Full wwPDB EM Validation Report

Dec 17, 2024 – 12:29 AM JST

PDB ID	:	8XJS
EMDB ID	:	EMD-38404
Title	:	Cryo-EM structure of human insulin receptor bound to 3 IGF-I
Authors	:	Xi, Z.
Deposited on	:	2023-12-22
Resolution	:	3.24 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:

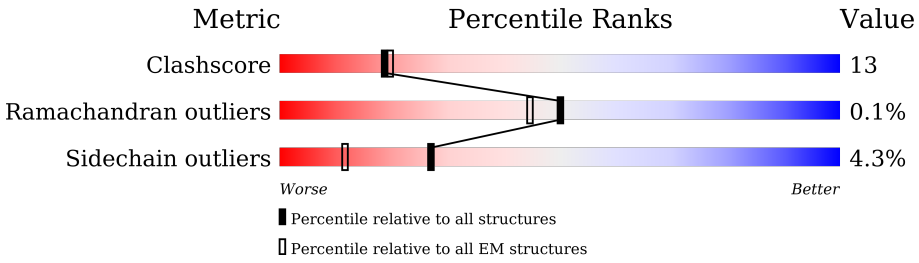
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 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 <=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	C	195	18% 5% 76%
1	D	195	95%
1	E	195	6% 10% 84%
2	A	1370	8% 44% 12% 43%
2	B	1370	5% 24% 13% 62%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Insulin-like growth factor I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	9	Total	C	N	O	S	0	0
			69	46	10	12	1		
1	C	46	Total	C	N	O	S	0	0
			359	225	60	67	7		
1	E	32	Total	C	N	O	S	0	0
			255	162	43	46	4		

- Molecule 2 is a protein called Isoform Short of Insulin receptor.

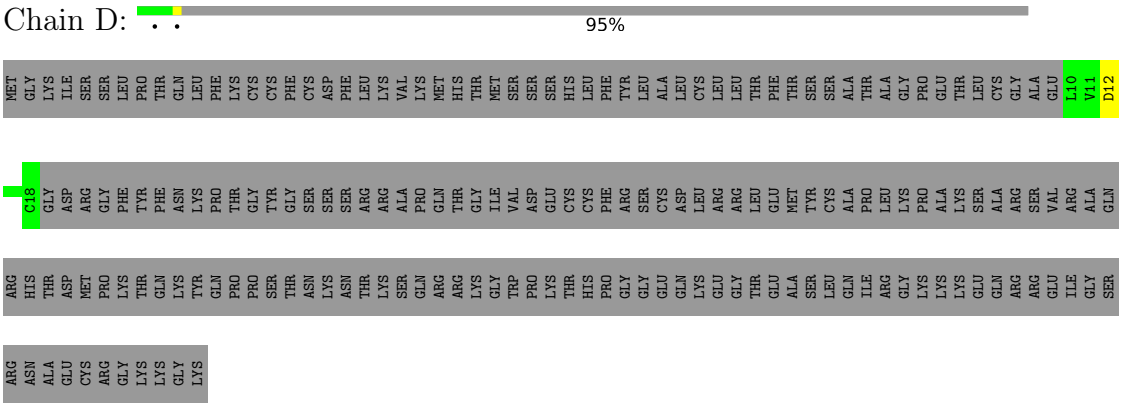
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	517	Total	C	N	O	S	0	0
			4193	2674	719	784	16		
2	A	781	Total	C	N	O	S	0	0
			6302	3999	1088	1167	48		

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.

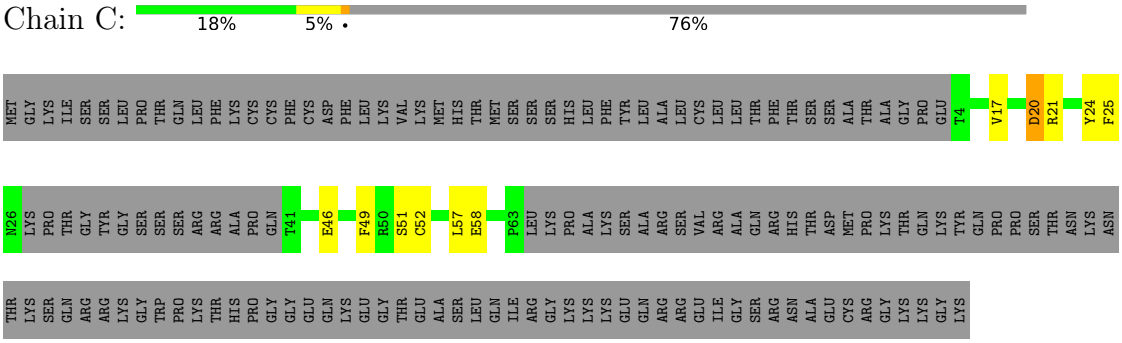
• Molecule 1: Insulin-like growth factor I

Chain D:



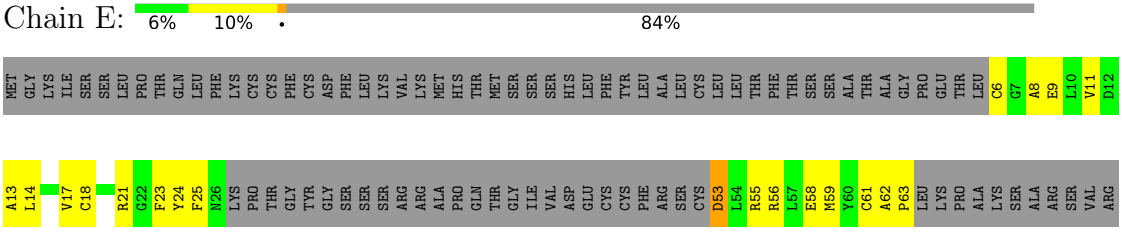
• Molecule 1: Insulin-like growth factor I

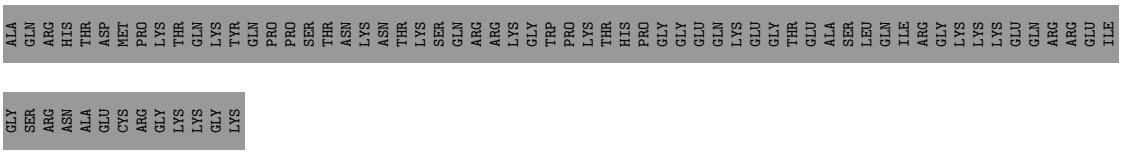
Chain C:



• Molecule 1: Insulin-like growth factor I

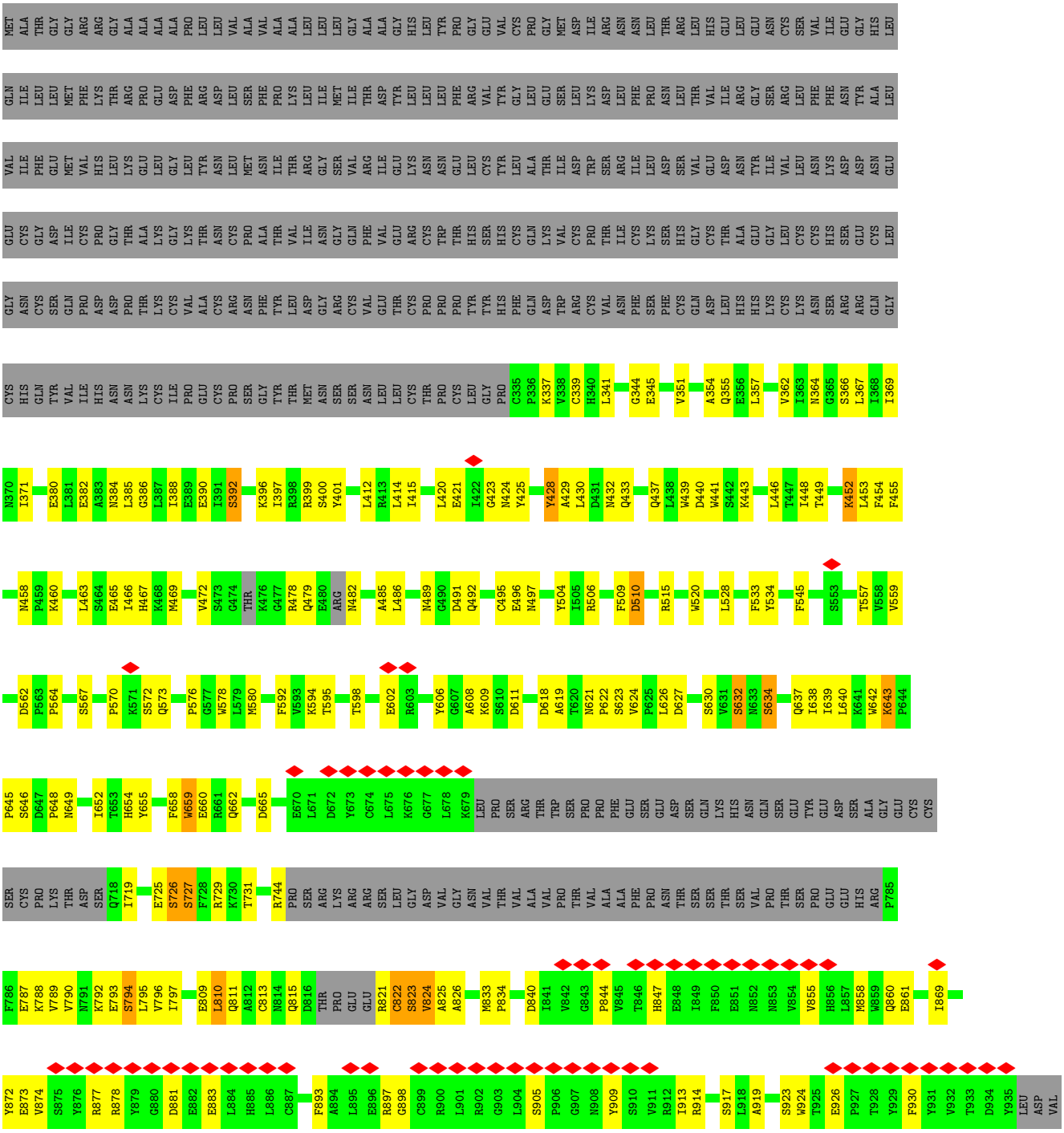
Chain E:

