



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 06:39 PM JST

PDB ID : 8WVY  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
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) : 2.39

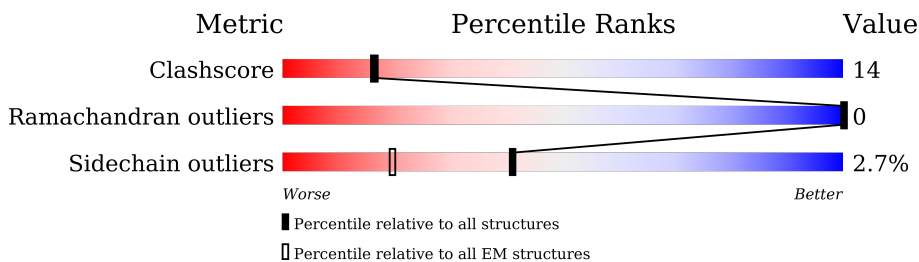
# 1 Overall quality at a glance

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  $\geq 3$ , 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	
2	E	103	
2	F	103	

## 2 Entry composition i

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

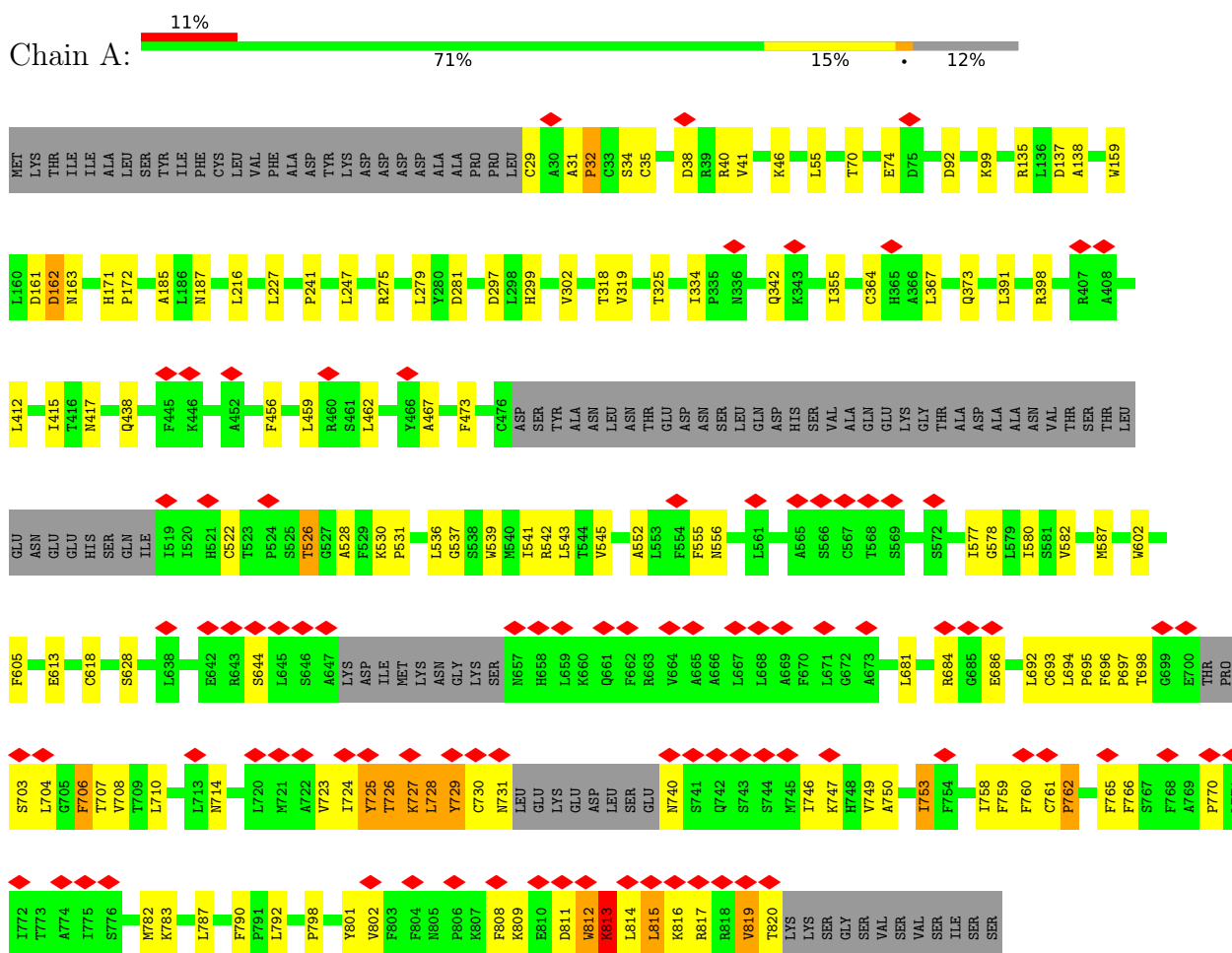
- Molecule 2 is a protein called Norrin.

