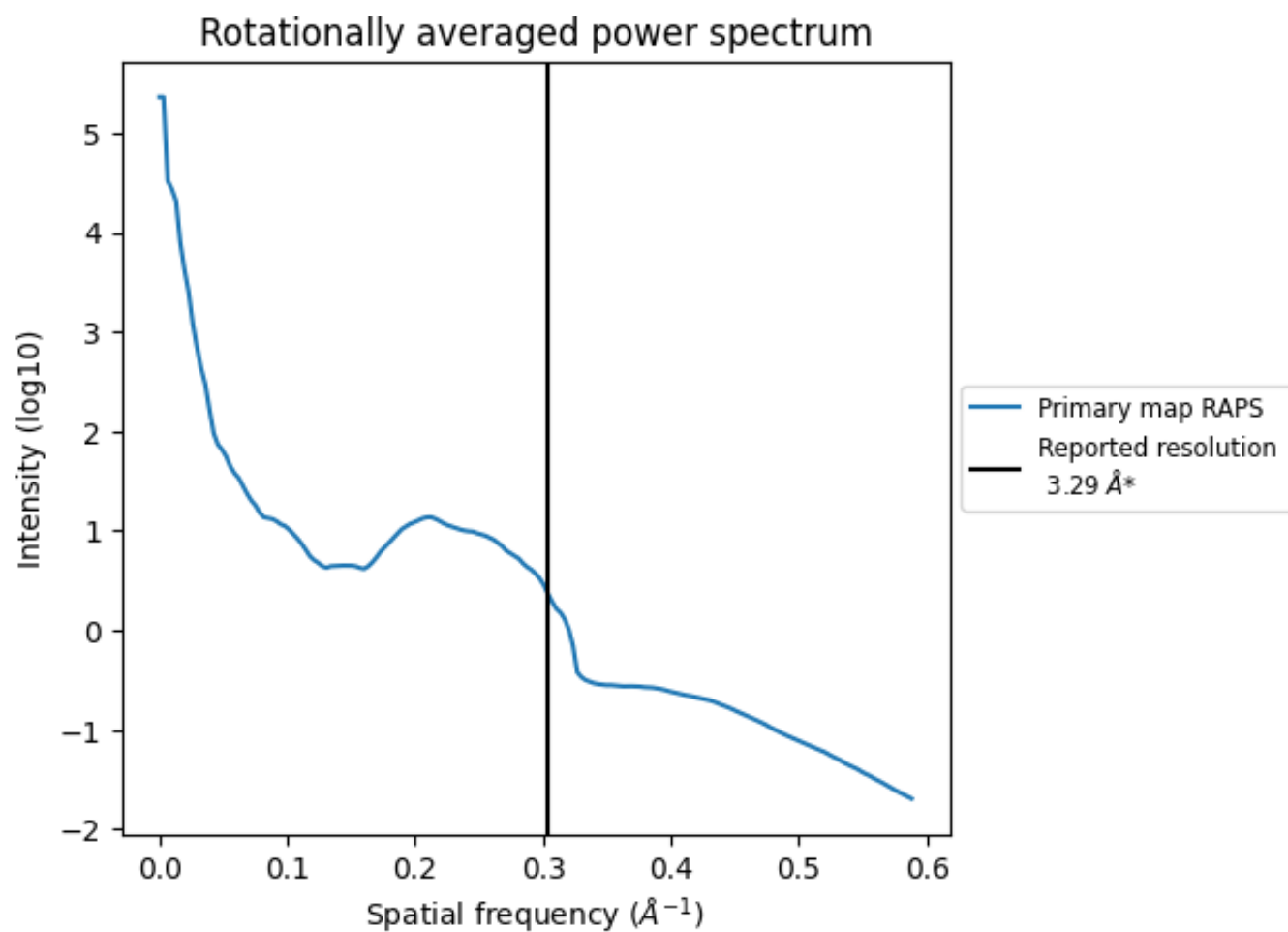
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 35 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 0.304 Å⁻¹