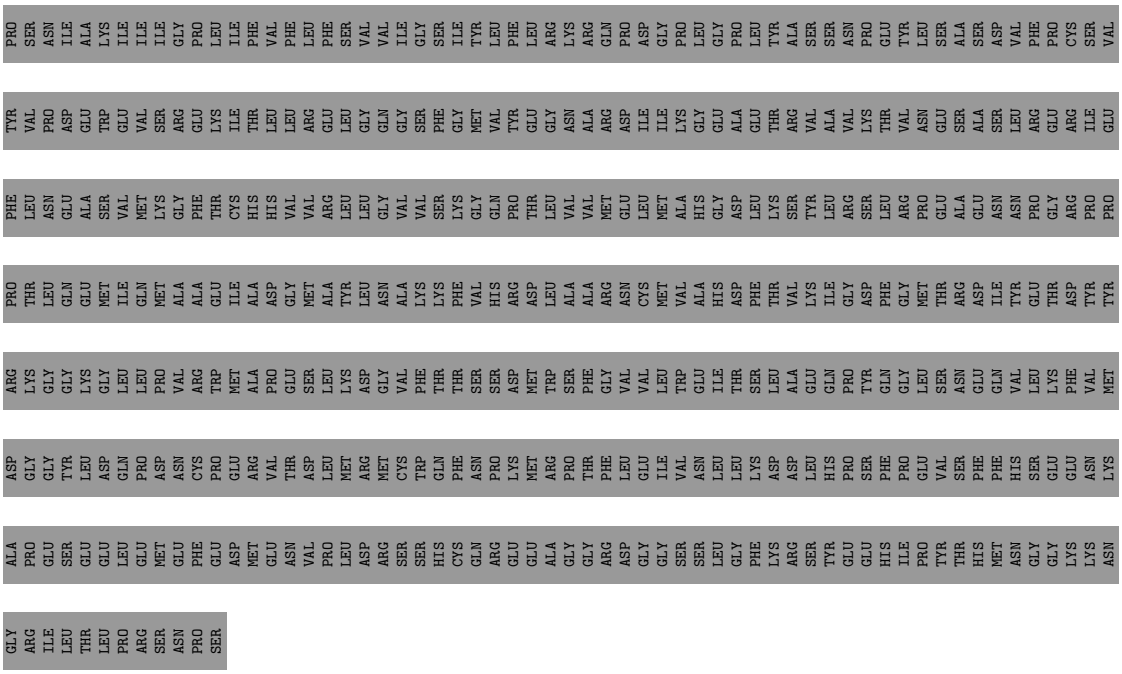




• Molecule 2: Isoform Short of Insulin receptor

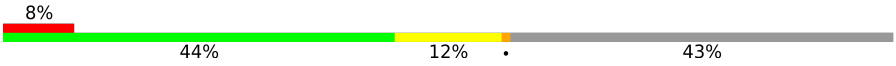
Chain B:

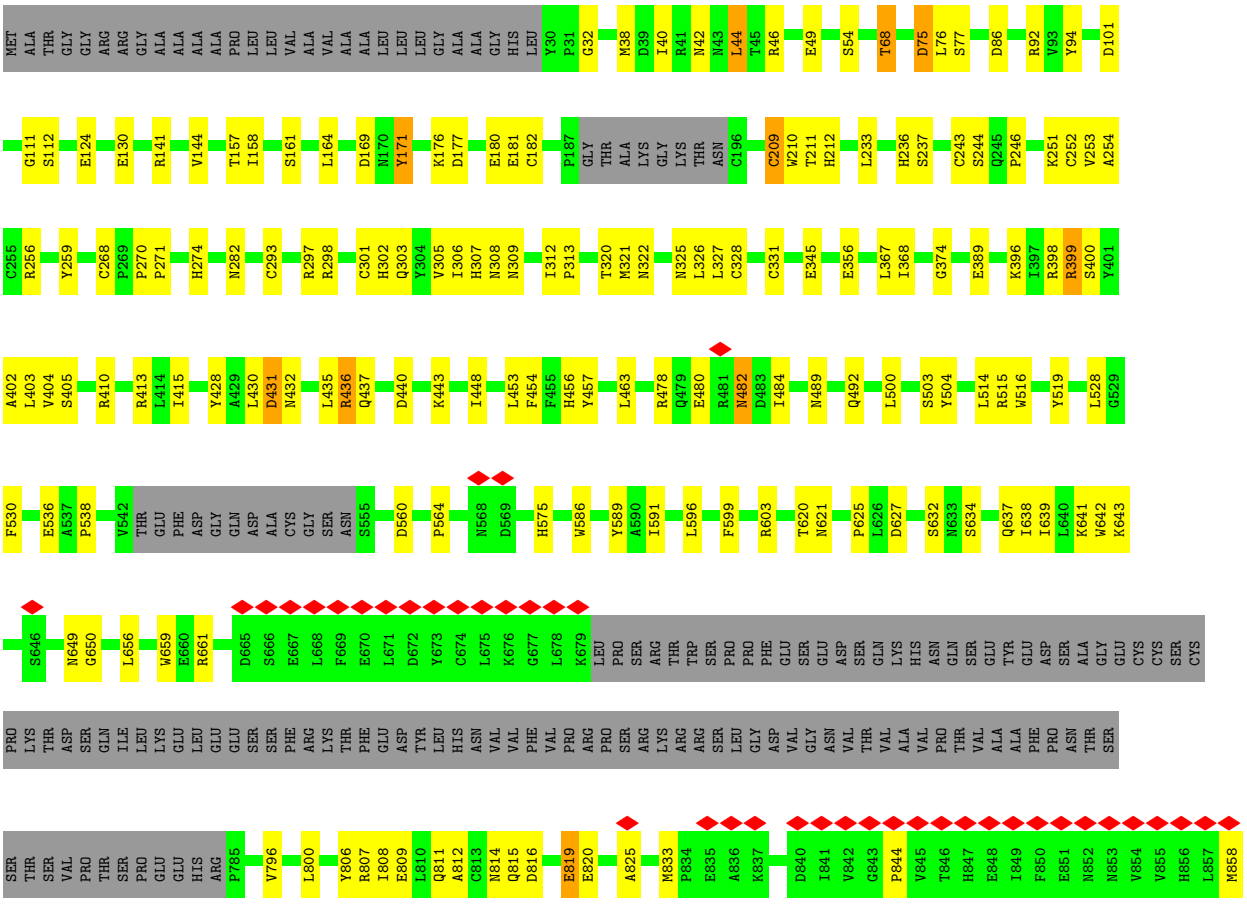


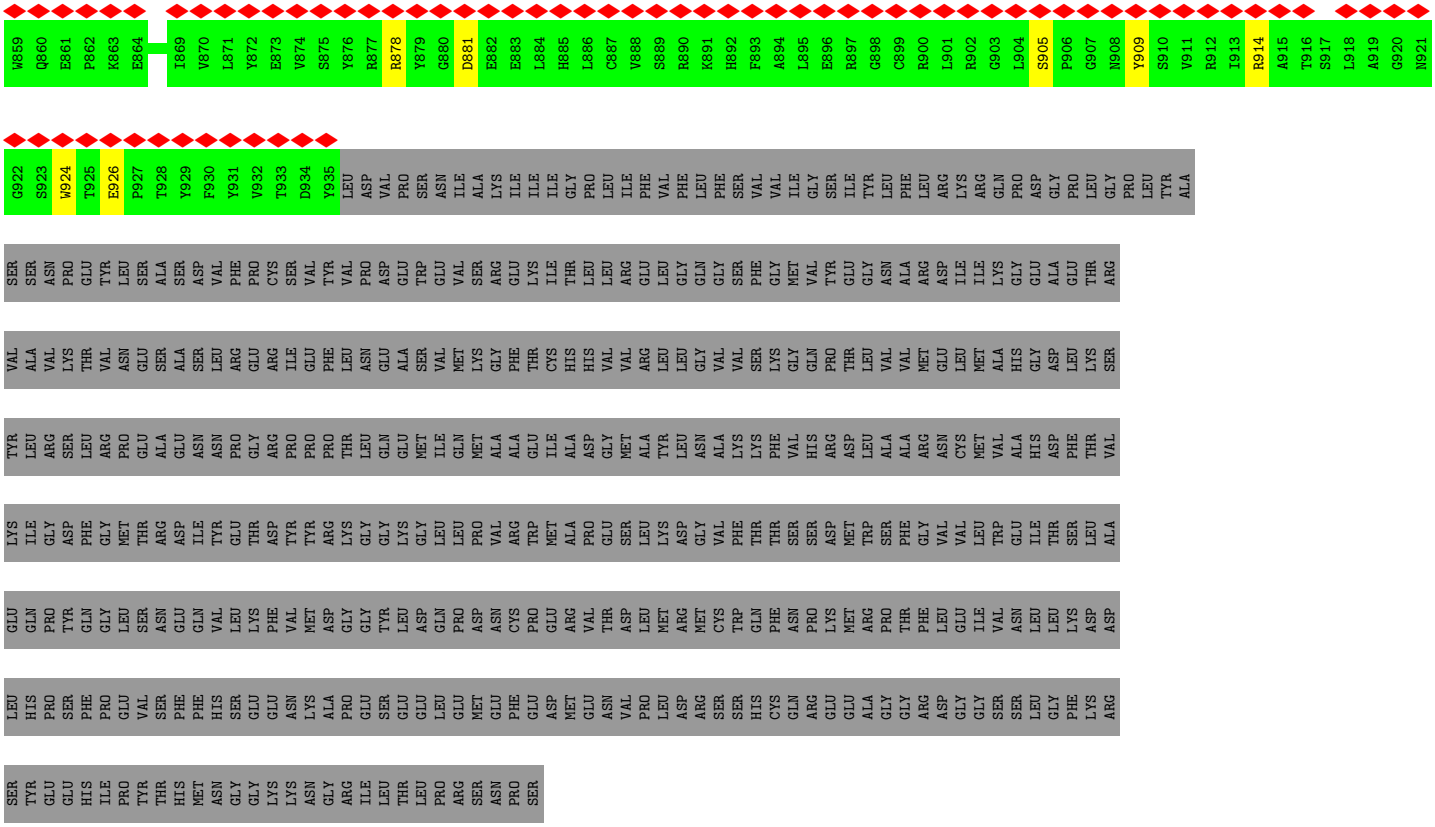


• Molecule 2: Isoform Short of Insulin receptor

Chain A:






W859 Q860 E861 P862 K863 E864
I869 V870 L871 Y872 E873 V874 S875 Y876 R877 R878 Y879 G880 D881 E882 E883 L884 H885 L886 C887 V888 S889 R890 K891 H892 F893 A894 L895 E896 R897 G898 C899 R900 L901 R902 G903 L904 S905 P906 G907 N908 Y909 S910 V911 R912 I913 R914 A915 T916 S917 L918 A919 G920 N921
G922 S923 W924 T925 E926 P927 T928 Y929 F930 Y931 V932 T933 D934 Y935
LEU ASP VAL PRO SER ASN ILE ALA LYS ILE ILE ILE GLY PRO LEU ILE PHE VAL PHE LEU PHE SER VAL VAL ILE GLY SER ILE TYR LEU PHE LEU ARG LYS GLY PRO ASP GLY PRO LEU GLY PRO LEU TYR ALA
SER SER ASN PRO GLU TYR LEU SER ALA SER ASP VAL PHE PRO CYS SER VAL TYR VAL PRO ASP GLU TRP GLU VAL SER ARG GLU LYS ILE THR LEU LEU ARG GLU LEU GLY GLN GLY SER PHE GLY MET VAL TYR GLU GLY ASN ALA ARG ASP ILE ILE LYS GLY GLU ALA GLU THR ARG
VAL ALA VAL LYS THR VAL ASN GLU SER ALA SER LEU ARG GLU ILE PHE LEU ASN GLU ALA SER VAL MET LYS GLY PHE THR CYS HIS HIS VAL VAL ARG LEU LEU GLY VAL VAL SER LYS GLY GLN PRO THR LEU VAL VAL MET GLU LEU MET ALA HIS GLY ASP LEU LYS SER
TYR LEU ARG SER LEU ARG PRO GLU ALA GLU ASN ASN PRO GLY ARG PRO PRO PRO THR LEU GLN GLU MET ILE GLN MET ALA ALA GLU ILE ALA ASP GLY MET ALA TYR LEU ASN ALA LYS LYS PHE VAL HIS ARG ASP LEU ALA ALA ARG ASN CYS MET VAL ALA HIS ASP PHE THR VAL
LYS ILE GLY ASP PHE GLY MET THR ARG ASP ILE TYR GLU THR ASP TYR TYR ARG LYS GLY GLY LYS GLY LEU LEU PRO VAL ARG TRP MET ALA PRO GLU SER LEU LYS ASP GLY VAL PHE THR THR SER SER ASP MET TRP SER PHE GLY VAL VAL LEU TRP GLU ILE THR SER LEU ALA
GLU GLN PRO TYR GLN GLY LEU SER ASN GLU GLN VAL LEU LYS PHE VAL MET ASP GLY GLY TYR LEU ASP GLN PRO ASP ASN CYS PRO GLU ARG VAL THR ASP LEU MET ARG MET CYS TRP GLN PHE ASN PRO LYS MET ARG PRO THR PHE LEU GLU ILE VAL ASN LEU LEU LYS ASP ASP
LEU HIS PRO SER PHE PRO GLU VAL SER PHE PHE HIS SER GLU GLU ASN LYS ALA PRO GLU SER GLU GLU LEU GLU MET GLU GLU PHE GLU ASP MET GLU ASN VAL PRO LEU ASP ARG SER SER HIS CYS GLN ARG GLU GLU ALA GLY GLY ARG ASP GLY GLY SER SER LEU GLY PHE LYS ARG
SER TYR GLU GLU HIS ILE PRO TYR THR HIS MET ASN GLY GLY LYS LYS ASN GLY ARG ILE LEU THR LEU PRO ARG SER ASN PRO SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148388	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	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	C	0.38	0/364	0.53	0/488
1	D	0.23	0/69	0.40	0/93
1	E	0.27	0/259	0.57	0/346
2	A	0.32	0/6458	0.53	2/8759 (0.0%)
2	B	0.32	0/4293	0.57	0/5814
All	All	0.32	0/11443	0.55	2/15500 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	75	ASP	CB-CG-OD1	5.67	123.40	118.30
2	A	101	ASP	CB-CG-OD1	5.34	123.11	118.30