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

### 3 Residue-property plots [i](#)

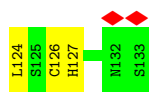
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Leucine-rich repeat-containing G-protein coupled receptor 4

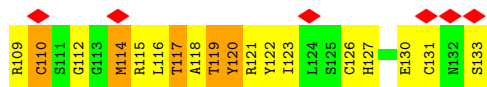
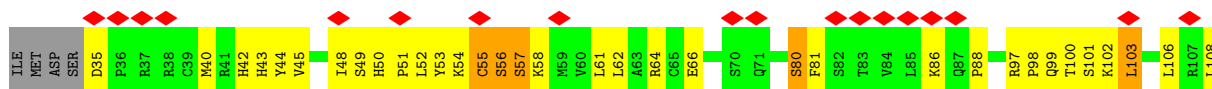
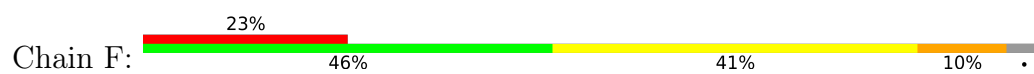


- Molecule 2: Norrin





## • 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 i

### 5.1 Standard geometry i

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	0.57	8/5806 (0.1%)	0.67	10/7902 (0.1%)
2	E	0.51	1/804 (0.1%)	0.69	1/1078 (0.1%)
2	F	0.90	5/798 (0.6%)	1.28	15/1070 (1.4%)
All	All	0.60	14/7408 (0.2%)	0.76	26/10050 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	100	THR	C-N	9.72	1.56	1.34
1	A	32	PRO	N-CD	-8.20	1.36	1.47
1	A	770	PRO	C-N	7.97	1.52	1.34
1	A	815	LEU	C-N	6.59	1.49	1.34
1	A	706	PHE	C-N	6.08	1.48	1.34
2	F	64	ARG	C-N	-5.79	1.20	1.34
1	A	819	VAL	C-N	5.69	1.47	1.34
1	A	526	THR	C-N	5.68	1.43	1.33
1	A	728	LEU	C-N	5.36	1.46	1.34
1	A	746	ILE	C-N	-5.36	1.21	1.34
2	F	56	SER	C-N	-5.31	1.21	1.34
2	F	35	ASP	C-N	5.23	1.44	1.34
2	F	40	MET	C-N	5.20	1.46	1.34
2	E	120	TYR	C-N	-5.04	1.22	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	56	SER	O-C-N	-13.26	101.48	122.70
2	F	42	HIS	O-C-N	-10.31	106.20	122.70
2	F	56	SER	CA-C-N	8.93	136.83	117.20
2	F	56	SER	C-N-CA	8.32	142.51	121.70
1	A	726	THR	O-C-N	7.96	135.44	122.70
2	F	80	SER	O-C-N	-7.08	111.37	122.70
2	F	102	LYS	O-C-N	6.87	133.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	110	CYS	O-C-N	6.72	133.46	122.70
2	F	42	HIS	C-N-CA	6.59	138.18	121.70
2	F	45	VAL	CA-C-N	-6.49	102.91	117.20
2	F	42	HIS	CA-C-N	6.10	130.63	117.20
1	A	726	THR	C-N-CA	-6.06	106.55	121.70
1	A	726	THR	CA-C-N	-6.03	103.94	117.20
2	F	45	VAL	O-C-N	5.84	132.05	122.70
1	A	32	PRO	CA-N-CD	5.80	119.82	111.70
1	A	762	PRO	CA-N-CD	-5.79	103.39	111.50
1	A	729	TYR	O-C-N	5.57	131.61	122.70
1	A	813	LYS	O-C-N	5.54	131.56	122.70
2	F	103	LEU	O-C-N	5.53	131.55	122.70
2	F	57	SER	O-C-N	5.30	131.19	122.70
2	F	102	LYS	CA-C-N	-5.24	105.66	117.20
1	A	727	LYS	O-C-N	5.24	131.08	122.70
2	E	107	ARG	O-C-N	5.24	131.08	122.70
1	A	817	ARG	O-C-N	5.11	130.87	122.70
2	F	45	VAL	C-N-CA	-5.09	108.98	121.70
1	A	730	CYS	O-C-N	5.05	130.79	122.70

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	A	5671	0	5682	118	0
2	E	788	0	776	29	0
2	F	782	0	772	62	0
All	All	7241	0	7230	200	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 14.

