



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 10:58 AM JST

PDB ID : 7YRR
EMDB ID : EMD-34065
Title : Cryo-EM structure of IGF1R with two IGF1 complex
Authors : Xi, Z.; Cang, W.
Deposited on : 2022-08-10
Resolution : 4.30 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) : 2.39

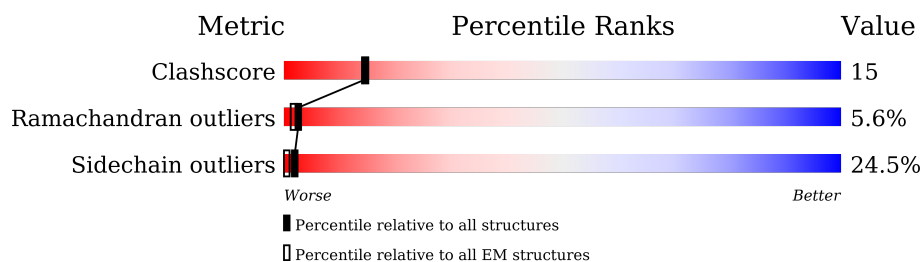
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	897	<p>15% 55% 27% 7% 11%</p>
1	B	897	<p>16% 52% 32% 6% 10%</p>
2	C	60	<p>15% 33% 25% 27%</p>
2	D	60	<p>8% 27% 27% 20% 27%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24937 atoms, of which 11408 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 1 receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	799	Total	C	H	N	O	S	0	0
			12029	4023	5649	1097	1210	50		
1	B	810	Total	C	H	N	O	S	0	0
			12242	4089	5759	1117	1227	50		

- Molecule 2 is a protein called Isoform 3 of Insulin-like growth factor I.

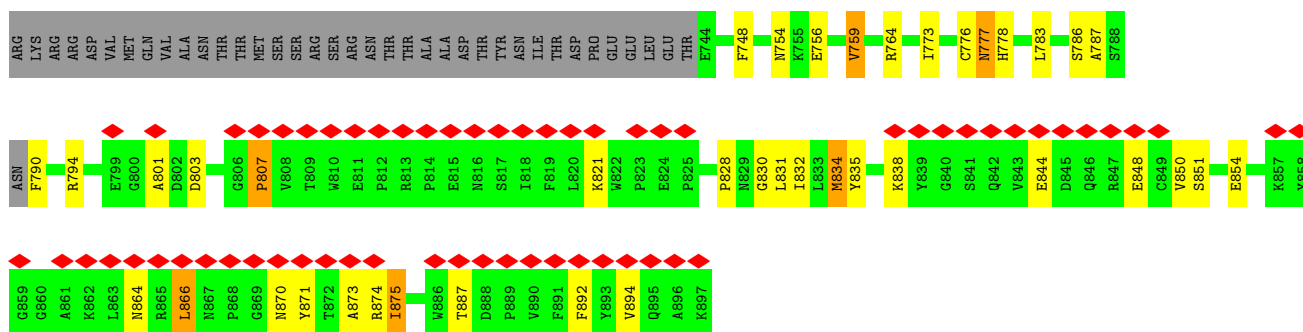
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	44	Total	C	N	O	S	0	0
			333	204	58	64	7		
2	D	44	Total	C	N	O	S	0	0
			333	204	58	64	7		

3 Residue-property plots

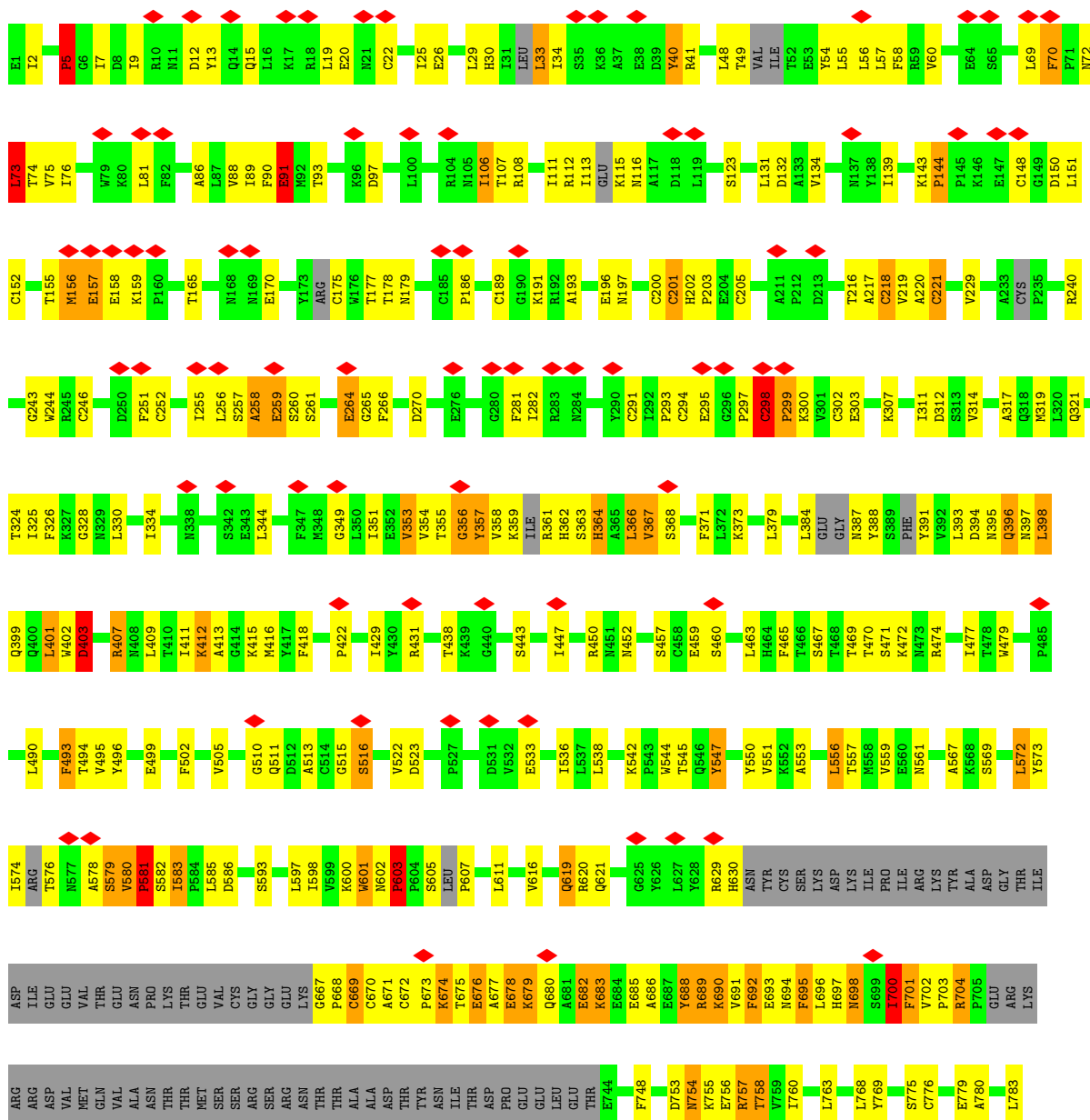
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

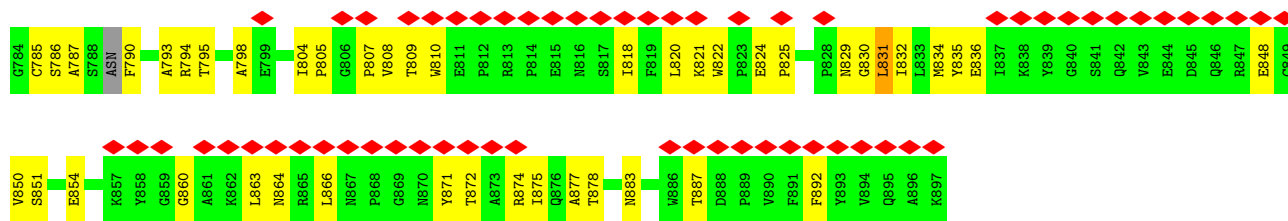
- Molecule 1: Insulin-like growth factor 1 receptor



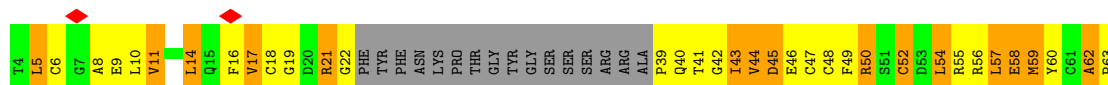


• Molecule 1: Insulin-like growth factor 1 receptor

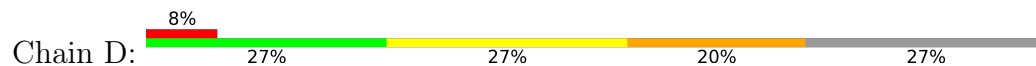




- Molecule 2: Isoform 3 of Insulin-like growth factor I



- Molecule 2: Isoform 3 of Insulin-like growth factor I



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	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	0.666	Depositor
Minimum map value	-0.421	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.062	Depositor
Map size (\AA)	297.72, 297.72, 297.72	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.827, 0.827, 0.827	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	0.65	0/6517	1.00	0/8813
1	B	0.64	0/6630	0.99	0/8977
2	C	0.62	0/336	0.70	0/450
2	D	0.61	0/336	0.65	0/450
All	All	0.64	0/13819	0.98	0/18690