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	C	359	0	331	6	0
1	D	69	0	70	0	0
1	E	255	0	235	14	0
2	A	6302	0	6129	119	0
2	B	4193	0	4099	145	0
All	All	11178	0	10864	280	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 13.

All (280) 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)
2:A:399:ARG:HH22	2:A:430:LEU:HG	1.09	1.12
2:A:399:ARG:HH21	2:A:430:LEU:HB3	0.98	1.09
2:A:399:ARG:NH2	2:A:430:LEU:HB3	1.73	1.02
2:A:399:ARG:NH2	2:A:430:LEU:HG	1.76	0.98
2:A:399:ARG:HH21	2:A:430:LEU:CB	1.77	0.98
2:B:811:GLN:NE2	2:B:822:CYS:SG	2.42	0.92
2:A:399:ARG:NH2	2:A:430:LEU:CB	2.36	0.88
2:B:632:SER:HB2	2:B:638:ILE:HG12	1.55	0.87
2:A:399:ARG:NH2	2:A:430:LEU:CG	2.37	0.87
2:B:627:ASP:HB2	2:B:643:LYS:HD2	1.62	0.81
2:B:380:GLU:HG3	2:B:384:ASN:HD21	1.46	0.81
2:A:432:ASN:HD22	2:A:435:LEU:HD22	1.45	0.80
2:B:528:LEU:HD21	2:B:598:THR:HG23	1.71	0.73
2:A:656:LEU:HB2	2:A:811:GLN:HB2	1.71	0.72
2:A:374:GLY:HA2	2:A:402:ALA:HB2	1.72	0.71
2:A:463:LEU:HD21	2:A:484:ILE:HG21	1.73	0.70
2:A:92:ARG:NE	2:A:124:GLU:OE1	2.23	0.70
2:B:354:ALA:HB1	2:B:385:LEU:HD21	1.76	0.68
2:B:369:ILE:HB	2:B:397:ILE:HD13	1.75	0.68
2:B:660:GLU:OE2	2:B:662:GLN:NE2	2.27	0.68
2:B:424:ASN:HB2	2:B:452:LYS:HZ2	1.57	0.67
2:B:622:PRO:HG2	2:B:823:SER:HB3	1.76	0.67
2:A:503:SER:H	2:A:516:TRP:HA	1.59	0.67
2:B:659:TRP:HE1	2:B:797:ILE:HD12	1.60	0.66
2:A:321:MET:SD	2:A:322:ASN:N	2.69	0.66
2:B:463:LEU:O	2:B:467:HIS:ND1	2.22	0.66
2:A:320:THR:OG1	2:A:331:CYS:SG	2.39	0.66
1:E:53:ASP:HB2	1:E:56:ARG:HG2	1.78	0.64
2:B:453:LEU:HB2	2:B:479:GLN:HE22	1.62	0.64
2:B:440:ASP:OD2	2:B:443:LYS:NZ	2.27	0.63
2:B:415:ILE:HB	2:B:448:ILE:HG12	1.80	0.63
2:B:504:TYR:HB3	2:B:515:ARG:HB2	1.81	0.63
2:B:824:VAL:HG23	2:B:825:ALA:H	1.64	0.62
1:E:21:ARG:HH11	1:E:62:ALA:HB1	1.63	0.62
2:B:399:ARG:HH12	2:B:401:TYR:HB2	1.64	0.62
2:B:623:SER:OG	2:B:624:VAL:N	2.32	0.62
2:B:528:LEU:HD21	2:B:598:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:456:HIS:NE2	2:A:482:ASN:OD1	2.28	0.61
2:A:297:ARG:HH21	2:A:303:GLN:HE22	1.46	0.61
1:E:24:TYR:HB3	1:E:25:PHE:HD2	1.67	0.60
2:B:491:ASP:OD1	2:B:491:ASP:N	2.34	0.60
2:B:834:PRO:HG3	2:B:919:ALA:HB1	1.83	0.60
2:A:112:SER:O	2:A:141:ARG:NH1	2.34	0.60
2:A:268:CYS:SG	2:A:274:HIS:ND1	2.71	0.60
2:A:815:GLN:NE2	2:A:819:GLU:O	2.35	0.60
2:B:877:ARG:NH1	2:B:883:GLU:OE1	2.35	0.59
2:B:424:ASN:HB2	2:B:452:LYS:NZ	2.17	0.59
2:A:428:TYR:HE1	2:A:430:LEU:HD22	1.68	0.59
2:B:630:SER:HB3	2:B:640:LEU:HD13	1.83	0.59
1:E:55:ARG:HA	1:E:58:GLU:HB3	1.85	0.59
2:B:659:TRP:NE1	2:B:797:ILE:HD12	2.18	0.58
2:A:307:HIS:HD2	2:A:328:CYS:HB2	1.69	0.58
2:A:800:LEU:HB3	2:A:806:TYR:HE2	1.69	0.58
2:A:807:ARG:HH12	2:A:809:GLU:N	2.02	0.58
2:B:623:SER:HB3	2:B:645:PRO:HB3	1.84	0.58
2:B:833:MET:SD	2:B:833:MET:N	2.74	0.58
2:A:244:SER:HB2	2:A:251:LYS:HB3	1.86	0.58
2:A:620:THR:O	2:A:814:ASN:ND2	2.36	0.58
2:B:840:ASP:HA	2:B:923:SER:H	1.69	0.57
2:A:144:VAL:HG23	2:A:164:LEU:HD21	1.84	0.57
2:A:297:ARG:NH1	2:A:301:CYS:SG	2.73	0.57
2:B:790:VAL:O	2:B:792:LYS:HG3	2.03	0.57
2:A:456:HIS:HB3	2:A:457:TYR:HD2	1.70	0.57
2:A:368:ILE:HD12	2:A:396:LYS:HB3	1.85	0.57
2:B:414:LEU:HD11	2:B:449:THR:HG23	1.87	0.57
2:B:429:ALA:HB1	2:B:432:ASN:HD21	1.69	0.57
2:A:621:ASN:O	2:A:649:ASN:ND2	2.32	0.57
1:C:20:ASP:OD1	1:C:20:ASP:N	2.34	0.56
2:B:809:GLU:OE1	2:B:809:GLU:N	2.38	0.56
2:B:646:SER:O	2:B:648:PRO:HD3	2.06	0.56
2:A:44:LEU:HD23	2:A:44:LEU:H	1.70	0.56
2:A:833:MET:SD	2:A:833:MET:N	2.78	0.56
2:B:492:GLN:HE22	2:A:457:TYR:HE1	1.53	0.56
2:B:420:LEU:HB3	2:B:424:ASN:HA	1.87	0.55
2:A:634:SER:HB3	2:A:637:GLN:HB2	1.87	0.55
2:A:268:CYS:H	2:A:274:HIS:HE1	1.54	0.55
2:A:453:LEU:H	2:A:480:GLU:HG2	1.72	0.55
2:A:44:LEU:HD22	2:A:68:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ILE:HG23	2:A:46:ARG:HB2	1.88	0.55
2:A:130:GLU:HG3	2:A:211:THR:HG22	1.88	0.55
2:B:795:LEU:HD12	2:B:796:VAL:N	2.22	0.54
2:A:536:GLU:HA	2:A:589:TYR:HD1	1.72	0.54
2:A:157:THR:OG1	2:A:209:CYS:O	2.25	0.54
2:B:458:ASN:ND2	2:B:489:ASN:OD1	2.41	0.54
2:A:586:TRP:CD1	2:A:650:GLY:HA2	2.43	0.54
2:A:638:ILE:HD12	2:A:808:ILE:HD11	1.89	0.54
2:A:844:PRO:HB3	2:A:926:GLU:HB2	1.89	0.54
2:B:622:PRO:HD2	2:B:823:SER:N	2.23	0.54
2:B:860:GLN:NE2	2:B:861:GLU:O	2.40	0.54
2:B:847:HIS:CD2	2:B:930:PHE:HB3	2.43	0.54
2:B:364:ASN:HA	2:B:392:SER:HB2	1.90	0.53
2:A:46:ARG:O	2:A:49:GLU:HG3	2.07	0.53
2:A:878:ARG:NE	2:A:881:ASP:OD2	2.37	0.53
2:B:858:MET:HE1	2:B:898:GLY:HA3	1.90	0.53
2:A:389:GLU:OE1	2:A:413:ARG:NH1	2.35	0.53
2:B:341:LEU:HD11	2:B:357:LEU:HD21	1.90	0.53
2:A:325:ASN:HD21	2:A:327:LEU:HD12	1.73	0.53
2:B:570:PRO:HA	2:B:573:GLN:HG2	1.91	0.53
2:B:420:LEU:HD13	2:B:424:ASN:HB3	1.91	0.52
2:A:398:ARG:HG2	2:A:399:ARG:NE	2.24	0.52
1:E:6:CYS:N	1:E:9:GLU:HB3	2.24	0.52
2:A:396:LYS:NZ	2:A:398:ARG:HH11	2.08	0.52
2:B:367:LEU:HD12	2:B:369:ILE:HD11	1.91	0.52
2:B:441:TRP:CZ3	2:B:472:VAL:HG11	2.44	0.52
2:B:423:GLY:O	2:B:452:LYS:NZ	2.42	0.52
2:B:533:PHE:HD2	2:B:592:PHE:CZ	2.28	0.52
2:A:293:CYS:SG	2:A:297:ARG:NH2	2.83	0.52
2:B:564:PRO:HG3	2:B:576:PRO:HB3	1.93	0.51
2:A:303:GLN:O	2:A:305:VAL:HG23	2.10	0.51
2:B:504:TYR:OH	2:B:506:ARG:HD3	2.11	0.51
2:A:625:PRO:HG3	2:A:812:ALA:HB2	1.91	0.51
2:B:632:SER:HA	2:B:638:ILE:HA	1.92	0.50
2:B:455:PHE:CD1	2:B:466:ILE:HD13	2.45	0.50
2:A:800:LEU:HB3	2:A:806:TYR:CE2	2.46	0.50
1:E:21:ARG:HD3	1:E:62:ALA:HA	1.92	0.50
2:B:567:SER:OG	2:B:572:SER:OG	2.24	0.50
2:A:236:HIS:HD2	2:A:237:SER:H	1.58	0.50
2:A:306:ILE:HB	2:A:326:LEU:O	2.13	0.49
2:A:399:ARG:NE	2:A:431:ASP:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:GLU:HG3	2:B:366:SER:HB2	1.94	0.49
2:B:869:ILE:HD13	2:B:917:SER:HB3	1.95	0.49
2:A:38:MET:HE3	2:A:49:GLU:HB2	1.93	0.49
2:B:725:GLU:OE2	2:B:729:ARG:NH1	2.46	0.49
2:B:602:GLU:HG2	1:C:49:PHE:CE2	2.47	0.49
2:B:655:TYR:HB2	2:B:789:VAL:HB	1.95	0.49
2:B:727:SER:O	2:B:731:THR:OG1	2.27	0.49
2:A:500:LEU:HD11	2:A:519:TYR:HB2	1.95	0.49
2:A:514:LEU:HD21	2:A:591:ILE:HG21	1.95	0.49
1:E:18:CYS:SG	1:E:21:ARG:HG3	2.53	0.49
2:B:654:HIS:O	2:B:813:CYS:HB2	2.14	0.48
2:B:337:LYS:O	2:B:362:VAL:HB	2.13	0.48
2:B:627:ASP:O	2:B:642:TRP:HA	2.13	0.48
2:B:658:PHE:HB2	2:B:809:GLU:CD	2.34	0.48
2:B:611:ASP:OD1	2:B:611:ASP:N	2.44	0.48
2:A:308:ASN:OD1	2:A:308:ASN:N	2.42	0.48
2:A:504:TYR:CZ	2:A:515:ARG:HG3	2.49	0.48
2:B:496:GLU:O	2:B:497:ASN:ND2	2.34	0.48
2:A:432:ASN:ND2	2:A:435:LEU:HD22	2.24	0.47
2:A:253:VAL:HG23	2:A:254:ALA:H	1.77	0.47
2:A:484:ILE:HG23	2:A:489:ASN:ND2	2.29	0.47
2:B:496:GLU:C	2:B:497:ASN:HD22	2.17	0.47