All (200) 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: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:109:ARG:C	2.42	0.98
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
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
2:E:102:LYS:HZ2	2:E:104:LYS:HE3	1.57	0.70
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:759:PHE:C	1:A:762:PRO:HD2	2.17	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: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:HH11	1:A:684:ARG:HA	1.68	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:HD12	2:F:116:LEU:N	2.22	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:114:MET:CE	2:F:115:ARG:O	2.61	0.48
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: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
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
1:A:162:ASP:N	1:A:162:ASP:OD1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:740:ASN:OD1	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
2:E:85:LEU:HD13	2:F:103:LEU:HD11	1.97	0.46
1:A:696:PHE:C	1:A:698:THR:N	2.69	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
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: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
1:A:759:PHE:C	1:A:762:PRO:CD	2.85	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
1:A:765:PHE:O	1:A:766:PHE:C	2.54	0.44
2:E:107:ARG:HB3	2:E:115:ARG:NH1	2.32	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
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
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
2:E:41:ARG:HD2	2:E:63:ALA:HB1	2.00	0.43
1:A:40:ARG:NH2	2:E:124:LEU:HD22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:O	1:A:187:ASN:ND2	2.51	0.43
2:F:122:TYR:O	2:F:123:ILE:C	2.58	0.42
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
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
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:541:ILE:H	1:A:541:ILE:HG12	1.71	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:812:TRP:C	2.94	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
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
2:F:114:MET:HE2	2:F:115:ARG:O	2.20	0.41
1:A:281:ASP:OD2	2:E:54:LYS:NZ	2.44	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
2:F:49:SER:OG	2:F:56:SER:O	2.31	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%)	621 (98%)	14 (2%)	47	69
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%)	798 (97%)	22 (3%)	41	65

All (22) 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	299	HIS
1	A	522	CYS

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	577	ILE
1	A	580	ILE
1	A	618	CYS
1	A	693	CYS
1	A	725	TYR
1	A	753	ILE
1	A	808	PHE
1	A	812	TRP
1	A	813	LYS
2	E	127	HIS
2	F	53	TYR
2	F	55	CYS
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 (14) 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	299	HIS
1	A	311	GLN
1	A	386	GLN
1	A	417	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

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.

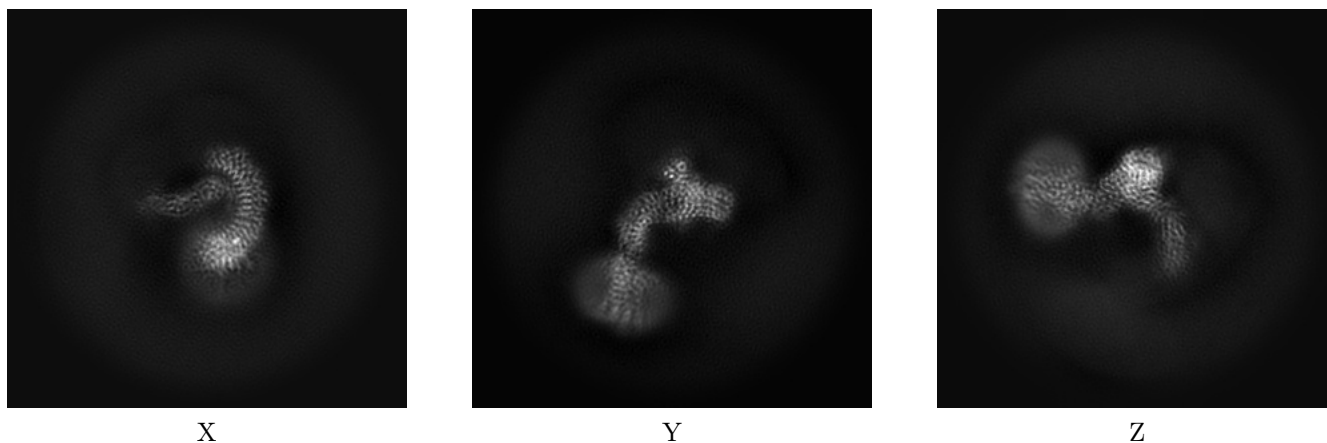
## 6 Map visualisation [i](#)

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](#)