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6380	5649	6153	168	0
1	B	6483	5759	6260	216	0
2	C	333	0	314	38	0
2	D	333	0	314	29	0
All	All	13529	11408	13041	400	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 (400) 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:90:PHE:CE2	1:B:689:ARG:HA	1.73	1.22
1:B:688:TYR:HA	1:B:691:VAL:HG22	1.29	1.11
1:B:693:GLU:HB2	2:C:44:VAL:HB	1.33	1.10
1:B:556:LEU:HD23	1:B:556:LEU:H	1.18	1.08
1:A:204:GLU:OE2	1:A:204:GLU:HA	1.40	1.07
1:B:556:LEU:HD23	1:B:556:LEU:N	1.71	1.05
1:A:240:ARG:HA	1:A:246:CYS:SG	1.98	1.03
1:A:580:VAL:HG11	1:A:783:LEU:HD13	1.42	0.99
1:B:822:TRP:CZ3	1:B:875:ILE:HG12	1.99	0.97
1:A:26:GLU:HG3	1:A:26:GLU:O	1.63	0.96
1:B:411:ILE:HG22	1:B:413:ALA:O	1.66	0.96
1:B:258:ALA:HB3	1:B:261:SER:HB3	1.47	0.94
2:C:62:ALA:HB1	2:C:63:PRO:HD2	1.50	0.93
1:A:866:LEU:HB2	1:A:894:VAL:HG21	1.50	0.93
2:D:17:VAL:HB	2:D:58:GLU:HB3	1.50	0.91
1:A:192:ARG:O	1:A:193:ALA:O	1.87	0.91
1:B:703:PRO:HB3	2:C:60:TYR:HA	1.50	0.91
1:B:398:LEU:HD23	1:B:399:GLN:N	1.85	0.91
2:C:5:LEU:H	2:C:48:CYS:HA	1.33	0.89
1:A:90:PHE:HE2	1:B:689:ARG:HA	1.14	0.89
2:D:5:LEU:H	2:D:48:CYS:HA	1.39	0.87
1:A:289:MET:HE3	1:A:289:MET:HA	1.54	0.86
1:B:294:CYS:HB2	1:B:297:PRO:HG3	1.56	0.85
1:B:586:ASP:HB3	1:B:602:ASN:HB3	1.59	0.84
1:A:683:LYS:HA	1:A:686:ALA:HB3	1.60	0.84
1:A:26:GLU:HB2	1:A:241:PHE:CZ	2.13	0.83
1:A:675:THR:HA	1:B:668:PRO:HA	1.59	0.82
2:C:21:ARG:HB2	2:C:62:ALA:HB3	1.63	0.80
1:A:603:PRO:O	1:A:604:PRO:O	2.00	0.80
1:B:7:ILE:HD11	1:B:22:CYS:SG	2.22	0.79
1:B:822:TRP:CE3	1:B:875:ILE:HD13	2.18	0.78
1:B:9:ILE:HG12	1:B:15:GLN:O	1.83	0.78
1:A:90:PHE:HE2	1:B:689:ARG:CA	1.95	0.78
1:B:692:PHE:HA	1:B:695:PHE:HB2	1.65	0.78
1:B:697:HIS:HA	2:C:60:TYR:OH	1.83	0.78
1:B:411:ILE:CG2	1:B:413:ALA:O	2.32	0.77
1:B:676:GLU:HB2	1:B:678:GLU:HG2	1.66	0.77
1:A:256:LEU:HD22	1:A:264:GLU:HG2	1.67	0.76
1:A:289:MET:HA	1:A:289:MET:CE	2.16	0.76
1:A:26:GLU:O	1:A:26:GLU:CG	2.35	0.75
1:B:7:ILE:HD12	1:B:25:ILE:HD11	1.67	0.75
1:B:328:GLY:O	1:B:354:VAL:HG12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:TRP:HE3	1:B:875:ILE:HD13	1.52	0.74
1:A:673:PRO:HG2	1:B:669:CYS:HB3	1.70	0.74
1:B:686:ALA:HA	1:B:689:ARG:HB3	1.71	0.73
1:A:495:VAL:HG21	1:A:536:ILE:HG21	1.70	0.73
1:B:367:VAL:HB	1:B:515:GLY:HA2	1.70	0.73
1:B:463:LEU:O	1:B:569:SER:CB	2.37	0.73
1:B:808:VAL:HG23	1:B:887:THR:HG21	1.71	0.72
1:B:493:PHE:CZ	1:B:553:ALA:HB2	2.23	0.72
2:C:47:CYS:HA	2:C:52:CYS:HB3	1.71	0.72
1:B:556:LEU:N	1:B:556:LEU:CD2	2.45	0.71
1:B:693:GLU:HB2	2:C:44:VAL:CB	2.18	0.71
1:A:602:ASN:O	1:A:604:PRO:HD3	1.92	0.70
2:C:42:GLY:H	2:C:45:ASP:HB2	1.56	0.70
1:B:48:LEU:HD23	1:B:70:PHE:HB3	1.73	0.70
1:A:549:VAL:HG22	1:A:549:VAL:O	1.91	0.70
1:B:572:LEU:HD12	1:B:573:TYR:N	2.07	0.70
1:B:822:TRP:CZ3	1:B:875:ILE:CG1	2.74	0.69
2:D:46:GLU:HA	2:D:50:ARG:HH12	1.55	0.69
1:B:572:LEU:HD12	1:B:572:LEU:C	2.13	0.69
2:D:14:LEU:HD11	2:D:60:TYR:HB3	1.74	0.69
1:A:204:GLU:OE2	1:A:204:GLU:CA	2.29	0.69
1:A:704:ARG:HG2	2:D:62:ALA:HB2	1.74	0.69
1:B:866:LEU:HD22	1:B:892:PHE:HZ	1.55	0.69
1:B:366:LEU:HD22	1:B:371:PHE:CE2	2.28	0.68
2:C:17:VAL:HG22	2:C:58:GLU:HB3	1.75	0.68
1:A:234:CYS:HB2	1:A:240:ARG:HG3	1.73	0.68
1:B:619:GLN:HG2	1:B:620:ARG:N	2.08	0.68
1:A:367:VAL:O	1:A:399:GLN:N	2.27	0.68
1:B:602:ASN:O	1:B:603:PRO:C	2.32	0.67
1:B:818:ILE:HG13	1:B:892:PHE:CD1	2.28	0.67
1:B:411:ILE:HG22	1:B:413:ALA:C	2.13	0.67
1:A:670:CYS:O	1:B:671:ALA:HA	1.94	0.66
1:B:822:TRP:CD2	1:B:875:ILE:HG21	2.30	0.66
1:B:463:LEU:O	1:B:569:SER:HB3	1.95	0.66
1:B:866:LEU:HD22	1:B:892:PHE:CZ	2.30	0.66
1:B:757:ARG:HG2	1:B:758:THR:N	2.09	0.66
1:B:493:PHE:CE1	1:B:553:ALA:HB2	2.30	0.66
1:B:822:TRP:CE3	1:B:875:ILE:CD1	2.79	0.65
1:A:477:ILE:HD13	1:A:574:ILE:HD11	1.79	0.65
2:C:14:LEU:HD21	2:C:43:ILE:HD11	1.79	0.64
1:A:411:ILE:O	1:A:441:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TYR:HA	1:A:691:VAL:HG23	1.78	0.64
1:A:677:ALA:HB2	1:B:668:PRO:HG3	1.80	0.64
1:B:398:LEU:CD2	1:B:399:GLN:N	2.61	0.64
1:B:463:LEU:HB2	1:B:569:SER:HB3	1.79	0.64
1:B:398:LEU:CD2	1:B:398:LEU:C	2.66	0.64
1:A:90:PHE:CE2	1:B:689:ARG:CA	2.67	0.63
1:A:553:ALA:HB3	1:A:567:ALA:HB3	1.80	0.63
1:B:356:GLY:O	1:B:357:TYR:HB3	1.97	0.63
1:B:822:TRP:CZ3	1:B:875:ILE:CD1	2.81	0.63
1:B:470:THR:OG1	1:B:578:ALA:HA	1.98	0.63
1:A:832:ILE:HG21	1:A:835:TYR:CE1	2.33	0.63
1:A:667:GLY:N	1:B:674:LYS:HA	2.13	0.63
1:B:822:TRP:CE3	1:B:875:ILE:HG12	2.32	0.63
2:D:62:ALA:HB1	2:D:63:PRO:HD2	1.80	0.62
1:A:377:LEU:HD12	1:A:377:LEU:C	2.20	0.62
1:A:495:VAL:O	1:A:522:VAL:CG1	2.47	0.61
1:B:465:PHE:CE2	1:B:572:LEU:HB3	2.34	0.61
2:D:17:VAL:HB	2:D:58:GLU:CB	2.26	0.61
1:A:240:ARG:CA	1:A:246:CYS:SG	2.83	0.61
1:B:311:ILE:HG23	1:B:317:ALA:HB2	1.82	0.61
1:A:580:VAL:HG21	1:A:783:LEU:HD22	1.82	0.61
1:B:364:HIS:HA	1:B:397:ASN:HB2	1.83	0.61
2:D:17:VAL:HG11	2:D:57:LEU:HB3	1.80	0.61
1:A:112:ARG:CZ	1:B:688:TYR:HB2	2.30	0.61
1:B:688:TYR:HA	1:B:691:VAL:CG2	2.20	0.60
1:B:822:TRP:CE3	1:B:875:ILE:CG1	2.84	0.60
1:B:463:LEU:CB	1:B:569:SER:HB3	2.31	0.60
1:B:465:PHE:CD1	1:B:477:ILE:HD11	2.37	0.60
2:D:47:CYS:HA	2:D:52:CYS:HB3	1.84	0.60
1:A:192:ARG:C	1:A:193:ALA:O	2.39	0.60
1:B:830:GLY:O	1:B:831:LEU:HB2	2.01	0.60
2:D:46:GLU:HA	2:D:50:ARG:NH1	2.17	0.60
1:A:339:ASN:C	1:A:341:ALA:H	2.04	0.60
1:B:193:ALA:HB3	1:B:201:CYS:CB	2.32	0.60
1:B:691:VAL:HG11	2:C:40:GLN:HG3	1.84	0.60
1:A:90:PHE:CZ	1:B:689:ARG:HA	2.33	0.59
1:A:495:VAL:O	1:A:522:VAL:HG12	2.02	0.59
1:B:472:LYS:HA	1:B:580:VAL:HG23	1.83	0.59
1:A:399:GLN:NE2	1:A:456:ALA:HB1	2.18	0.59
1:B:790:PHE:CE1	2:C:54:LEU:HB3	2.37	0.59
1:A:411:ILE:O	1:A:441:ARG:CZ	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LEU:HD23	1:B:399:GLN:H	1.68	0.59
1:A:692:PHE:HA	1:B:112:ARG:NH1	2.18	0.58
1:B:704:ARG:HB2	2:C:59:MET:HG2	1.83	0.58
1:A:611:LEU:HD21	1:A:614:TYR:CZ	2.39	0.58
1:B:818:ILE:HG13	1:B:892:PHE:CE1	2.39	0.58
1:B:411:ILE:O	1:B:413:ALA:N	2.37	0.57
1:A:674:LYS:HA	1:B:670:CYS:HB3	1.86	0.57
1:B:597:LEU:HD21	1:B:793:ALA:HB3	1.87	0.57
1:A:697:HIS:CB	2:D:44:VAL:HB	2.34	0.57
1:A:697:HIS:HB3	2:D:44:VAL:HB	1.87	0.57
1:A:495:VAL:C	1:A:522:VAL:HG12	2.25	0.57
1:B:302:CYS:HB3	1:B:326:PHE:CA	2.35	0.57
1:B:580:VAL:HG11	1:B:783:LEU:HD12	1.86	0.57
1:A:33:LEU:HB2	1:B:700:ILE:HD12	1.85	0.57
1:A:557:THR:HG22	1:A:564:ILE:HG21	1.87	0.57
1:B:583:ILE:HB	1:B:787:ALA:HB3	1.86	0.57
1:B:12:ASP:OD1	1:B:13:TYR:N	2.38	0.56
1:B:820:LEU:HD11	1:B:863:LEU:HD21	1.86	0.56
2:C:8:ALA:HA	2:C:11:VAL:HG13	1.86	0.56
1:A:611:LEU:HD21	1:A:614:TYR:CE1	2.39	0.56
1:A:263:SER:HB2	1:A:275:GLN:HG3	1.87	0.56
1:B:302:CYS:HB3	1:B:326:PHE:HA	1.87	0.56
1:B:463:LEU:O	1:B:569:SER:HB2	2.05	0.56
1:A:790:PHE:CE1	2:D:54:LEU:HB3	2.39	0.56
1:B:824:GLU:HG3	1:B:825:PRO:HD2	1.87	0.56
1:B:411:ILE:O	1:B:412:LYS:C	2.44	0.56
2:C:62:ALA:HB1	2:C:63:PRO:CD	2.31	0.56
1:A:58:PHE:CE2	1:B:696:LEU:HD21	2.41	0.56
1:A:866:LEU:CB	1:A:894:VAL:HG21	2.31	0.56
1:B:619:GLN:OE1	1:B:621:GLN:HA	2.06	0.56
1:A:675:THR:HB	1:B:670:CYS:SG	2.46	0.55
1:B:553:ALA:HB3	1:B:567:ALA:HB3	1.87	0.55
1:B:398:LEU:HD23	1:B:398:LEU:C	2.25	0.55
1:A:425:CYS:SG	1:A:428:GLU:OE2	2.63	0.55
1:B:396:GLN:O	1:B:398:LEU:O	2.25	0.55
1:B:688:TYR:O	1:B:692:PHE:HB2	2.07	0.55
2:D:14:LEU:HA	2:D:17:VAL:HG22	1.89	0.55
1:B:863:LEU:HB2	1:B:866:LEU:HD11	1.87	0.55
1:A:495:VAL:O	1:A:495:VAL:HG12	2.06	0.54
1:A:704:ARG:CG	2:D:62:ALA:HB2	2.37	0.54
1:B:691:VAL:HG12	2:C:40:GLN:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:HE2	1:A:675:THR:H	1.73	0.54
1:B:29:LEU:HD23	1:B:55:LEU:CD1	2.36	0.54
1:B:477:ILE:HD12	1:B:574:ILE:CD1	2.38	0.54
1:A:26:GLU:HB2	1:A:241:PHE:HZ	1.68	0.54
1:A:495:VAL:HG13	1:A:551:VAL:HG22	1.89	0.54
1:A:583:ILE:HB	1:A:787:ALA:HB3	1.90	0.54
1:A:33:LEU:HD12	1:B:700:ILE:HD11	1.89	0.54
1:B:693:GLU:HA	1:B:697:HIS:HB2	1.88	0.54
1:A:418:PHE:HB2	1:A:447:ILE:HG23	1.90	0.53
1:A:577:ASN:HB2	1:A:778:HIS:CE1	2.43	0.53
2:D:6:CYS:HA	2:D:10:LEU:HD22	1.90	0.53
1:B:111:ILE:HD11	1:B:139:ILE:HD11	1.90	0.53
1:B:679:LYS:O	1:B:682:GLU:HB2	2.08	0.53
1:B:697:HIS:HA	2:C:60:TYR:CZ	2.43	0.53
1:A:377:LEU:HD12	1:A:378:ILE:N	2.23	0.53
1:A:12:ASP:C	1:A:34:ILE:HG23	2.29	0.52
1:A:13:TYR:CD1	1:A:34:ILE:HG22	2.44	0.52
1:B:600:LYS:HG2	1:B:601:TRP:H	1.74	0.52
1:A:686:ALA:O	1:A:689:ARG:HB2	2.10	0.52
1:A:702:VAL:N	1:A:703:PRO:HD2	2.24	0.52
1:B:692:PHE:CA	1:B:695:PHE:HB2	2.37	0.52
1:A:173:TYR:HD1	1:A:173:TYR:N	2.06	0.52
1:B:367:VAL:CB	1:B:515:GLY:HA2	2.39	0.52
1:B:669:CYS:HA	1:B:672:CYS:HB3	1.92	0.52
1:B:763:LEU:HD22	1:B:769:TYR:CE1	2.45	0.52
1:B:202:HIS:O	1:B:203:PRO:C	2.48	0.52
1:A:677:ALA:HB2	1:B:668:PRO:CG	2.40	0.52
1:A:3:CYS:SG	1:A:7:ILE:HD11	2.50	0.51
1:A:258:ALA:HB3	1:A:261:SER:HB3	1.91	0.51
1:A:573:TYR:O	1:A:574:ILE:C	2.49	0.51
1:B:34:ILE:HB	1:B:60:VAL:HG13	1.91	0.51
1:B:282:ILE:HG22	1:B:325:ILE:HD11	1.93	0.51
1:A:339:ASN:C	1:A:341:ALA:N	2.63	0.51
1:B:19:LEU:HD22	1:B:48:LEU:HD22	1.93	0.51
1:B:703:PRO:CB	2:C:60:TYR:HA	2.32	0.51
1:B:755:LYS:HD2	1:B:757:ARG:NH1	2.25	0.51