2:B:844:PRO:HB3	2:B:926:GLU:HB2	1.96	0.47
2:A:400:SER:HB3	2:A:403:LEU:HB2	1.96	0.47
2:B:626:LEU:O	2:B:643:LYS:N	2.47	0.47
2:B:362:VAL:HG13	2:B:390:GLU:HB2	1.97	0.47
2:B:811:GLN:HG3	2:B:824:VAL:O	2.15	0.47
2:B:905:SER:HG	2:B:909:TYR:HH	1.62	0.47
2:A:528:LEU:HB2	2:A:596:LEU:HG	1.96	0.47
1:E:21:ARG:HB2	1:E:63:PRO:HD2	1.96	0.47
2:B:905:SER:OG	2:B:909:TYR:OH	2.31	0.47
2:A:312:ILE:HG22	2:A:313:PRO:HD2	1.97	0.47
2:B:790:VAL:H	2:B:792:LYS:NZ	2.13	0.47
2:B:621:ASN:O	2:B:649:ASN:ND2	2.37	0.46
2:A:158:ILE:HD11	2:A:210:TRP:CD2	2.50	0.46
2:A:396:LYS:HG3	2:A:428:TYR:HB3	1.97	0.46
1:C:21:ARG:NH2	1:C:58:GLU:OE2	2.48	0.46
1:E:14:LEU:HD21	1:E:61:CYS:HB3	1.97	0.46
2:B:385:LEU:HB3	2:B:388:ILE:HD12	1.98	0.46
2:B:622:PRO:HD2	2:B:823:SER:CA	2.45	0.46
2:A:905:SER:OG	2:A:909:TYR:OH	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ILE:HG23	2:B:796:VAL:HG22	1.97	0.46
2:A:639:ILE:HG12	2:A:796:VAL:HG22	1.96	0.46
2:B:621:ASN:OD1	2:B:823:SER:HA	2.16	0.46
2:B:914:ARG:HB2	2:B:924:TRP:CD2	2.51	0.46
2:A:405:SER:HB2	2:A:437:GLN:HB3	1.97	0.45
2:A:503:SER:N	2:A:515:ARG:O	2.48	0.45
2:B:595:THR:HB	2:B:608:ALA:H	1.80	0.45
2:A:176:LYS:HG2	2:A:182:CYS:SG	2.56	0.45
2:A:396:LYS:NZ	2:A:398:ARG:HD3	2.31	0.45
2:B:744:ARG:HA	1:C:24:TYR:CE1	2.52	0.45
2:B:648:PRO:HB3	2:B:652:ILE:HD11	1.99	0.45
2:B:344:GLY:O	2:B:366:SER:N	2.39	0.45
2:B:465:GLU:OE1	2:B:465:GLU:N	2.50	0.45
2:B:788:LYS:HE2	2:B:788:LYS:HA	1.98	0.45
2:A:403:LEU:HD12	2:A:403:LEU:HA	1.86	0.45
2:B:441:TRP:HE1	2:B:469:MET:CE	2.29	0.45
2:A:430:LEU:HD13	2:A:454:PHE:HE1	1.82	0.45
2:B:463:LEU:HB2	2:B:495:CYS:SG	2.57	0.45
2:B:485:ALA:O	2:B:489:ASN:ND2	2.49	0.44
2:A:367:LEU:C	2:A:368:ILE:HD13	2.37	0.44
2:B:453:LEU:HB2	2:B:479:GLN:NE2	2.29	0.44
2:A:321:MET:SD	2:A:326:LEU:HA	2.57	0.44
2:A:86:ASP:O	2:A:111:GLY:HA2	2.17	0.44
2:A:430:LEU:O	2:A:457:TYR:HB2	2.17	0.44
2:A:632:SER:OG	2:A:634:SER:O	2.36	0.44
2:A:632:SER:HA	2:A:638:ILE:HA	1.99	0.44
2:B:719:ILE:HD12	2:B:719:ILE:HA	1.84	0.44
2:B:382:GLU:O	2:B:386:GLY:N	2.47	0.44
2:B:726:SER:HA	2:B:729:ARG:NH1	2.32	0.44
2:A:404:VAL:HG13	2:A:436:ARG:HE	1.82	0.44
2:A:661:ARG:HA	2:A:806:TYR:CD1	2.53	0.44
2:A:816:ASP:O	2:A:820:GLU:HG2	2.18	0.44
2:B:623:SER:CB	2:B:645:PRO:HB3	2.48	0.44
2:A:92:ARG:NH1	2:A:94:TYR:OH	2.50	0.44
2:A:399:ARG:CZ	2:A:431:ASP:HB3	2.47	0.44
2:A:410:ARG:HA	2:A:410:ARG:HD3	1.70	0.44
2:A:503:SER:N	2:A:516:TRP:HA	2.30	0.43
2:B:534:TYR:CD1	2:B:580:MET:HE3	2.53	0.43
2:B:665:ASP:OD1	2:B:665:ASP:N	2.48	0.43
2:B:428:TYR:HE1	2:B:430:LEU:HD21	1.83	0.43
2:A:627:ASP:O	2:A:642:TRP:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:811:GLN:HE22	2:A:825:ALA:HA	1.82	0.43
2:B:622:PRO:HD2	2:B:823:SER:HA	1.99	0.43
2:B:639:ILE:HG12	2:B:796:VAL:HG13	1.99	0.43
2:A:492:GLN:N	2:A:492:GLN:OE1	2.52	0.43
2:B:399:ARG:HD2	2:B:399:ARG:HA	1.71	0.43
2:B:421:GLU:HB3	2:B:425:TYR:HB2	2.00	0.43
2:B:634:SER:OG	2:B:637:GLN:HG3	2.19	0.43
2:B:874:VAL:HG13	2:B:913:ILE:HG12	2.01	0.43
2:B:562:ASP:N	2:B:562:ASP:OD1	2.51	0.43
2:B:623:SER:O	2:B:824:VAL:HG22	2.19	0.43
2:B:847:HIS:HD2	2:B:930:PHE:HB3	1.84	0.43
2:B:520:TRP:CH2	2:B:564:PRO:HD2	2.54	0.43
1:E:11:VAL:HG13	1:E:24:TYR:CE2	2.54	0.43
2:B:479:GLN:HG2	2:B:482:ASN:HA	2.01	0.43
2:B:652:ILE:HG22	2:B:655:TYR:HE2	1.83	0.43
2:A:440:ASP:OD2	2:A:443:LYS:NZ	2.47	0.43
2:B:652:ILE:HG22	2:B:655:TYR:CE2	2.55	0.42
2:B:869:ILE:HG21	2:B:872:TYR:CZ	2.54	0.42
2:A:536:GLU:HG3	2:A:538:PRO:HD3	2.01	0.42
2:B:559:VAL:HG11	2:B:578:TRP:NE1	2.34	0.42
2:A:270:PRO:N	2:A:271:PRO:HD2	2.34	0.42
2:A:307:HIS:ND1	2:A:308:ASN:OD1	2.51	0.42
2:A:530:PHE:CZ	2:A:564:PRO:HD3	2.53	0.42
1:E:53:ASP:N	1:E:53:ASP:OD1	2.52	0.42
2:B:793:GLU:N	2:B:793:GLU:OE1	2.52	0.42
2:B:824:VAL:O	2:B:825:ALA:HB2	2.19	0.42
2:A:914:ARG:HB2	2:A:924:TRP:CD2	2.55	0.42
2:B:725:GLU:HG2	2:A:171:TYR:OH	2.20	0.42
2:A:282:ASN:OD1	2:A:282:ASN:N	2.53	0.42
2:A:302:HIS:CG	2:A:313:PRO:HB3	2.55	0.42
2:A:560:ASP:OD2	2:A:560:ASP:N	2.50	0.42
2:A:603:ARG:HA	2:A:603:ARG:HD2	1.87	0.42
2:B:351:VAL:O	2:B:355:GLN:HG2	2.20	0.42
2:B:428:TYR:HA	2:B:454:PHE:HB3	2.02	0.42
2:B:619:ALA:HB3	2:B:821:ARG:NH2	2.35	0.42
2:B:858:MET:HE3	2:B:897:ARG:O	2.20	0.42
2:A:627:ASP:HB3	2:A:643:LYS:HG3	2.01	0.42
2:A:237:SER:O	2:A:256:ARG:NH1	2.53	0.42
1:C:17:VAL:HG21	1:C:57:LEU:HD23	2.02	0.42
2:B:640:LEU:O	2:B:794:SER:HA	2.20	0.41
2:A:76:LEU:HA	2:A:76:LEU:HD12	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:307:HIS:O	2:A:309:ASN:N	2.53	0.41
2:A:515:ARG:NH1	2:A:575:HIS:O	2.52	0.41
2:B:412:LEU:HD23	2:B:439:TRP:CZ2	2.55	0.41
2:B:496:GLU:O	2:B:606:TYR:HD2	2.03	0.41
2:A:415:ILE:HB	2:A:448:ILE:HG12	2.02	0.41
1:E:13:ALA:O	1:E:17:VAL:HG23	2.20	0.41
2:B:437:GLN:OE1	2:B:545:PHE:HB2	2.20	0.41
2:B:815:GLN:OE1	2:B:821:ARG:HB2	2.20	0.41
2:B:787:GLU:OE1	2:B:788:LYS:N	2.40	0.41
2:B:789:VAL:HG13	2:B:792:LYS:NZ	2.35	0.41
2:B:813:CYS:HB3	2:B:822:CYS:HB2	1.76	0.41
2:B:873:GLU:N	2:B:914:ARG:O	2.39	0.41
2:A:32:GLY:HA3	2:A:54:SER:HB2	2.01	0.41
2:B:396:LYS:HG3	2:B:428:TYR:HB3	2.03	0.41
2:B:497:ASN:ND2	2:B:606:TYR:HB2	2.35	0.41
2:B:509:PHE:CD1	2:B:510:ASP:HB3	2.55	0.41
2:B:914:ARG:HD3	2:B:924:TRP:NE1	2.36	0.41
2:B:463:LEU:HD13	2:B:463:LEU:HA	1.96	0.41
2:A:181:GLU:O	2:A:182:CYS:C	2.59	0.41
1:E:8:ALA:O	1:E:11:VAL:HB	2.20	0.41
2:B:371:ILE:O	2:B:400:SER:HA	2.21	0.41
2:A:432:ASN:HB3	2:A:435:LEU:HB2	2.02	0.41
2:B:463:LEU:HB3	2:B:467:HIS:CE1	2.56	0.41
2:B:624:VAL:H	2:B:645:PRO:HB3	1.86	0.41
2:B:810:LEU:HD23	2:B:826:ALA:HB3	2.03	0.41
2:A:233:LEU:HD12	2:A:246:PRO:HG3	2.02	0.41
2:B:362:VAL:HA	2:B:390:GLU:O	2.21	0.41
2:B:893:PHE:O	2:B:897:ARG:NH1	2.53	0.41
2:B:437:GLN:HB2	2:B:545:PHE:CD1	2.55	0.40
2:B:441:TRP:CH2	2:B:472:VAL:HG11	2.56	0.40
2:A:243:CYS:HA	2:A:252:CYS:HA	2.04	0.40
1:C:46:GLU:O	1:C:52:CYS:HB3	2.21	0.40
2:B:855:VAL:HG21	2:B:930:PHE:CD2	2.56	0.40
1:E:11:VAL:HG13	1:E:24:TYR:CZ	2.57	0.40
2:B:533:PHE:HA	2:B:557:THR:O	2.22	0.40
2:A:169:ASP:OD1	2:A:169:ASP:N	2.55	0.40
2:B:878:ARG:HB3	2:B:881:ASP:HB2	2.04	0.40
2:A:298:ARG:H	2:A:298:ARG:HG2	1.71	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	C	42/195 (22%)	41 (98%)	1 (2%)	0	100 100
1	D	7/195 (4%)	7 (100%)	0	0	100 100
1	E	28/195 (14%)	26 (93%)	2 (7%)	0	100 100
2	A	773/1370 (56%)	737 (95%)	35 (4%)	1 (0%)	48 78
2	B	505/1370 (37%)	471 (93%)	33 (6%)	1 (0%)	44 73
All	All	1355/3325 (41%)	1282 (95%)	71 (5%)	2 (0%)	50 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASN
2	B	823	SER