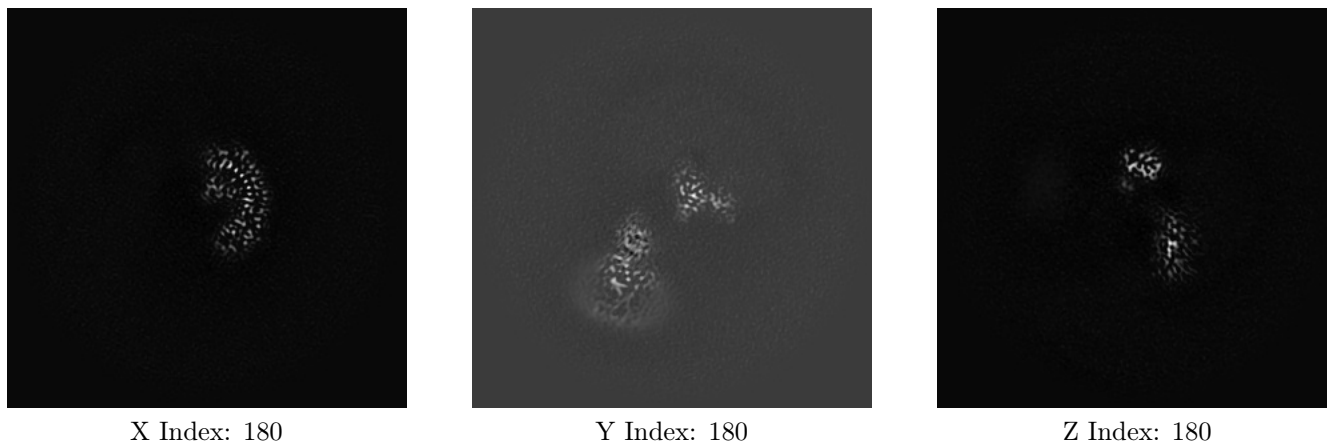
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

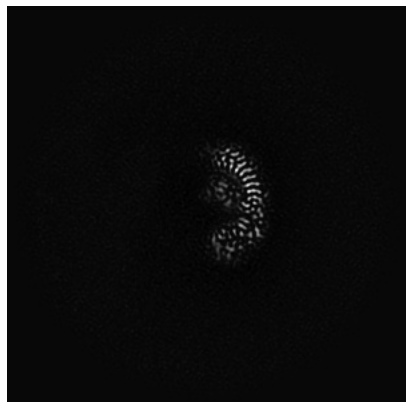
#### 6.2.1 Primary map



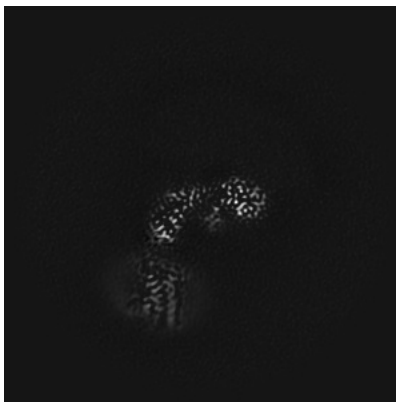
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

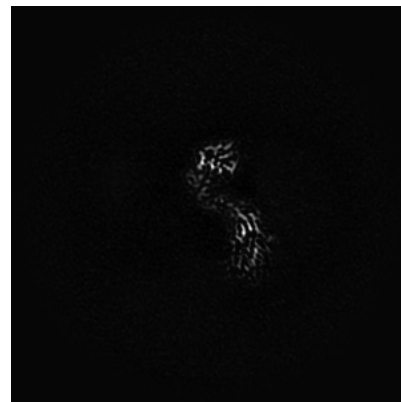
### 6.3.1 Primary map



X Index: 173



Y Index: 206

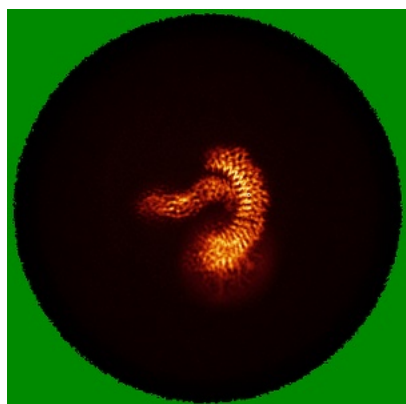


Z Index: 187

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

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

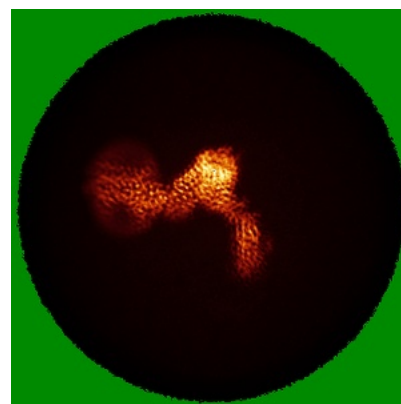
### 6.4.1 Primary map



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.