1:A:173:TYR:N	1:A:173:TYR:CD1	2.77	0.51
1:A:677:ALA:HA	1:A:679:LYS:HE3	1.92	0.51
1:B:220:ALA:O	1:B:221:CYS:HB3	2.11	0.51
1:B:359:LYS:HD2	1:B:384:LEU:HD11	1.92	0.51
1:B:416:MET:CG	1:B:438:THR:HG21	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:PRO:HG3	1:B:824:GLU:O	2.11	0.51
1:A:193:ALA:HB2	1:A:206:LEU:CA	2.40	0.51
1:A:495:VAL:HG22	1:A:551:VAL:HG13	1.92	0.51
1:B:808:VAL:HG22	1:B:822:TRP:HB3	1.93	0.50
1:A:289:MET:CE	1:A:289:MET:CA	2.84	0.50
1:B:193:ALA:HB3	1:B:201:CYS:SG	2.51	0.50
1:B:299:PRO:HD2	1:B:324:THR:HG21	1.94	0.50
1:B:583:ILE:HG13	2:C:55:ARG:HD3	1.93	0.50
2:D:10:LEU:HD21	2:D:43:ILE:HG23	1.93	0.50
1:A:339:ASN:O	1:A:341:ALA:N	2.45	0.50
1:A:468:THR:HG22	1:A:477:ILE:CD1	2.42	0.50
1:B:701:PHE:CE2	2:C:22:GLY:HA2	2.46	0.50
2:C:10:LEU:CD2	2:C:44:VAL:HG23	2.41	0.50
1:A:7:ILE:HD11	1:A:22:CYS:SG	2.52	0.50
1:A:263:SER:HB2	1:A:275:GLN:CG	2.42	0.50
1:B:49:THR:HG22	1:B:72:ASN:O	2.11	0.50
2:D:8:ALA:HA	2:D:11:VAL:HG13	1.93	0.50
1:B:86:ALA:HB3	1:B:106:ILE:CG1	2.41	0.49
1:B:495:VAL:HG21	1:B:536:ILE:HG21	1.92	0.49
1:B:677:ALA:HA	1:B:679:LYS:HE3	1.94	0.49
1:B:697:HIS:HA	2:C:60:TYR:CE1	2.47	0.49
2:D:55:ARG:O	2:D:58:GLU:HG3	2.12	0.49
1:A:129:LEU:HD12	1:A:165:THR:HG21	1.94	0.49
1:B:832:ILE:HG21	1:B:835:TYR:CE1	2.47	0.49
1:A:425:CYS:SG	1:A:428:GLU:HG2	2.52	0.49
1:A:580:VAL:HG11	1:A:783:LEU:CD1	2.27	0.49
2:C:49:PHE:HB3	2:C:50:ARG:NH2	2.27	0.49
1:B:820:LEU:HD21	1:B:863:LEU:HD11	1.95	0.49
1:A:581:PRO:HD3	1:A:777:ASN:HB3	1.94	0.49
1:A:689:ARG:O	1:A:693:GLU:HG2	2.13	0.49
2:C:10:LEU:HD23	2:C:44:VAL:HG23	1.94	0.49
1:A:24:VAL:HG11	1:A:244:TRP:CD1	2.48	0.48
1:A:580:VAL:HG12	1:A:581:PRO:HD2	1.95	0.48
1:A:26:GLU:HB2	1:A:241:PHE:CE2	2.47	0.48
1:A:398:LEU:HD23	1:A:399:GLN:N	2.29	0.48
1:A:673:PRO:HD2	1:B:669:CYS:O	2.14	0.48
1:A:238:THR:O	1:A:239:TYR:CD1	2.67	0.48
1:A:667:GLY:N	1:B:675:THR:H	2.12	0.48
1:B:411:ILE:C	1:B:413:ALA:N	2.68	0.47
1:A:601:TRP:CE3	1:A:773:ILE:HD12	2.48	0.47
1:A:801:ALA:HB1	1:A:828:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:CYS:CB	1:B:297:PRO:HG3	2.36	0.47
1:B:691:VAL:HA	1:B:694:ASN:ND2	2.28	0.47
1:A:334:ILE:CG2	1:A:366:LEU:HD21	2.45	0.47
1:A:494:THR:HG22	1:A:554:VAL:HG23	1.95	0.47
1:B:151:LEU:HD23	1:B:156:MET:HA	1.95	0.47
1:A:479:TRP:CE3	1:A:551:VAL:HG11	2.49	0.47
1:A:677:ALA:HB2	1:B:668:PRO:HB3	1.96	0.47
1:B:418:PHE:HB2	1:B:447:ILE:HG23	1.96	0.47
1:A:416:MET:CG	1:A:438:THR:HG21	2.44	0.47
1:B:556:LEU:H	1:B:556:LEU:CD2	1.97	0.47
2:C:59:MET:HE2	2:C:59:MET:HB3	1.90	0.47
1:A:88:VAL:HG21	1:B:688:TYR:CE2	2.50	0.47
1:B:264:GLU:H	1:B:264:GLU:HG3	1.46	0.47
1:B:402:TRP:O	1:B:403:ASP:C	2.52	0.47
1:A:59:ARG:HA	1:A:93:THR:HG23	1.97	0.47
1:A:402:TRP:O	1:A:403:ASP:C	2.53	0.47
1:A:89:ILE:HG22	1:A:116:ASN:HD21	1.80	0.46
1:A:495:VAL:HB	1:A:536:ILE:HD13	1.97	0.46
1:B:810:TRP:CE3	1:B:818:ILE:HD12	2.51	0.46
1:A:356:GLY:O	1:A:357:TYR:HB3	2.15	0.46
1:B:479:TRP:CD2	1:B:551:VAL:HG11	2.51	0.46
1:B:581:PRO:HG2	1:B:780:ALA:HA	1.97	0.46
1:A:495:VAL:HG21	1:A:536:ILE:CG2	2.42	0.46
1:A:592:ASN:HD21	1:A:759:VAL:HG21	1.79	0.46
1:A:193:ALA:HB2	1:A:206:LEU:C	2.35	0.46
1:B:398:LEU:HD11	1:B:401:LEU:HD23	1.96	0.46
1:A:579:SER:O	1:A:580:VAL:HG13	2.16	0.46
2:D:14:LEU:HD11	2:D:60:TYR:CB	2.46	0.46
1:A:679:LYS:H	1:A:679:LYS:HG2	1.46	0.45
1:A:351:ILE:HD11	1:A:354:VAL:HG22	1.98	0.45
1:A:549:VAL:O	1:A:549:VAL:CG2	2.60	0.45
1:A:234:CYS:SG	1:A:239:TYR:C	2.95	0.45
1:A:510:GLY:HA2	1:A:516:SER:HB3	1.97	0.45
1:B:384:LEU:HD12	1:B:388:TYR:HB2	1.99	0.45
1:B:579:SER:C	1:B:580:VAL:HG22	2.36	0.45
1:A:393:LEU:HD12	1:A:419:ALA:O	2.17	0.45
1:A:583:ILE:HA	1:A:787:ALA:O	2.17	0.45
1:B:808:VAL:HA	1:B:821:LYS:O	2.17	0.45
1:A:701:PHE:HB2	1:B:33:LEU:HD13	1.99	0.45
2:C:45:ASP:HA	2:C:49:PHE:CD1	2.52	0.45
1:A:129:LEU:HD13	1:A:184:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:CYS:O	1:A:295:GLU:HB2	2.16	0.45
1:A:603:PRO:HA	1:A:611:LEU:HD11	1.99	0.45
1:B:495:VAL:O	1:B:496:TYR:C	2.56	0.45
1:A:310:THR:HG22	1:A:331:LEU:HB3	1.99	0.44
1:A:491:ILE:O	1:A:492:SER:C	2.55	0.44
1:A:700:ILE:HG13	1:B:33:LEU:HD12	1.98	0.44
1:A:790:PHE:CD1	2:D:54:LEU:HB3	2.52	0.44
1:B:820:LEU:HD13	1:B:875:ILE:HD11	1.99	0.44
1:A:88:VAL:HG11	1:B:688:TYR:CD2	2.52	0.44
1:B:81:LEU:CD2	1:B:86:ALA:HB2	2.48	0.44
1:A:496:TYR:CZ	1:A:521:MET:SD	3.11	0.44
1:B:177:THR:OG1	1:B:179:ASN:OD1	2.36	0.44
1:B:256:LEU:HA	1:B:264:GLU:HA	2.00	0.44
1:B:298:CYS:H	1:B:299:PRO:CD	2.31	0.44
1:B:863:LEU:CB	1:B:866:LEU:HD11	2.48	0.44
2:D:56:ARG:HA	2:D:59:MET:HE3	1.99	0.44
1:B:688:TYR:CE2	1:B:695:PHE:HE2	2.35	0.44
2:D:6:CYS:HA	2:D:10:LEU:HB2	1.98	0.44
1:B:416:MET:HG2	1:B:438:THR:HG21	1.99	0.44
1:A:58:PHE:HE2	1:B:696:LEU:HD21	1.79	0.43
1:A:88:VAL:HG22	1:A:112:ARG:HB3	1.99	0.43
1:A:700:ILE:HG12	1:B:58:PHE:CE2	2.53	0.43
2:C:6:CYS:HB3	2:C:48:CYS:HB2	1.46	0.43
1:A:873:ALA:HB2	1:A:892:PHE:CE1	2.53	0.43
1:B:34:ILE:HG22	1:B:34:ILE:O	2.19	0.43
1:B:692:PHE:O	1:B:696:LEU:HD23	2.18	0.43
1:A:393:LEU:HD13	1:A:417:TYR:HE2	1.82	0.43
1:A:495:VAL:O	1:A:522:VAL:HG11	2.16	0.43
1:B:686:ALA:HB1	1:B:690:LYS:HD3	2.00	0.43
1:B:780:ALA:HB1	1:B:785:CYS:HA	2.00	0.43
1:A:393:LEU:HD13	1:A:417:TYR:CE2	2.53	0.43
1:B:619:GLN:OE1	1:B:621:GLN:OE1	2.36	0.43
1:A:338:ASN:C	1:A:340:ILE:H	2.21	0.43
1:B:463:LEU:HD23	1:B:567:ALA:HB1	2.00	0.43
1:B:688:TYR:HE2	1:B:695:PHE:HE2	1.65	0.43
1:B:875:ILE:O	1:B:887:THR:HG23	2.18	0.43
1:B:616:VAL:HG11	1:B:760:ILE:HD11	2.01	0.43
2:C:17:VAL:CG2	2:C:58:GLU:HB3	2.45	0.43
2:D:56:ARG:HA	2:D:59:MET:HB3	2.00	0.43
2:D:56:ARG:H	2:D:56:ARG:HG3	1.59	0.43
1:A:160:PRO:HG3	1:A:173:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PHE:HB2	1:A:351:ILE:CD1	2.49	0.43
1:B:353:VAL:CG1	1:B:354:VAL:N	2.82	0.43
2:C:10:LEU:HD11	2:C:57:LEU:HD21	2.01	0.43
1:A:431:ARG:NH1	1:A:435:VAL:HG21	2.33	0.43
1:A:695:PHE:O	1:A:696:LEU:HB2	2.18	0.43
1:B:298:CYS:N	1:B:299:PRO:HD2	2.34	0.42
1:B:493:PHE:CZ	1:B:553:ALA:CB	2.99	0.42
2:C:14:LEU:HD13	2:C:14:LEU:HA	1.80	0.42
1:A:875:ILE:O	1:A:887:THR:HG23	2.18	0.42
1:B:367:VAL:C	1:B:398:LEU:HA	2.40	0.42
2:D:6:CYS:HB3	2:D:48:CYS:HB2	1.43	0.42
1:A:326:PHE:HB2	1:A:351:ILE:HD11	2.02	0.42
1:A:700:ILE:HG23	1:B:33:LEU:HD12	2.02	0.42
1:B:73:LEU:HD21	1:B:76:ILE:HD11	1.99	0.42
1:A:544:TRP:CG	1:A:607:PRO:HD2	2.55	0.42
1:A:69:LEU:HD12	1:A:70:PHE:CE1	2.55	0.42
1:A:367:VAL:CG1	1:A:368:SER:N	2.83	0.42
1:A:689:ARG:CZ	1:A:689:ARG:HB3	2.50	0.42
1:A:330:LEU:HD11	1:A:351:ILE:HG12	2.01	0.42
1:A:334:ILE:HG21	1:A:366:LEU:HD21	2.01	0.42
1:B:88:VAL:HG22	1:B:112:ARG:HB3	2.02	0.42
1:B:362:HIS:CE1	1:B:394:ASP:HB3	2.55	0.42
1:B:499:GLU:HB2	1:B:545:THR:HG21	2.02	0.42
1:B:683:LYS:HE3	1:B:683:LYS:HB3	1.39	0.42
1:B:689:ARG:HD2	1:B:690:LYS:HE3	2.02	0.42
1:B:89:ILE:HB	1:B:113:ILE:HG23	2.00	0.42
1:B:822:TRP:CE3	1:B:875:ILE:HG21	2.54	0.42
1:A:151:LEU:HD22	1:A:156:MET:HA	2.02	0.42
1:B:5:PRO:HB3	1:B:260:SER:HB2	2.02	0.42
1:B:90:PHE:O	1:B:91:GLU:C	2.58	0.42
1:B:256:LEU:HD23	1:B:265:GLY:H	1.85	0.42
1:B:693:GLU:CB	2:C:44:VAL:HB	2.24	0.42
1:A:623:GLN:HE22	1:A:830:GLY:HA2	1.83	0.41
1:A:672:CYS:H	1:A:673:PRO:CD	2.33	0.41
1:B:356:GLY:O	1:B:357:TYR:CB	2.67	0.41
1:B:251:PHE:O	1:B:255:ILE:HG12	2.19	0.41
1:B:580:VAL:HG12	1:B:779:GLU:HB2	2.02	0.41
1:A:493:PHE:CZ	1:A:553:ALA:HB2	2.55	0.41
1:A:577:ASN:HB3	1:A:609:GLY:HA2	2.02	0.41
2:D:14:LEU:HD22	2:D:57:LEU:HD13	2.02	0.41
1:A:603:PRO:C	1:A:604:PRO:O	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:O	1:B:218:CYS:C	2.58	0.41
1:B:330:LEU:HB2	1:B:358:VAL:HG13	2.02	0.41
1:B:493:PHE:CD1	1:B:553:ALA:HA	2.55	0.41
2:C:54:LEU:HD12	2:C:54:LEU:HA	1.74	0.41
1:A:252:CYS:O	1:A:255:ILE:HG13	2.20	0.41
1:A:495:VAL:HG22	1:A:551:VAL:HG22	2.02	0.41
1:A:577:ASN:O	1:A:578:ALA:HB3	2.20	0.41
1:A:602:ASN:O	1:A:604:PRO:CD	2.64	0.41
1:B:298:CYS:N	1:B:299:PRO:CD	2.84	0.41
1:B:697:HIS:HB3	2:C:43:ILE:HG23	2.02	0.41
1:B:586:ASP:CB	1:B:602:ASN:HB3	2.40	0.41
2:C:62:ALA:CB	2:C:63:PRO:HD2	2.36	0.41
2:D:54:LEU:HD12	2:D:54:LEU:HA	1.89	0.41
1:B:152:CYS:O	1:B:156:MET:HG2	2.21	0.41
1:B:493:PHE:CE1	1:B:553:ALA:CB	3.01	0.41
1:B:755:LYS:HD2	1:B:757:ARG:CZ	2.51	0.41
1:B:804:ILE:HD13	1:B:877:ALA:HB2	2.03	0.41
1:B:311:ILE:HG22	1:B:311:ILE:O	2.21	0.41
1:B:74:THR:HG21	1:B:219:VAL:HG11	2.03	0.40
1:B:580:VAL:HG21	1:B:783:LEU:HD12	2.04	0.40
1:A:676:GLU:HB2	1:B:667:GLY:N	2.36	0.40
1:A:832:ILE:HG22	1:A:834:MET:O	2.22	0.40
1:B:510:GLY:HA2	1:B:516:SER:HB3	2.01	0.40
1:B:691:VAL:CG1	2:C:40:GLN:HG3	2.50	0.40
2:C:18:CYS:O	2:C:21:ARG:HG2	2.21	0.40
2:D:6:CYS:CA	2:D:10:LEU:HB2	2.51	0.40
1:B:40:TYR:CE1	1:B:41:ARG:HG3	2.56	0.40
2:C:17:VAL:HG13	2:C:58:GLU:HB3	2.04	0.40
1:B:216:THR:HG22	1:B:229:VAL:HG22	2.03	0.40
1:B:86:ALA:HB3	1:B:106:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	757/897 (84%)	544 (72%)	173 (23%)	40 (5%)	1	16
1	B	782/897 (87%)	574 (73%)	161 (21%)	47 (6%)	1	14
2	C	40/60 (67%)	32 (80%)	5 (12%)	3 (8%)	1	10
2	D	40/60 (67%)	32 (80%)	8 (20%)	0	100	100
All	All	1619/1914 (85%)	1182 (73%)	347 (21%)	90 (6%)	2	15