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	C	39/167 (23%)	36 (92%)	3 (8%)	10 36
1	D	8/167 (5%)	7 (88%)	1 (12%)	3 17
1	E	26/167 (16%)	23 (88%)	3 (12%)	4 20
2	A	709/1215 (58%)	686 (97%)	23 (3%)	34 62
2	B	463/1215 (38%)	440 (95%)	23 (5%)	20 51
All	All	1245/2931 (42%)	1192 (96%)	53 (4%)	27 54

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	ASP
2	B	339	CYS
2	B	392	SER
2	B	428	TYR
2	B	433	GLN
2	B	446	LEU
2	B	452	LYS
2	B	460	LYS
2	B	478	ARG
2	B	486	LEU
2	B	510	ASP
2	B	594	LYS
2	B	609	LYS
2	B	618	ASP
2	B	632	SER
2	B	634	SER
2	B	643	LYS
2	B	659	TRP
2	B	726	SER
2	B	727	SER
2	B	794	SER
2	B	810	LEU
2	B	822	CYS
2	B	824	VAL
2	A	44	LEU
2	A	68	THR
2	A	75	ASP
2	A	77	SER
2	A	161	SER
2	A	171	TYR
2	A	177	ASP
2	A	180	GLU
2	A	209	CYS
2	A	212	HIS
2	A	259	TYR
2	A	345	GLU
2	A	356	GLU
2	A	399	ARG
2	A	431	ASP
2	A	436	ARG
2	A	478	ARG
2	A	482	ASN

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Mol	Chain	Res	Type
2	A	599	PHE
2	A	641	LYS
2	A	659	TRP
2	A	819	GLU
2	A	858	MET
1	C	20	ASP
1	C	25	PHE
1	C	51	SER
1	E	23	PHE
1	E	53	ASP
1	E	59	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	384	ASN
2	B	432	ASN
2	A	42	ASN
2	A	322	ASN
2	A	325	ASN
2	A	815	GLN

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.

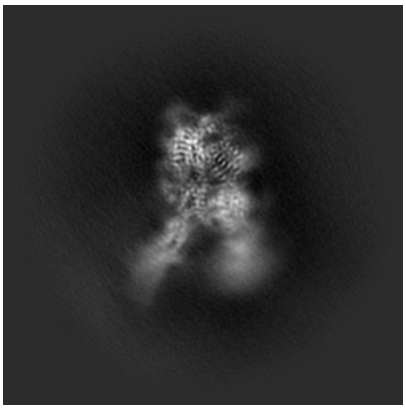
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38404. These allow visual inspection of the internal detail of the map and identification of artifacts.

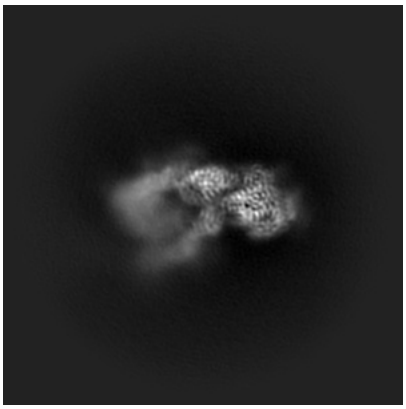
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

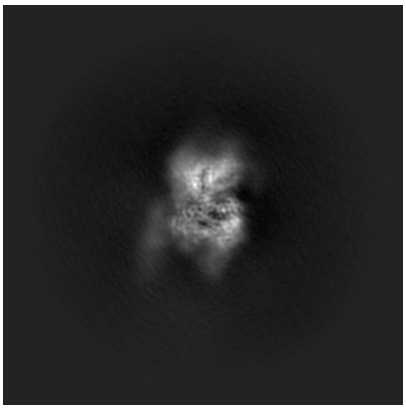
6.1.1 Primary map



X

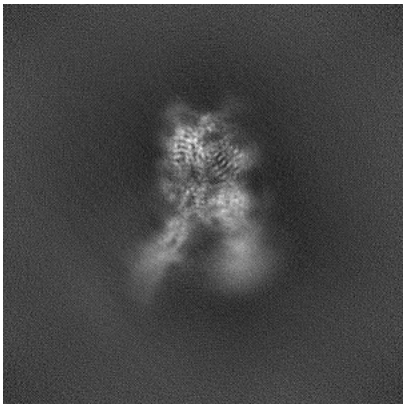


Y

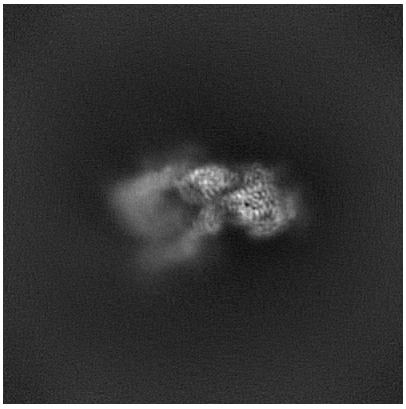


Z

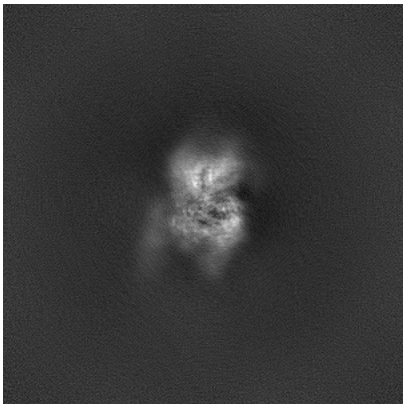
6.1.2 Raw map



X



Y

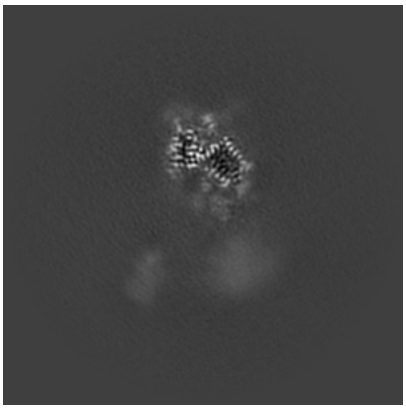


Z

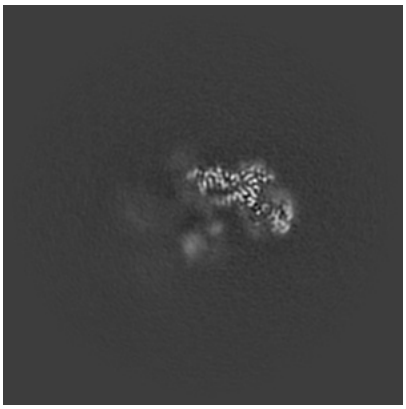
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