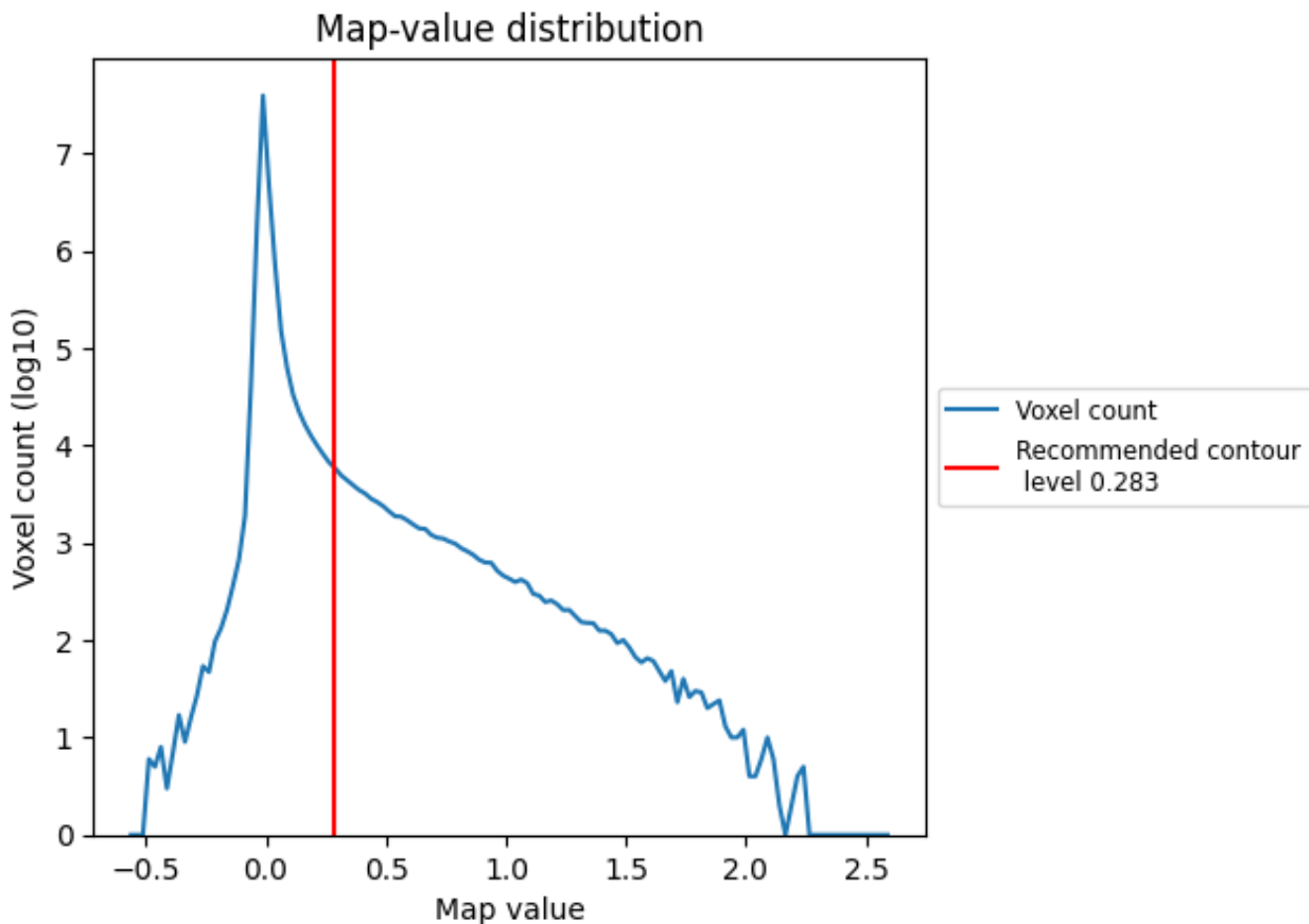
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