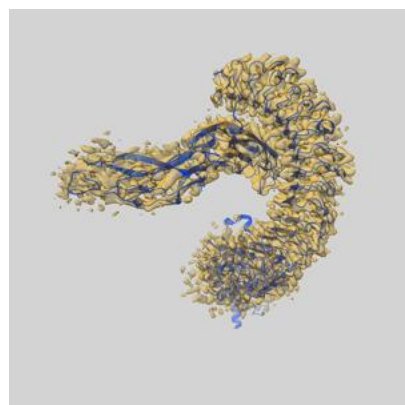
8 Fourier-Shell correlation

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

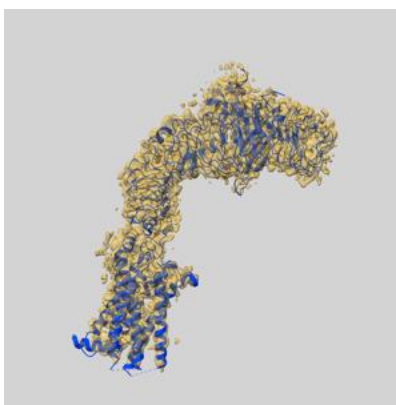
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37876 and PDB model 8WVY. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

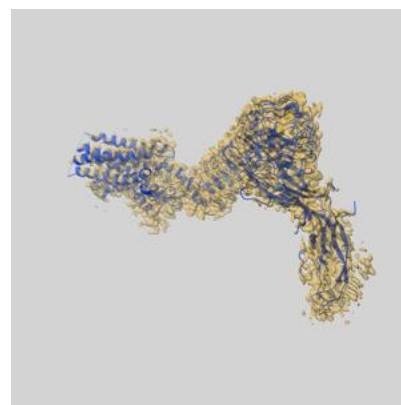
9.1 Map-model overlay [i](#)



X



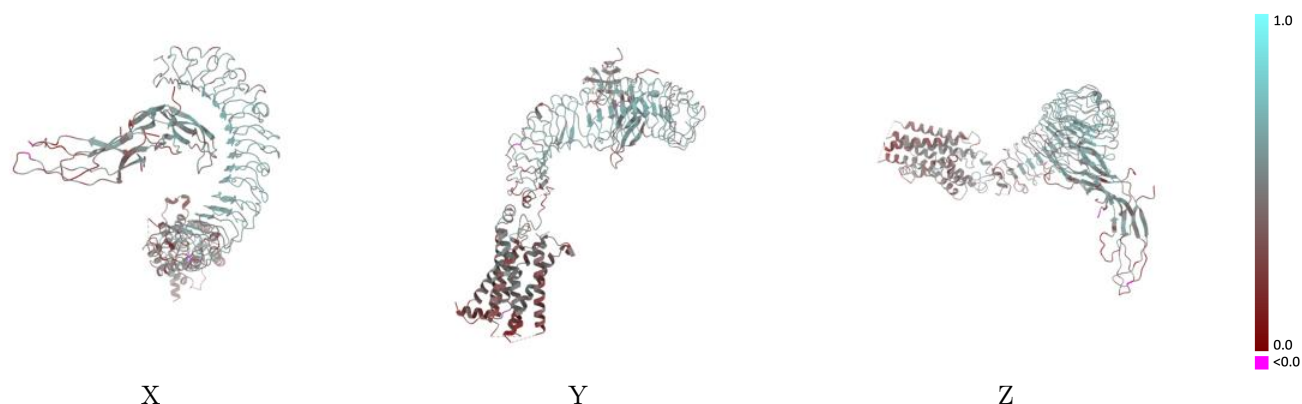
Y



Z

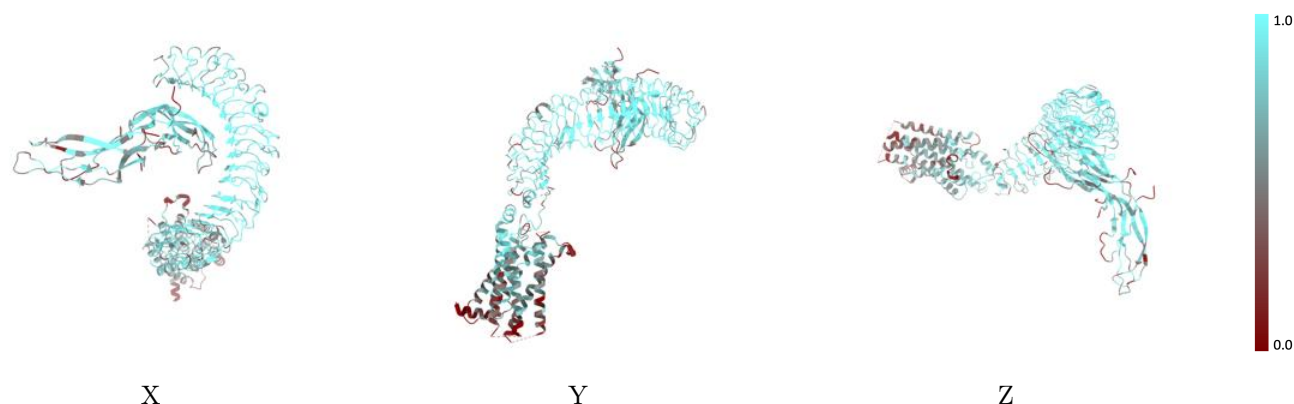
The images above show the 3D surface view of the map at the recommended contour level 0.283 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