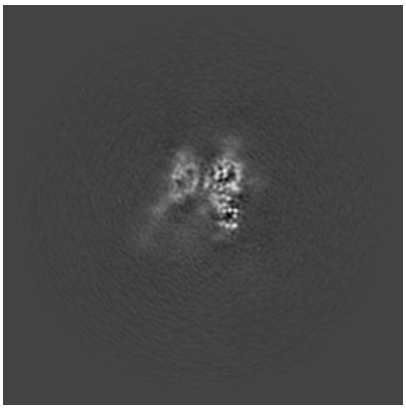
6.2.1 Primary map



X Index: 256

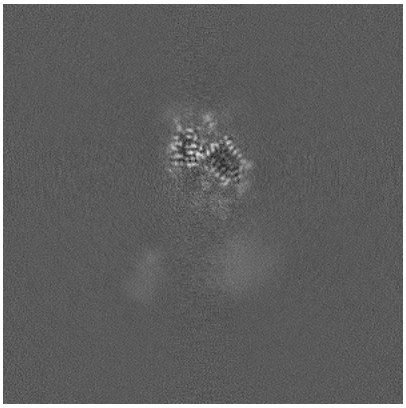


Y Index: 256

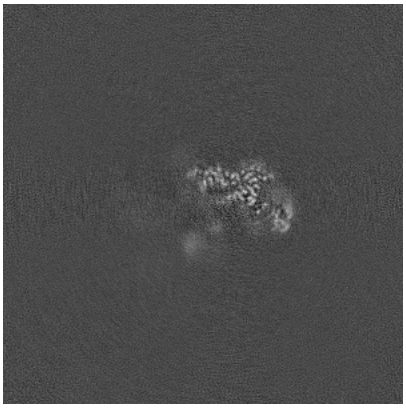


Z Index: 256

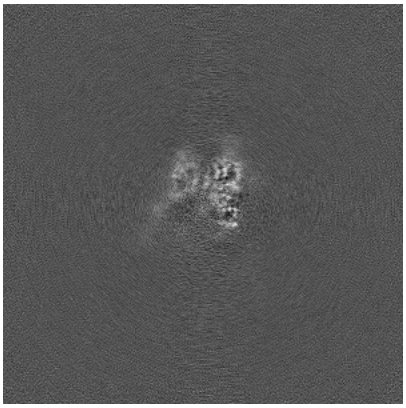
6.2.2 Raw map



X Index: 256



Y Index: 256



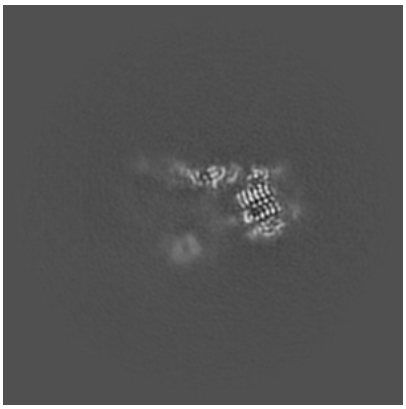
Z Index: 256

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

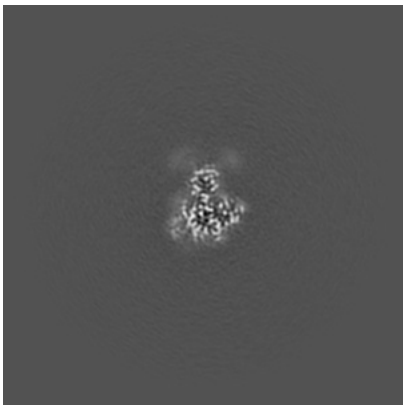
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 265



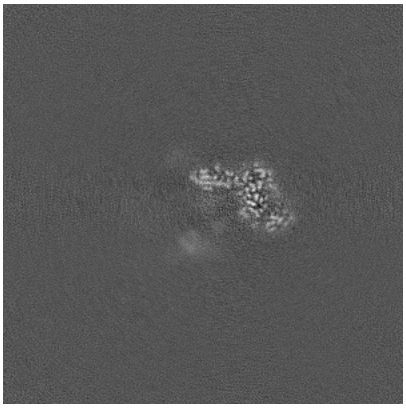
Y Index: 236



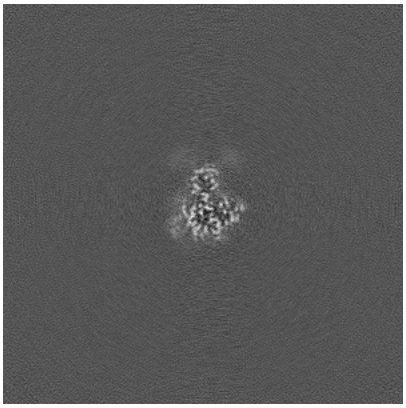
Z Index: 324

6.3.2 Raw map

X Index: 266



Y Index: 249

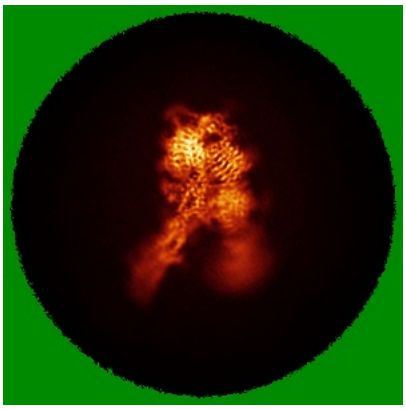


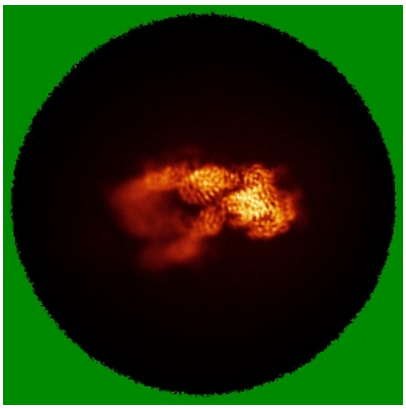
Z Index: 324

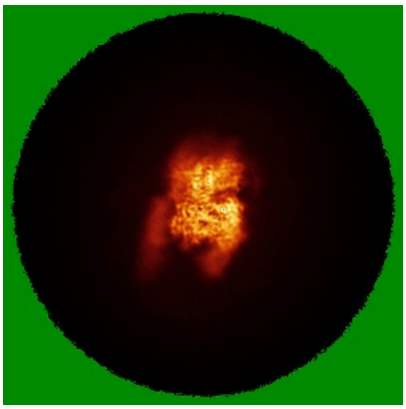
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

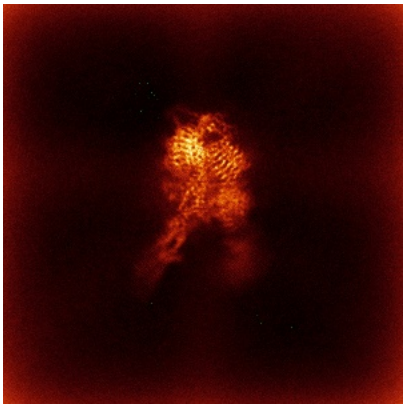
6.4.1 Primary map

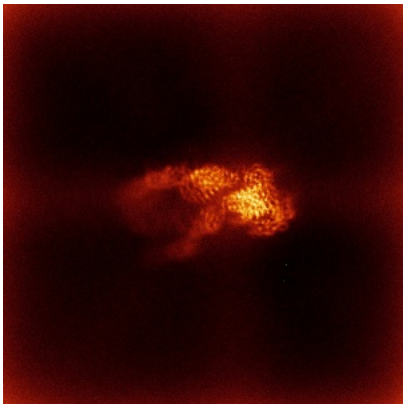

X

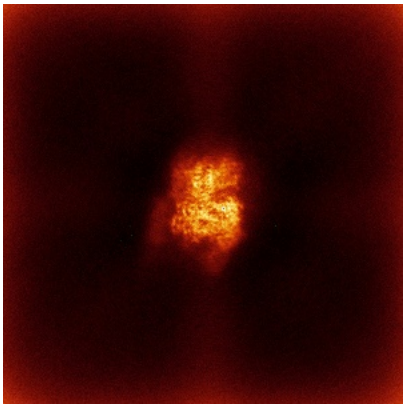

Y


Z

6.4.2 Raw 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.

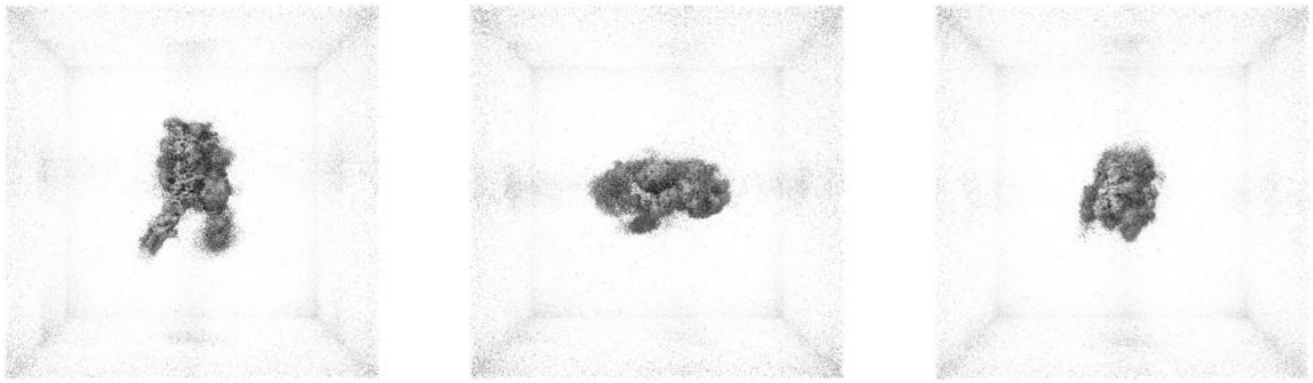
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

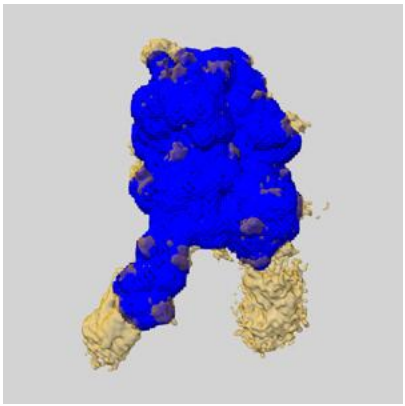
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

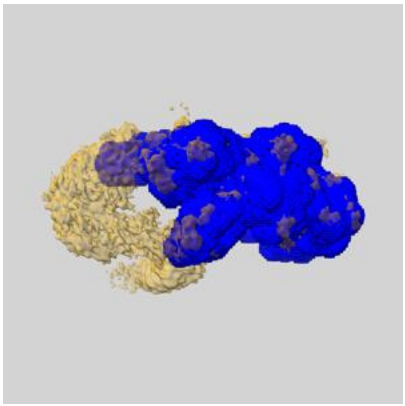
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

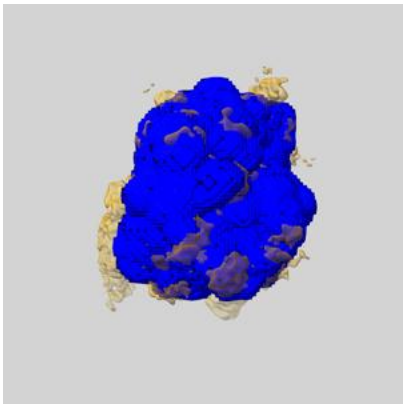
6.6.1 emd_38404_msk_1.map (i)