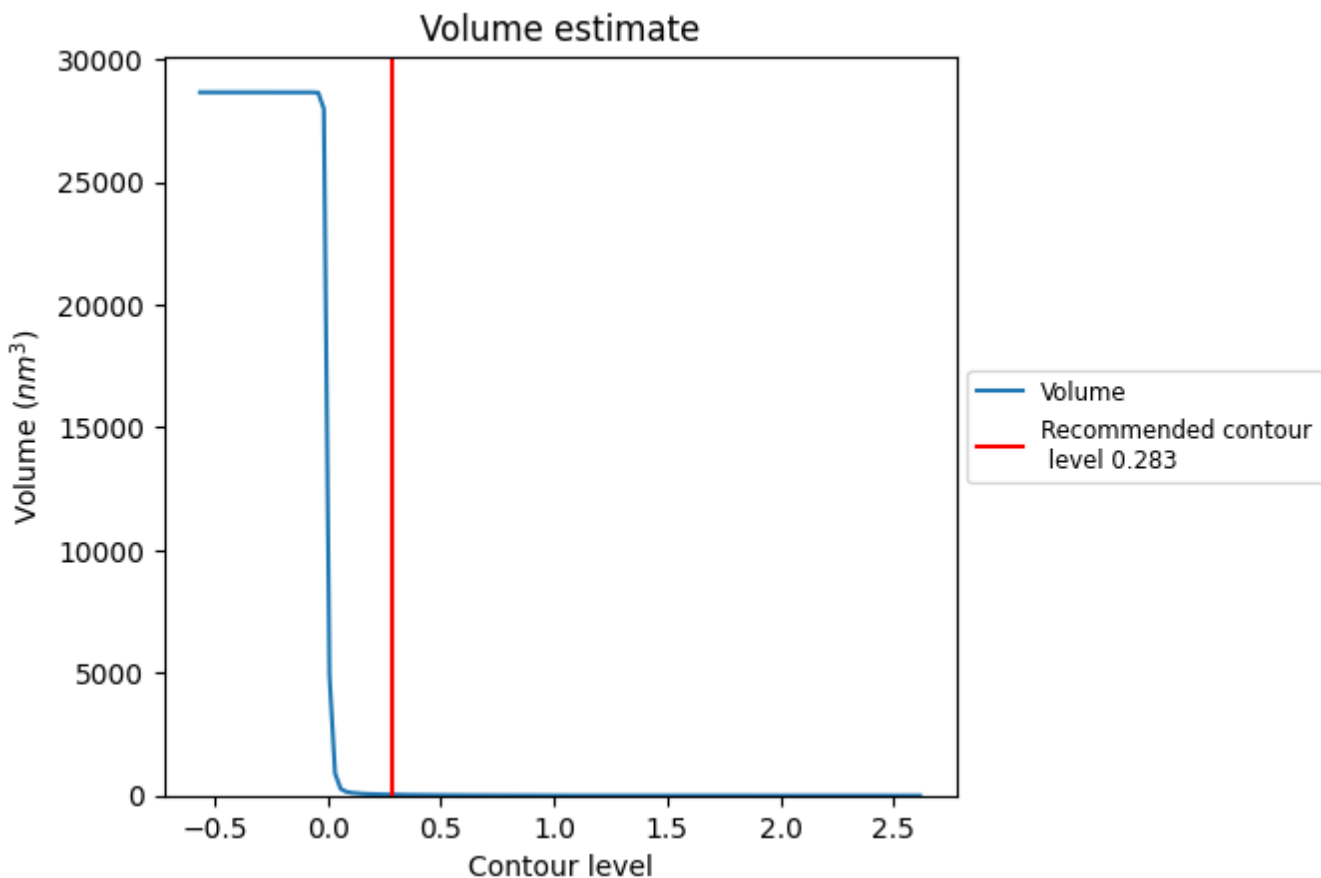
This section contains the results of statistical analysis of the map.

### 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.

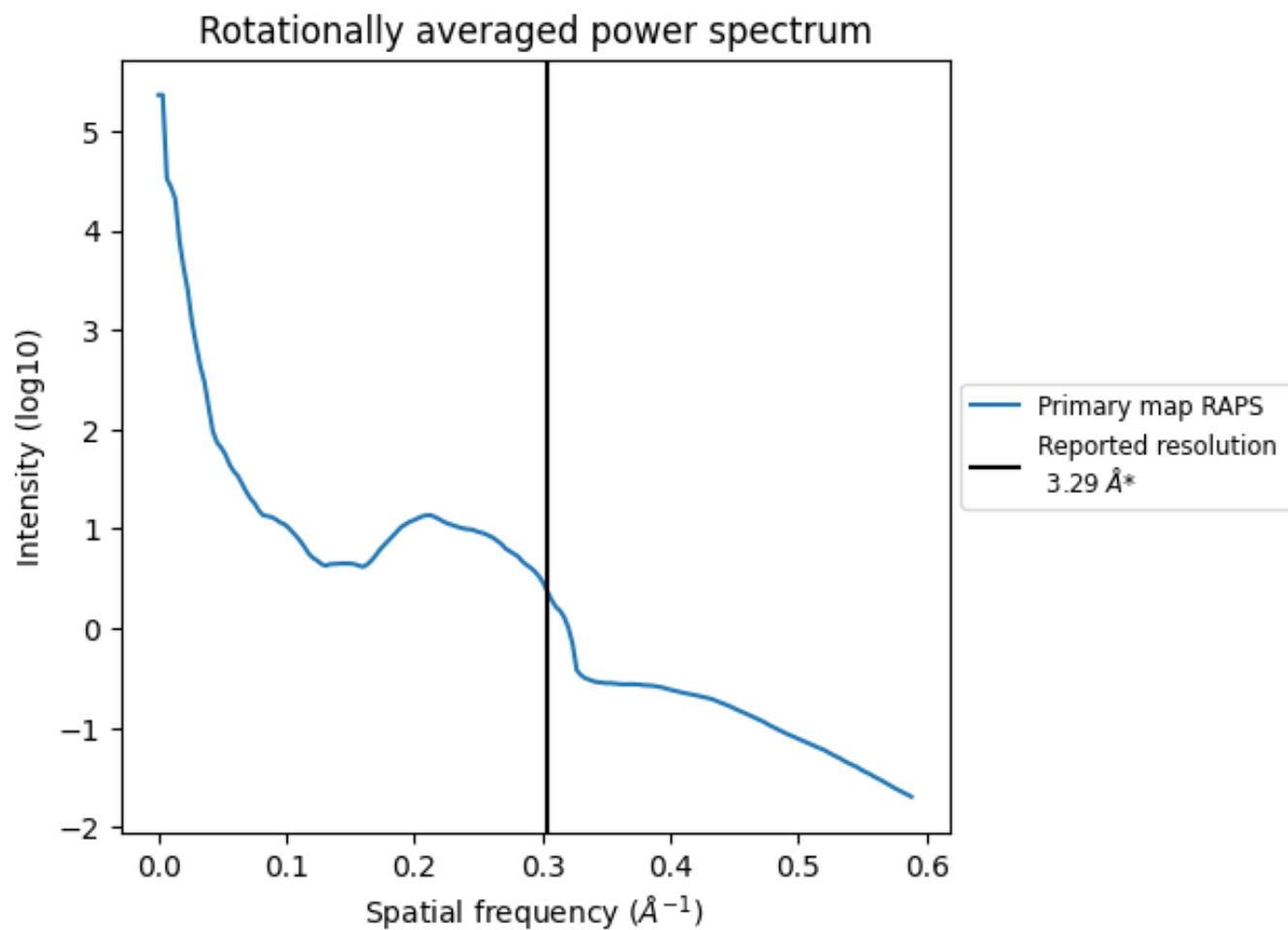
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.304 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