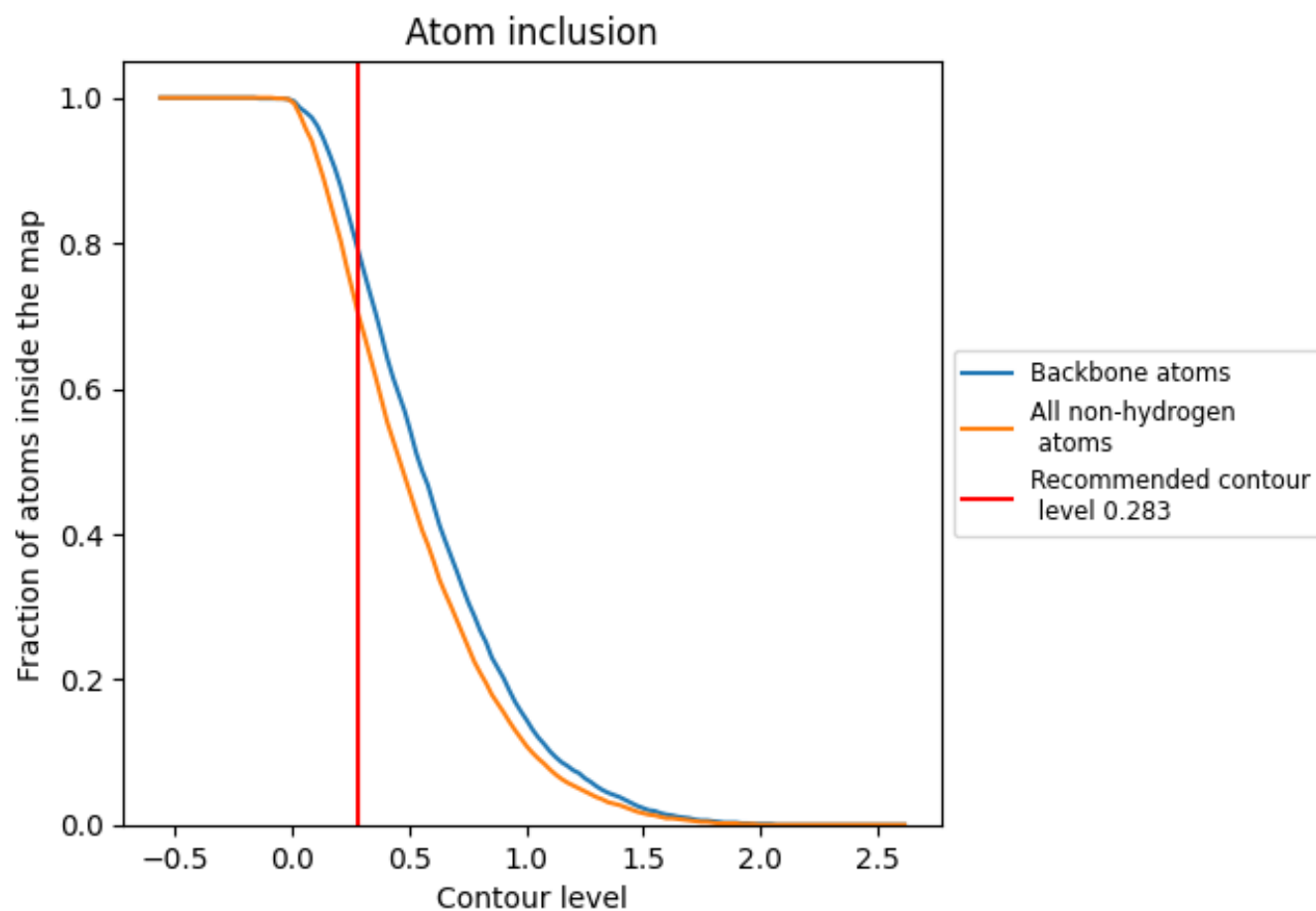
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.283).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.283) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7010	<div></div> 0.4670
A	<div></div> 0.7200	<div></div> 0.4770
E	<div></div> 0.6710	<div></div> 0.4560
F	<div></div> 0.5950	<div></div> 0.4040