X



Y

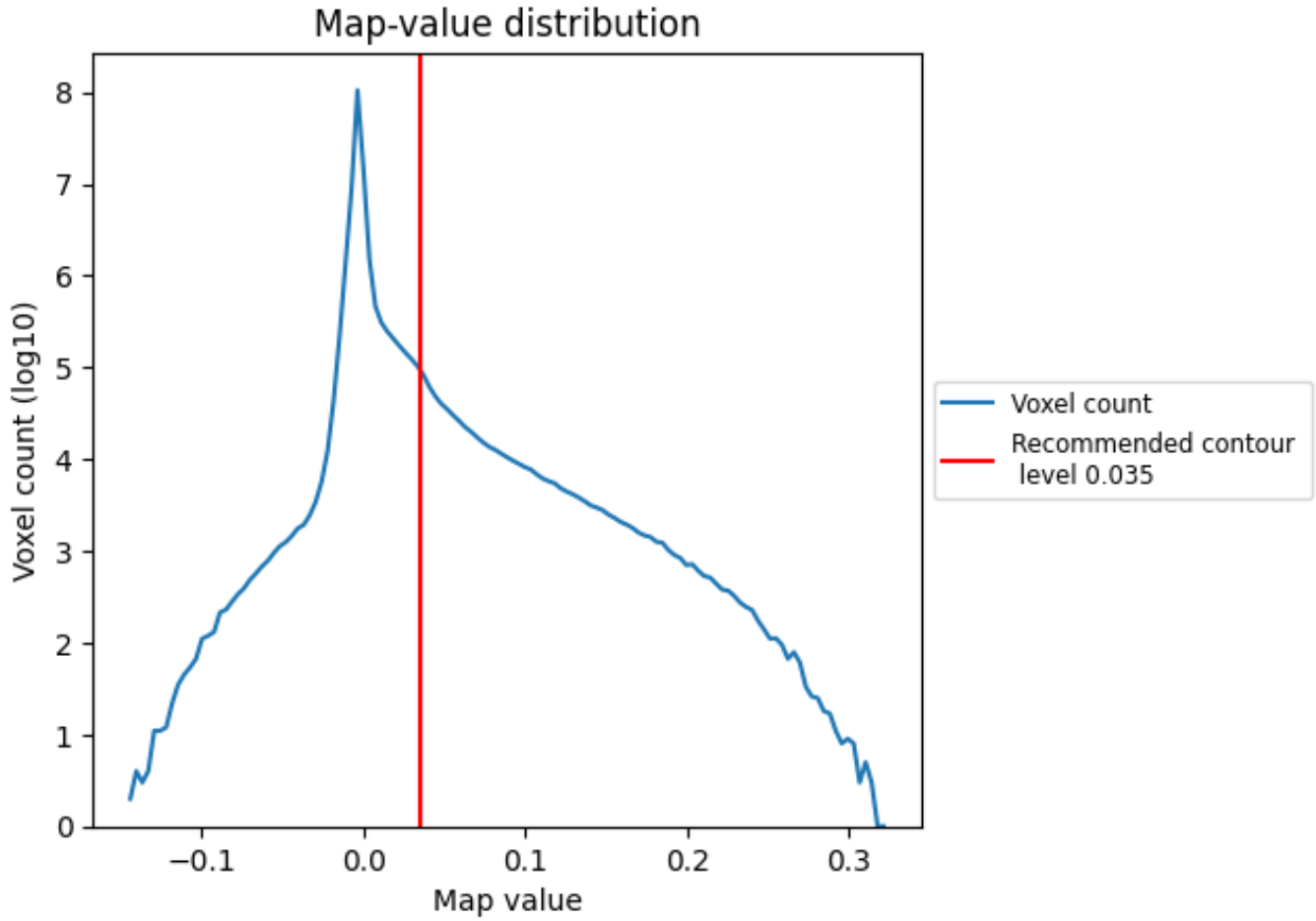


Z

7 Map analysis

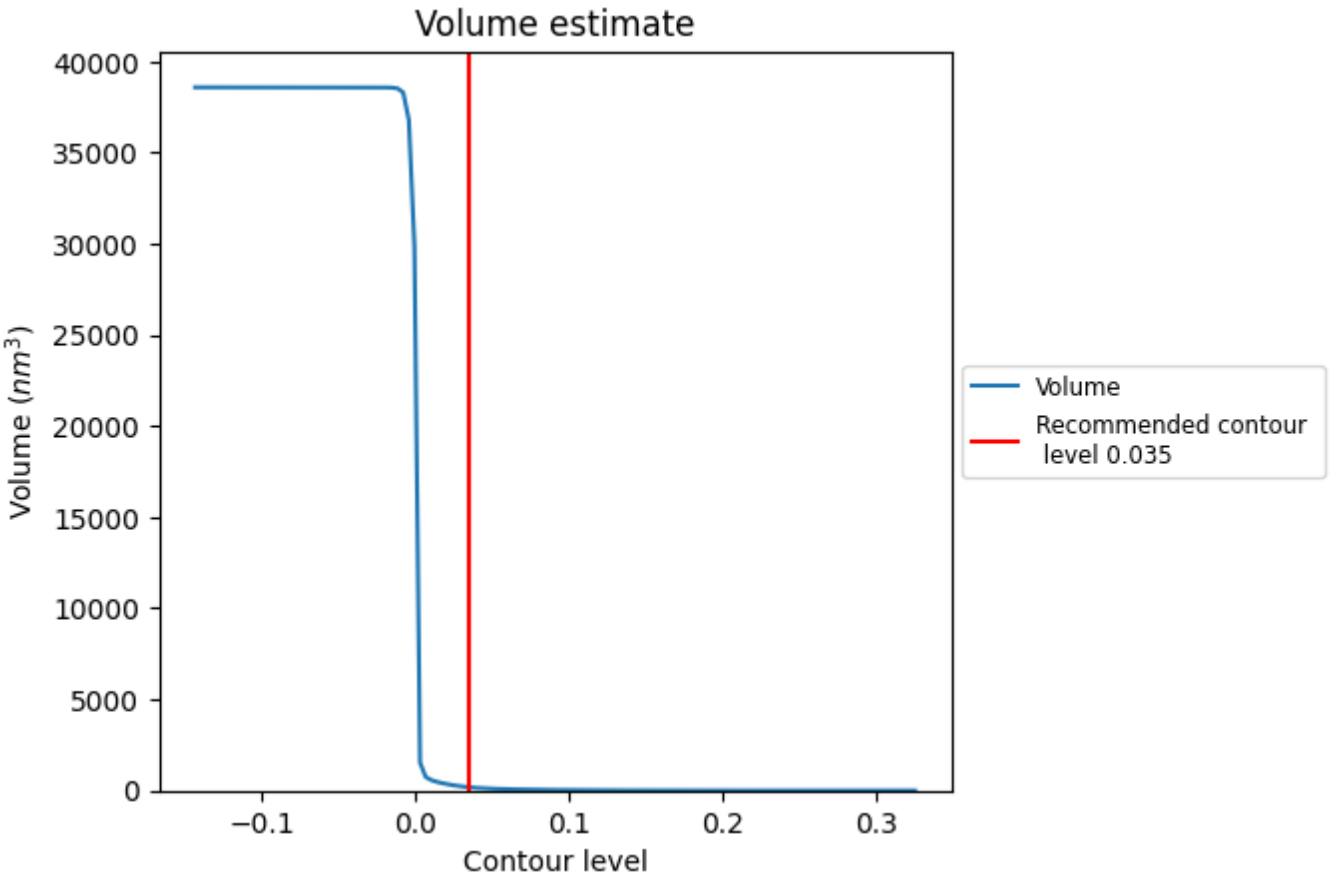
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

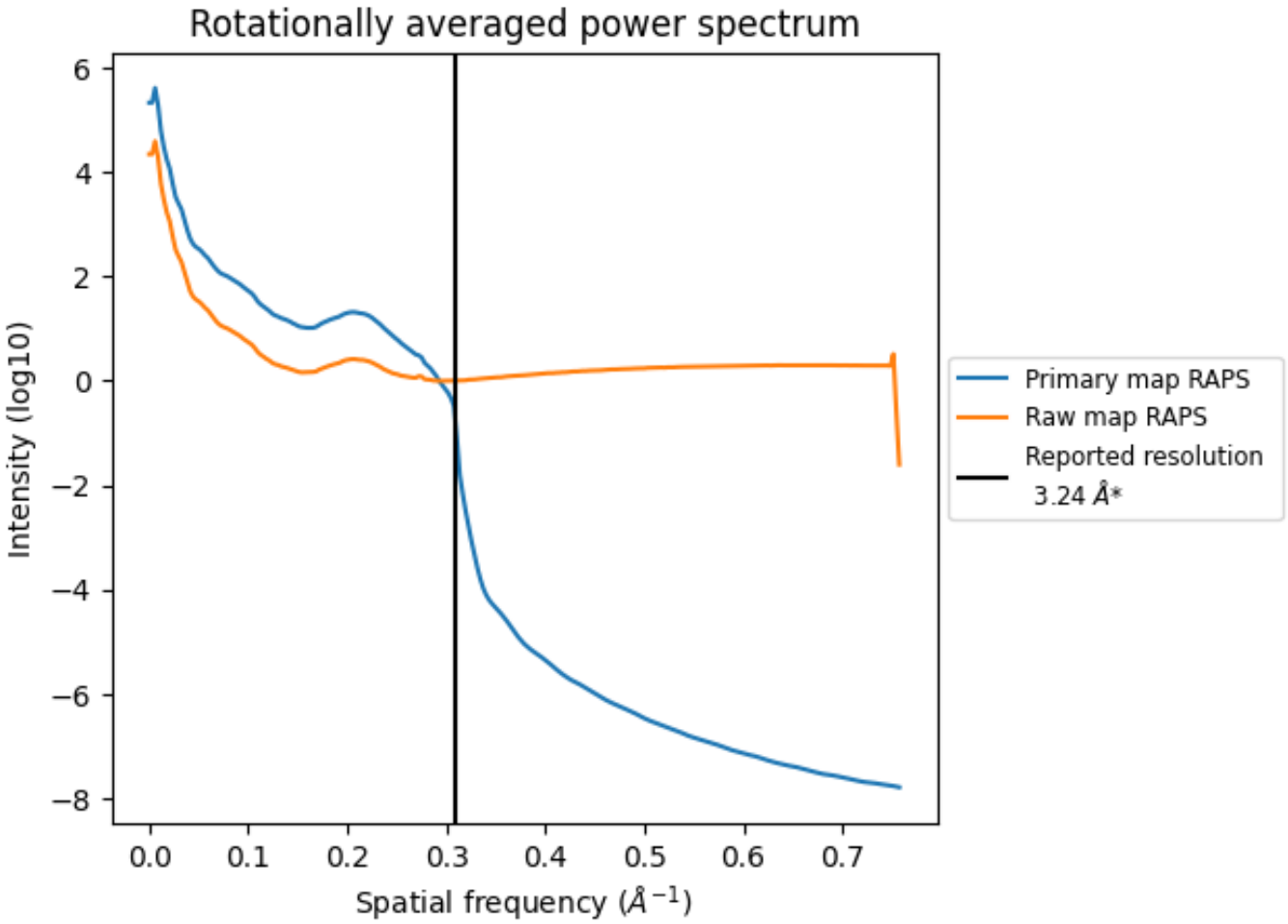
7.2 Volume estimate



The volume at the recommended contour level is 180 nm^3; this corresponds to an approximate mass of 163 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)