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	193	ALA
1	A	401	LEU
1	A	511	GLN
1	A	574	ILE
1	A	581	PRO
1	A	604	PRO
1	A	672	CYS
1	A	696	LEU
1	A	700	ILE
1	A	754	ASN
1	A	786	SER
1	B	5	PRO
1	B	240	ARG
1	B	403	ASP
1	B	754	ASN
1	A	144	PRO
1	A	258	ALA
1	A	340	ILE
1	A	403	ASP
1	A	460	SER
1	A	492	SER
1	A	544	TRP
1	A	549	VAL
1	B	91	GLU
1	B	218	CYS
1	B	258	ALA
1	B	349	GLY
1	B	412	LYS
1	B	460	SER

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Mol	Chain	Res	Type
1	B	522	VAL
1	B	559	VAL
1	B	698	ASN
1	B	700	ILE
1	B	775	SER
1	A	379	LEU
1	A	518	SER
1	A	807	PRO
1	B	54	TYR
1	B	157	GLU
1	B	244	TRP
1	B	266	PHE
1	B	357	TYR
1	B	401	LEU
1	B	407	ARG
1	B	452	ASN
1	B	603	PRO
1	B	673	PRO
1	B	831	LEU
2	C	46	GLU
1	A	213	ASP
1	A	259	GLU
1	A	513	ALA
1	A	561	ASN
1	A	673	PRO
1	B	107	THR
1	B	259	GLU
1	B	298	CYS
1	B	513	ALA
1	B	581	PRO
1	A	133	ALA
1	A	532	VAL
1	A	611	LEU
1	B	186	PRO
1	B	221	CYS
1	B	422	PRO
1	B	511	GLN
1	B	561	ASN
1	B	798	ALA
1	B	829	ASN
1	A	160	PRO
1	A	221	CYS