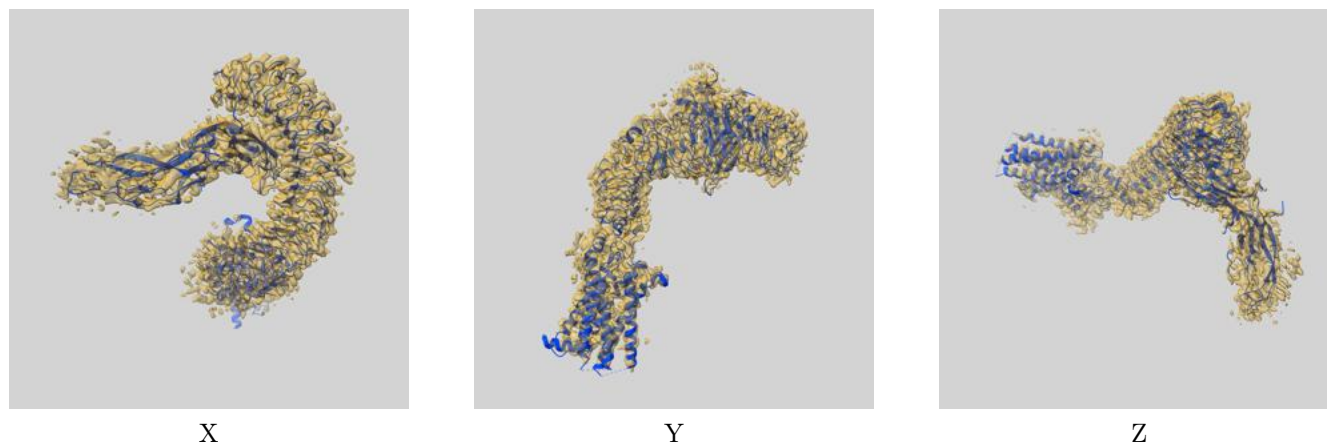
This section was not generated. No FSC curve or half-maps provided.



## 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](#)



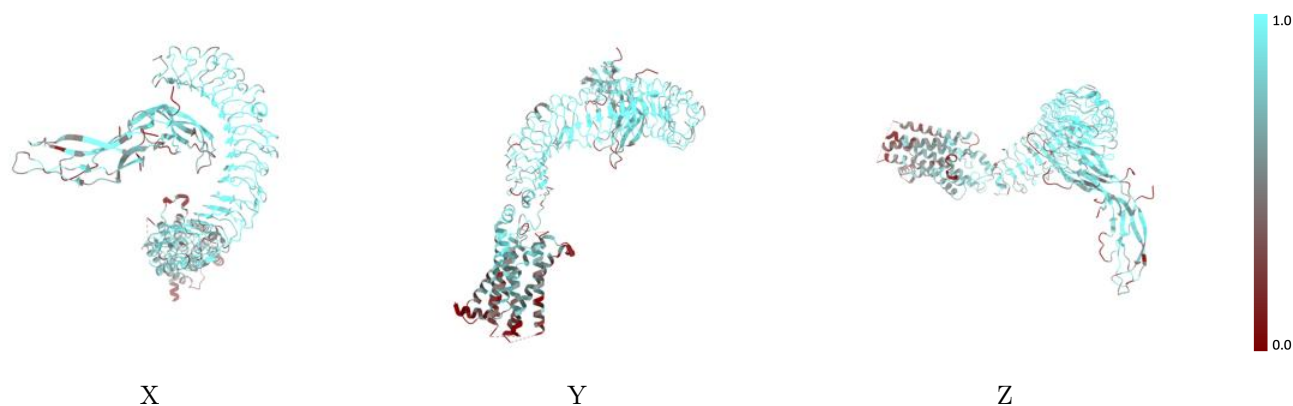
The images above show the 3D surface view of the map at the recommended contour level 0.283 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