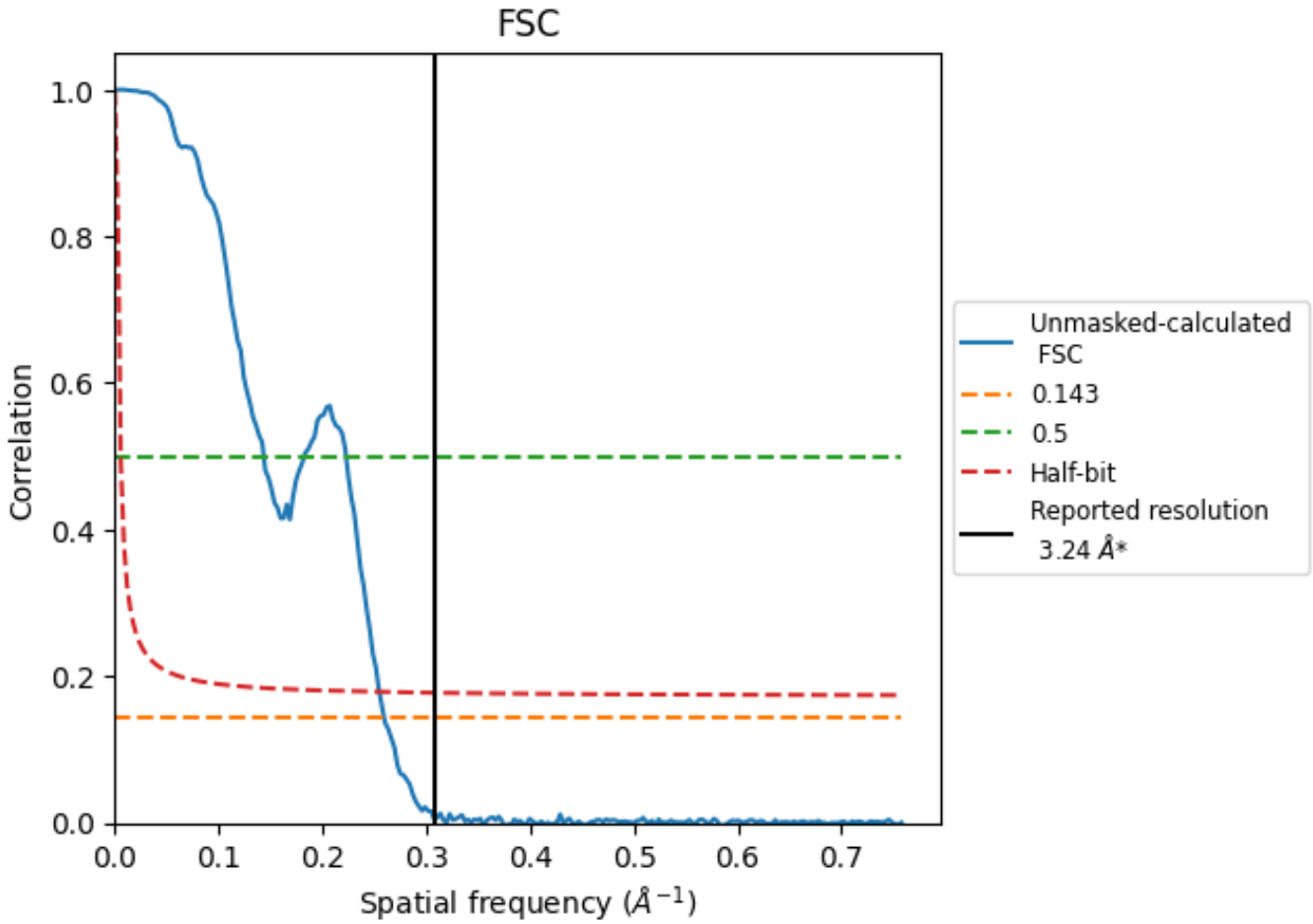


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8.2 Resolution estimates (i)

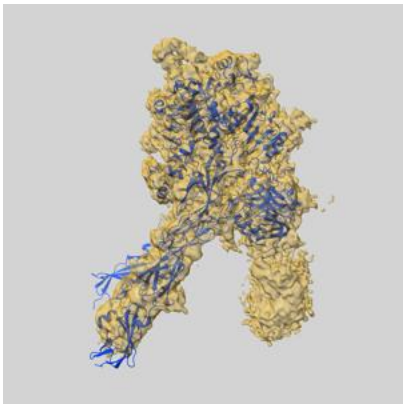
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.97	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.24 by more than 10 %

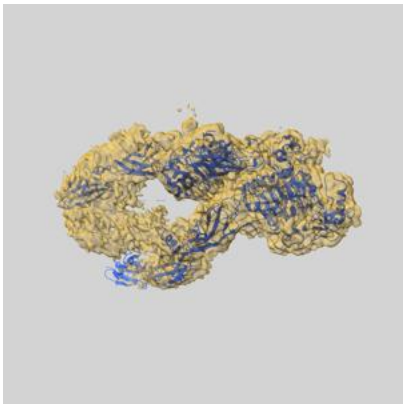
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38404 and PDB model 8XJS. Per-residue inclusion information can be found in section 3 on page 4.

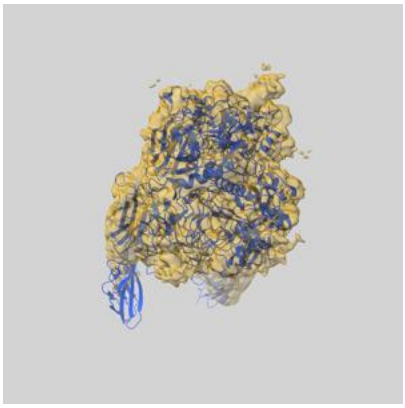
9.1 Map-model overlay



X



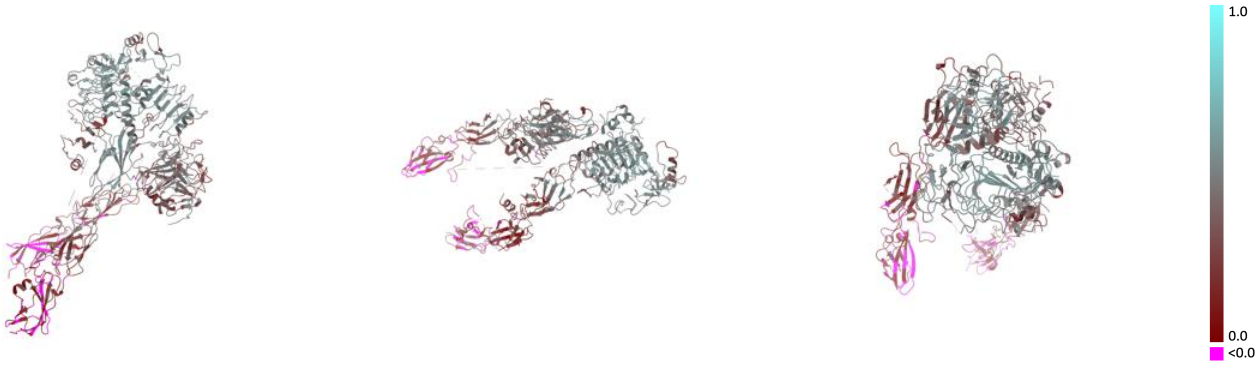
Y



Z

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

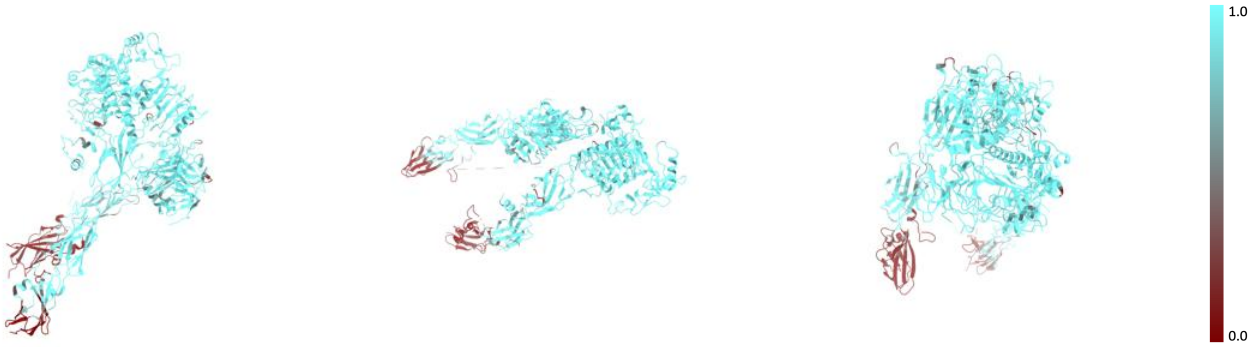
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

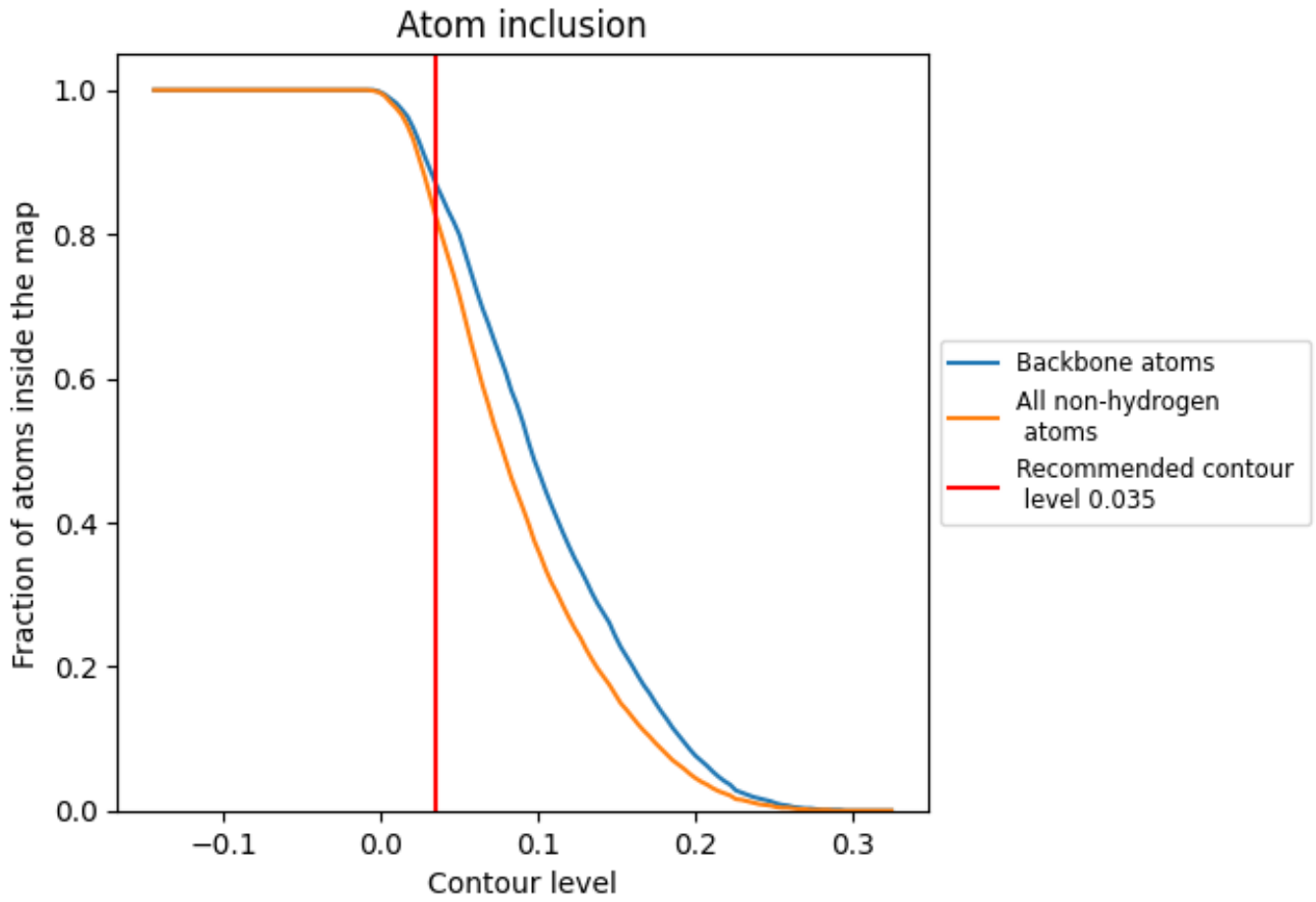
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.3620
A	0.8160	0.3730
B	0.8280	0.3370
C	0.9860	0.5100
D	0.8840	0.2780
E	0.8580	0.3330