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Mol	Chain	Res	Type
1	A	471	SER
1	B	73	LEU
1	B	144	PRO
1	B	293	PRO
1	B	334	ILE
1	B	356	GLY
1	B	547	TYR
1	A	243	GLY
1	A	356	GLY
1	A	285	GLY
1	A	559	VAL
1	B	243	GLY
1	A	510	GLY
1	B	860	GLY
1	B	2	ILE
2	C	19	GLY
1	A	2	ILE
2	C	62	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	710/800 (89%)	547 (77%)	163 (23%)	0	4
1	B	721/800 (90%)	551 (76%)	170 (24%)	0	4
2	C	37/50 (74%)	18 (49%)	19 (51%)	0	0
2	D	37/50 (74%)	20 (54%)	17 (46%)	0	0
All	All	1505/1700 (88%)	1136 (76%)	369 (24%)	2	3

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	12	ASP
1	A	14	GLN

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Mol	Chain	Res	Type
1	A	36	LYS
1	A	39	ASP
1	A	40	TYR
1	A	42	SER
1	A	63	LEU
1	A	69	LEU
1	A	74	THR
1	A	75	VAL
1	A	84	ASN
1	A	87	LEU
1	A	90	PHE
1	A	91	GLU
1	A	93	THR
1	A	107	THR
1	A	108	ARG
1	A	111	ILE
1	A	115	LYS
1	A	116	ASN
1	A	123	SER
1	A	128	SER
1	A	129	LEU
1	A	135	SER
1	A	138	TYR
1	A	143	LYS
1	A	144	PRO
1	A	148	CYS
1	A	155	THR
1	A	157	GLU
1	A	158	GLU
1	A	159	LYS
1	A	162	CYS
1	A	165	THR
1	A	167	ILE
1	A	168	ASN
1	A	172	ASN
1	A	173	TYR
1	A	180	ARG
1	A	181	CYS
1	A	189	CYS
1	A	191	LYS
1	A	196	GLU
1	A	199	GLU