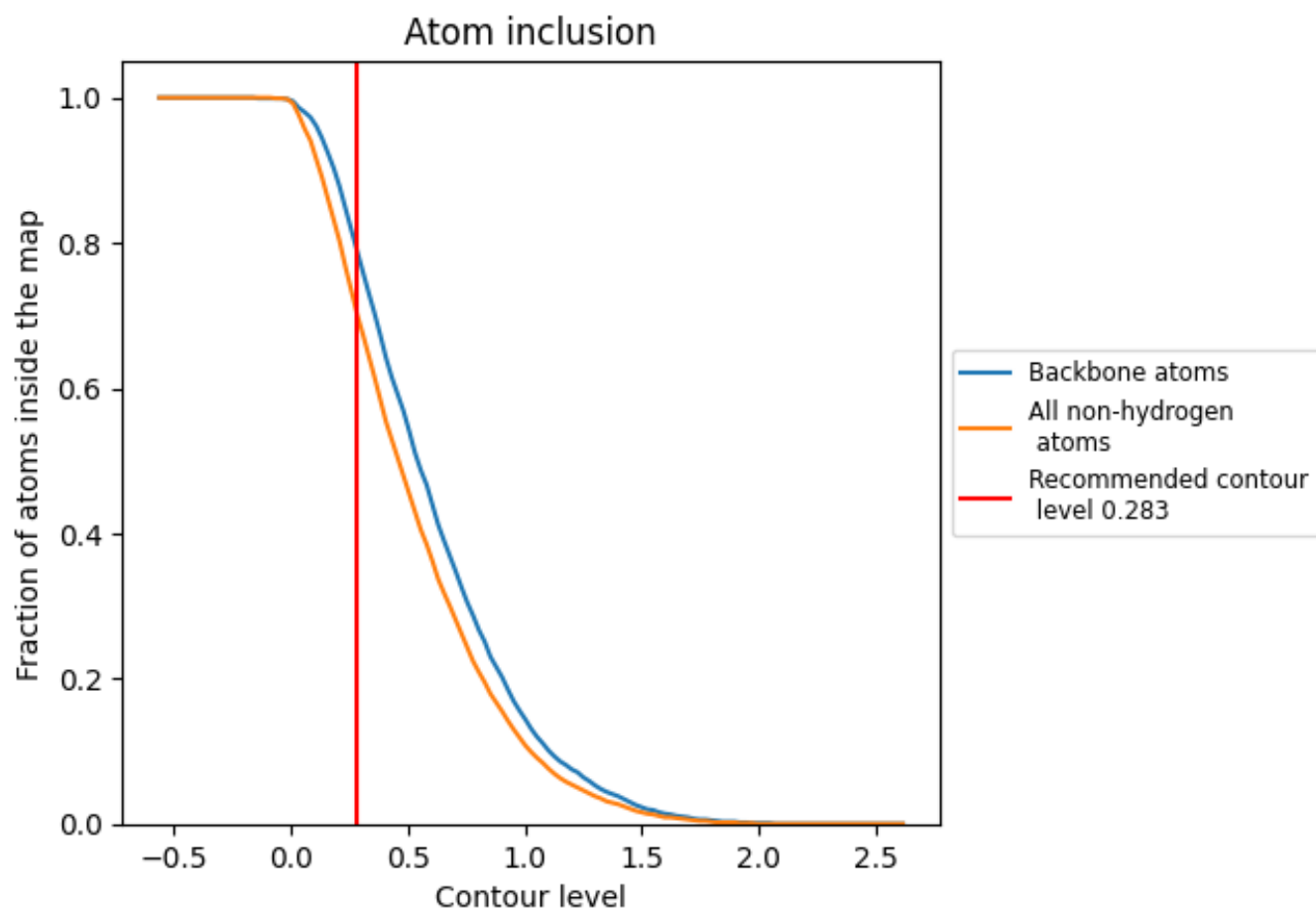
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 [i](#)

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	 0.7010	 0.4670
A	 0.7200	 0.4770
E	 0.6710	 0.4560
F	 0.5950	 0.4040