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Mol	Chain	Res	Type
1	A	200	CYS
1	A	201	CYS
1	A	204	GLU
1	A	205	CYS
1	A	222	ARG
1	A	234	CYS
1	A	237	ASN
1	A	246	CYS
1	A	254	ASN
1	A	257	SER
1	A	259	GLU
1	A	272	GLU
1	A	279	SER
1	A	284	ASN
1	A	289	MET
1	A	291	CYS
1	A	300	LYS
1	A	303	GLU
1	A	307	LYS
1	A	308	THR
1	A	309	LYS
1	A	314	VAL
1	A	319	MET
1	A	324	THR
1	A	333	ASN
1	A	336	ARG
1	A	339	ASN
1	A	345	GLU
1	A	351	ILE
1	A	361	ARG
1	A	368	SER
1	A	373	LYS
1	A	374	ASN
1	A	379	LEU
1	A	382	GLU
1	A	385	GLU
1	A	389	SER
1	A	400	GLN
1	A	407	ARG
1	A	409	LEU
1	A	410	THR
1	A	415	LYS

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Mol	Chain	Res	Type
1	A	425	CYS
1	A	427	SER
1	A	433	GLU
1	A	436	THR
1	A	455	ARG
1	A	457	SER
1	A	460	SER
1	A	464	HIS
1	A	467	SER
1	A	470	THR
1	A	473	ASN
1	A	476	ILE
1	A	486	ASP
1	A	489	ASP
1	A	491	ILE
1	A	493	PHE
1	A	502	PHE
1	A	504	ASN
1	A	505	VAL
1	A	518	SER
1	A	538	LEU
1	A	542	LYS
1	A	545	THR
1	A	550	TYR
1	A	556	LEU
1	A	579	SER
1	A	580	VAL
1	A	583	ILE
1	A	585	LEU
1	A	588	LEU
1	A	593	SER
1	A	597	LEU
1	A	601	TRP
1	A	608	ASN
1	A	622	PRO
1	A	629	ARG
1	A	630	HIS
1	A	669	CYS
1	A	672	CYS
1	A	674	LYS
1	A	675	THR
1	A	679	LYS

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Mol	Chain	Res	Type
1	A	683	LYS
1	A	684	GLU
1	A	685	GLU
1	A	688	TYR
1	A	689	ARG
1	A	690	LYS
1	A	691	VAL
1	A	701	PHE
1	A	702	VAL
1	A	704	ARG
1	A	748	PHE
1	A	756	GLU
1	A	759	VAL
1	A	764	ARG
1	A	776	CYS
1	A	777	ASN
1	A	794	ARG
1	A	803	ASP
1	A	807	PRO
1	A	821	LYS
1	A	831	LEU
1	A	834	MET
1	A	838	LYS
1	A	844	GLU
1	A	848	GLU
1	A	850	VAL
1	A	851	SER
1	A	854	GLU
1	A	864	ASN
1	A	866	LEU
1	A	870	ASN
1	A	871	TYR
1	A	874	ARG
1	A	875	ILE
1	B	5	PRO
1	B	20	GLU
1	B	26	GLU
1	B	30	HIS
1	B	33	LEU
1	B	40	TYR
1	B	56	LEU
1	B	57	LEU

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	70	PHE
1	B	73	LEU
1	B	75	VAL
1	B	91	GLU
1	B	93	THR
1	B	97	ASP
1	B	106	ILE
1	B	108	ARG
1	B	115	LYS
1	B	116	ASN
1	B	123	SER
1	B	131	LEU
1	B	132	ASP
1	B	134	VAL
1	B	143	LYS
1	B	144	PRO
1	B	148	CYS
1	B	150	ASP
1	B	155	THR
1	B	156	MET
1	B	157	GLU
1	B	158	GLU
1	B	159	LYS
1	B	165	THR
1	B	170	GLU
1	B	175	CYS
1	B	178	THR
1	B	189	CYS
1	B	191	LYS
1	B	196	GLU
1	B	197	ASN
1	B	200	CYS
1	B	201	CYS
1	B	205	CYS
1	B	246	CYS
1	B	252	CYS
1	B	257	SER
1	B	259	GLU
1	B	264	GLU
1	B	270	ASP
1	B	281	PHE

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Mol	Chain	Res	Type
1	B	291	CYS
1	B	295	GLU
1	B	298	CYS
1	B	299	PRO
1	B	300	LYS
1	B	303	GLU
1	B	307	LYS
1	B	312	ASP
1	B	314	VAL
1	B	319	MET
1	B	321	GLN
1	B	344	LEU
1	B	351	ILE
1	B	353	VAL
1	B	355	THR
1	B	361	ARG
1	B	363	SER
1	B	364	HIS
1	B	366	LEU
1	B	367	VAL
1	B	368	SER
1	B	373	LYS
1	B	379	LEU
1	B	387	ASN
1	B	391	TYR
1	B	393	LEU
1	B	395	ASN
1	B	396	GLN
1	B	398	LEU
1	B	403	ASP
1	B	407	ARG
1	B	409	LEU
1	B	415	LYS
1	B	429	ILE
1	B	431	ARG
1	B	443	SER
1	B	450	ARG
1	B	457	SER
1	B	459	GLU
1	B	467	SER
1	B	469	THR
1	B	471	SER

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Mol	Chain	Res	Type
1	B	474	ARG
1	B	490	LEU
1	B	493	PHE
1	B	494	THR
1	B	502	PHE
1	B	505	VAL
1	B	516	SER
1	B	523	ASP
1	B	533	GLU
1	B	538	LEU
1	B	542	LYS
1	B	544	TRP
1	B	547	TYR
1	B	550	TYR
1	B	556	LEU
1	B	557	THR
1	B	572	LEU
1	B	576	THR
1	B	579	SER
1	B	580	VAL
1	B	581	PRO
1	B	582	SER
1	B	583	ILE
1	B	585	LEU
1	B	593	SER
1	B	598	ILE
1	B	601	TRP
1	B	603	PRO
1	B	605	SER
1	B	607	PRO
1	B	611	LEU
1	B	619	GLN
1	B	629	ARG
1	B	630	HIS
1	B	669	CYS
1	B	674	LYS
1	B	676	GLU
1	B	678	GLU
1	B	679	LYS
1	B	680	GLN
1	B	682	GLU
1	B	683	LYS

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Mol	Chain	Res	Type
1	B	685	GLU
1	B	688	TYR
1	B	689	ARG
1	B	690	LYS
1	B	692	PHE
1	B	695	PHE
1	B	698	ASN
1	B	700	ILE
1	B	701	PHE
1	B	702	VAL
1	B	704	ARG
1	B	748	PHE
1	B	753	ASP
1	B	754	ASN
1	B	756	GLU
1	B	757	ARG
1	B	758	THR
1	B	768	LEU
1	B	776	CYS
1	B	786	SER
1	B	794	ARG
1	B	795	THR
1	B	807	PRO
1	B	809	THR
1	B	834	MET
1	B	836	GLU
1	B	848	GLU
1	B	850	VAL
1	B	851	SER
1	B	854	GLU
1	B	864	ASN
1	B	871	TYR
1	B	872	THR
1	B	874	ARG
1	B	878	THR
1	B	883	ASN
2	C	5	LEU
2	C	9	GLU
2	C	11	VAL
2	C	14	LEU
2	C	16	PHE
2	C	17	VAL

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Mol	Chain	Res	Type
2	C	21	ARG
2	C	39	PRO
2	C	41	THR
2	C	43	ILE
2	C	44	VAL
2	C	45	ASP
2	C	50	ARG
2	C	52	CYS
2	C	54	LEU
2	C	56	ARG
2	C	57	LEU
2	C	58	GLU
2	C	59	MET
2	D	5	LEU
2	D	9	GLU
2	D	11	VAL
2	D	14	LEU
2	D	15	GLN
2	D	20	ASP
2	D	21	ARG
2	D	41	THR
2	D	43	ILE
2	D	44	VAL
2	D	50	ARG
2	D	52	CYS
2	D	54	LEU
2	D	56	ARG
2	D	57	LEU
2	D	58	GLU
2	D	59	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	254	ASN
1	A	329	ASN
1	A	387	ASN
1	A	520	ASN
1	A	623	GLN
1	A	680	GLN
1	B	198	ASN

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Mol	Chain	Res	Type
1	B	333	ASN
1	B	395	ASN
1	B	473	ASN
1	B	697	HIS
1	B	698	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

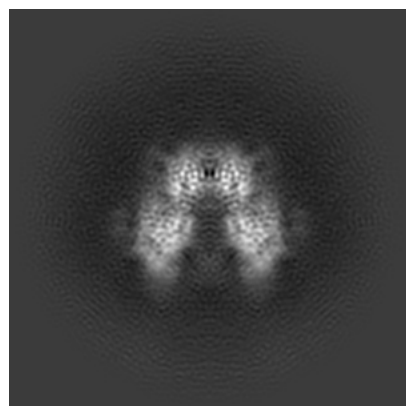
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34065. These allow visual inspection of the internal detail of the map and identification of artifacts.

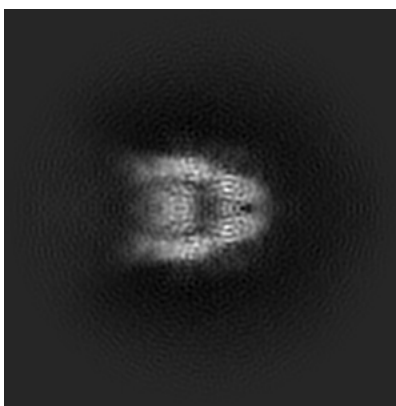
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

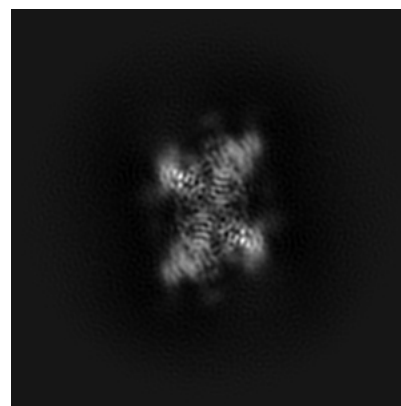
6.1.1 Primary map



X

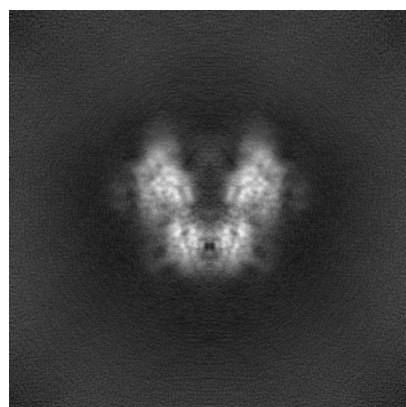


Y

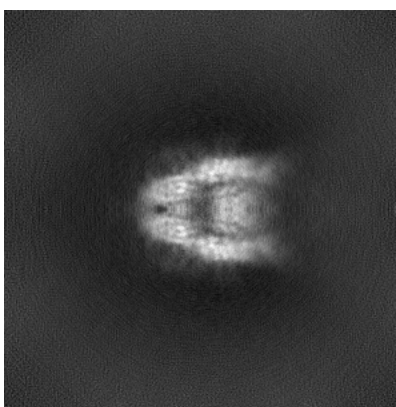


Z

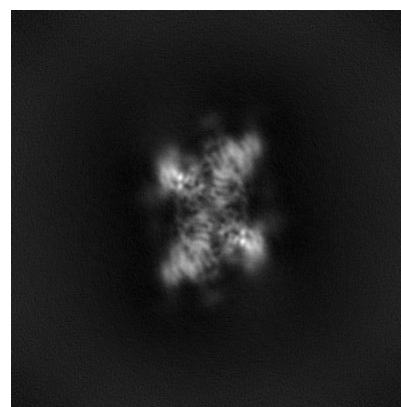
6.1.2 Raw map



X



Y

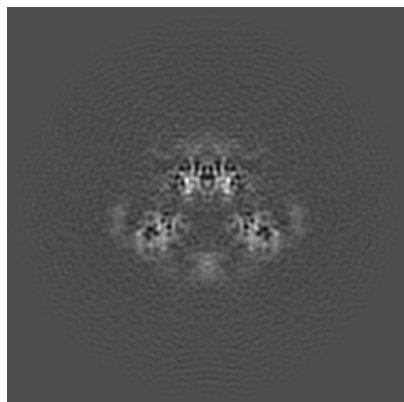


Z

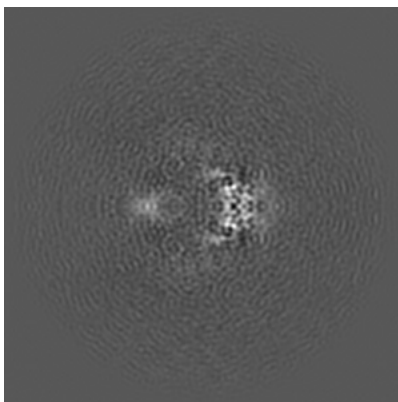
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

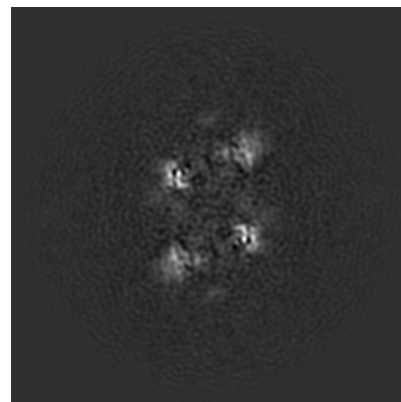
6.2.1 Primary map



X Index: 180

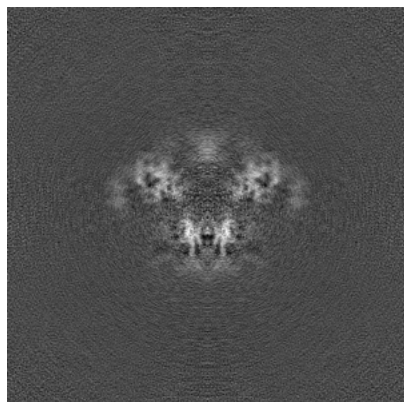


Y Index: 180

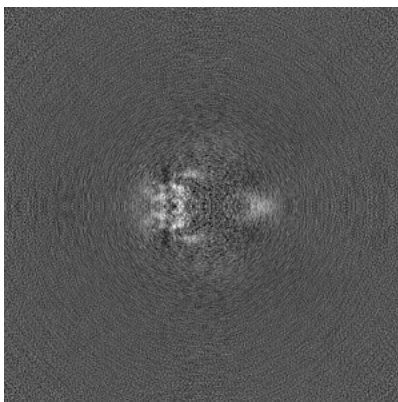


Z Index: 180

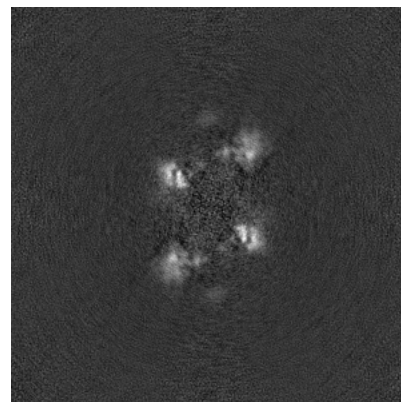
6.2.2 Raw map



X Index: 180



Y Index: 180

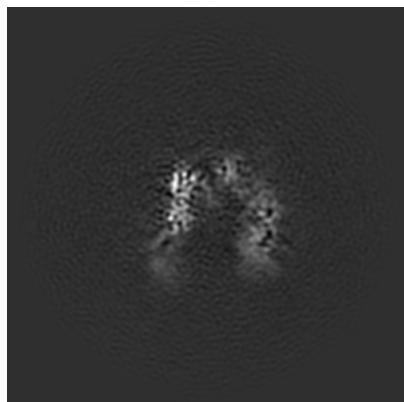


Z Index: 180

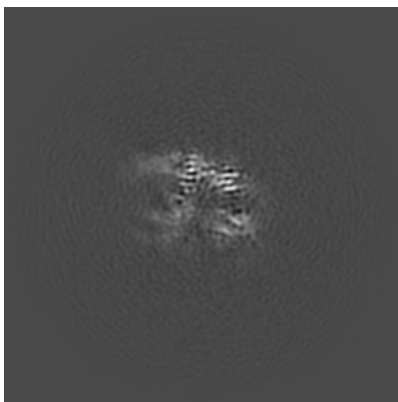
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

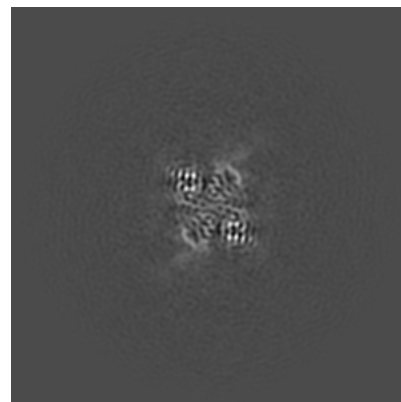
6.3.1 Primary map



X Index: 208

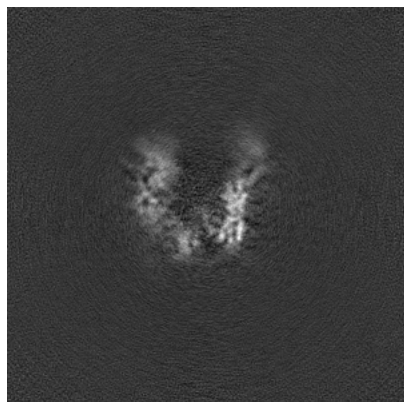


Y Index: 151

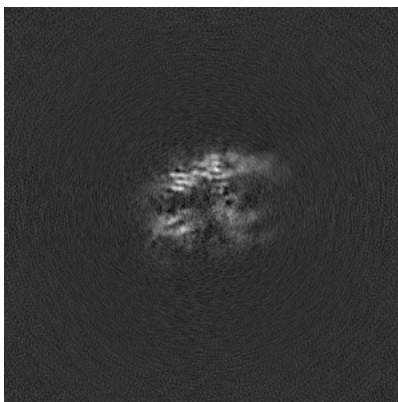


Z Index: 201

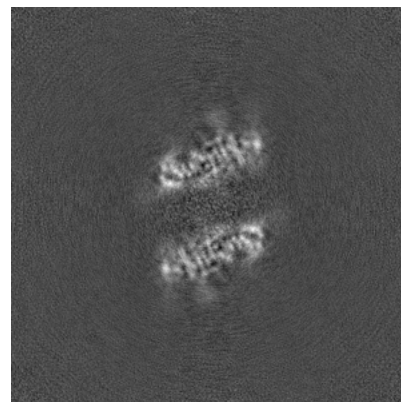
6.3.2 Raw map



X Index: 152



Y Index: 151

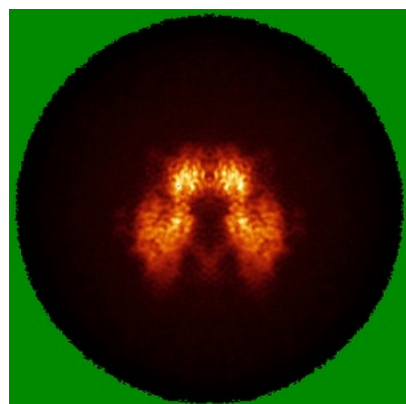


Z Index: 198

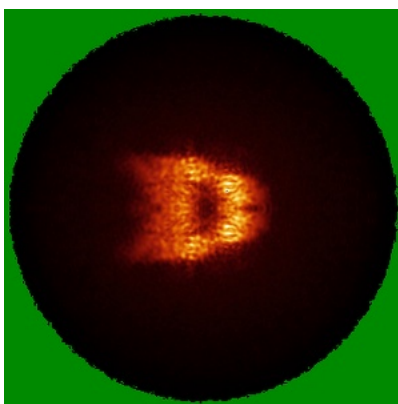
The images above show the largest variance slices of the map in three orthogonal directions.

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

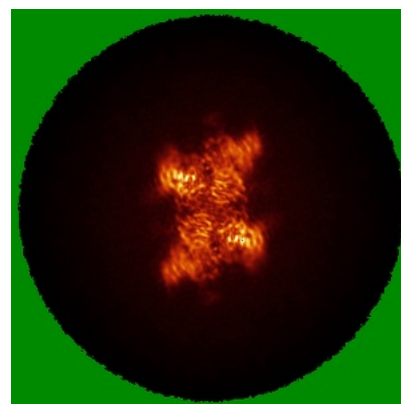
6.4.1 Primary map



X

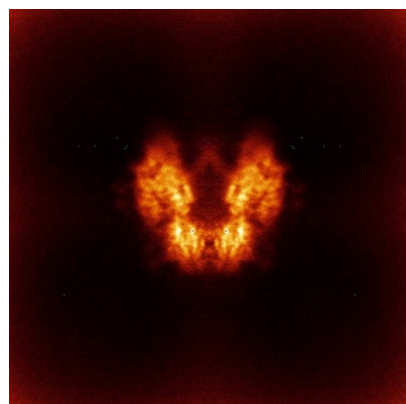


Y

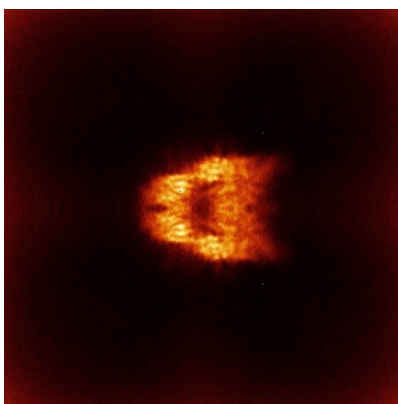


Z

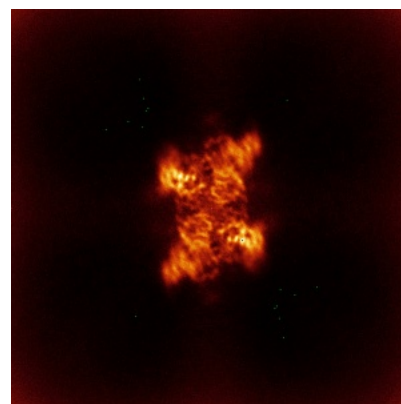
6.4.2 Raw map



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.

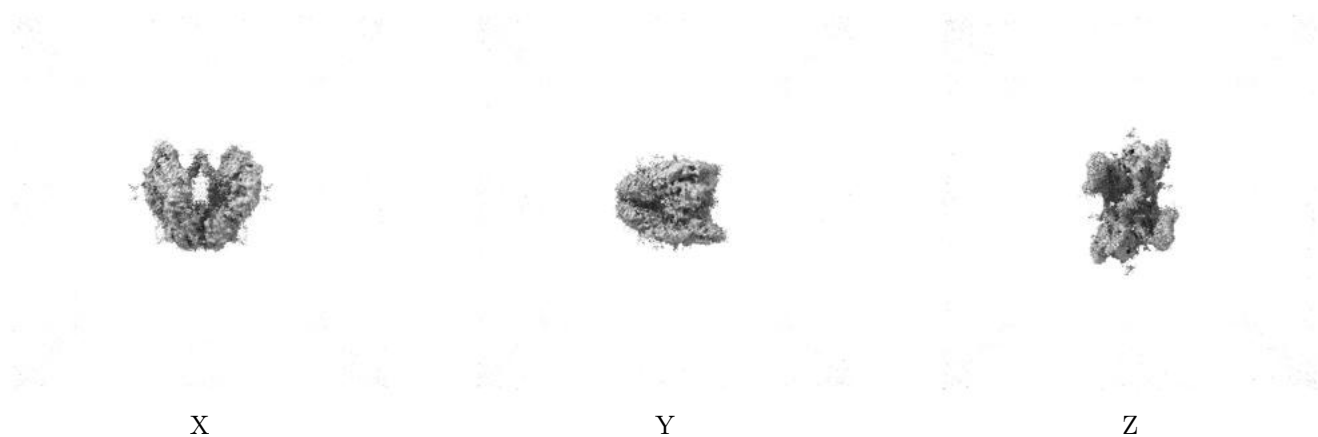
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.062. 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



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.

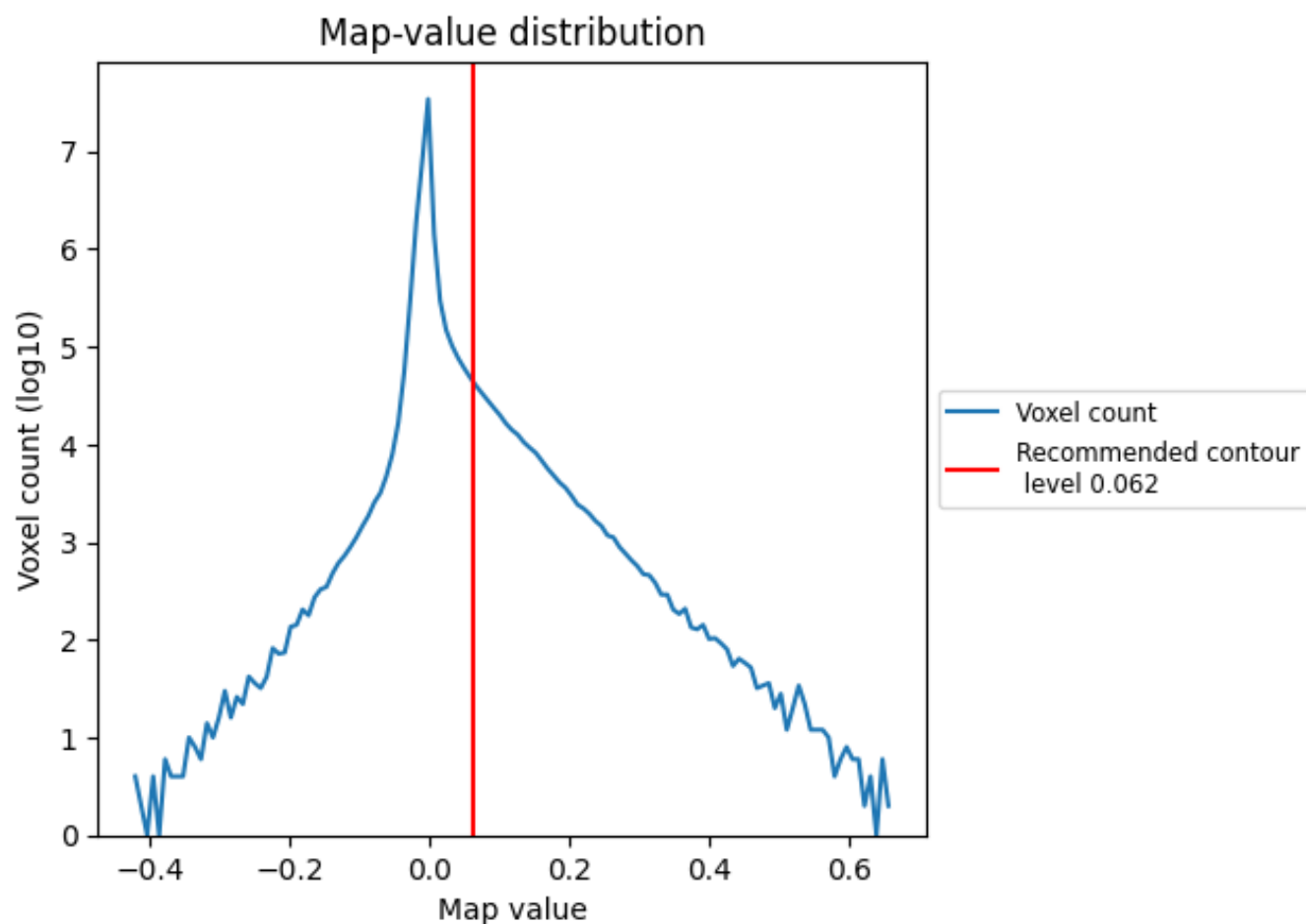
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

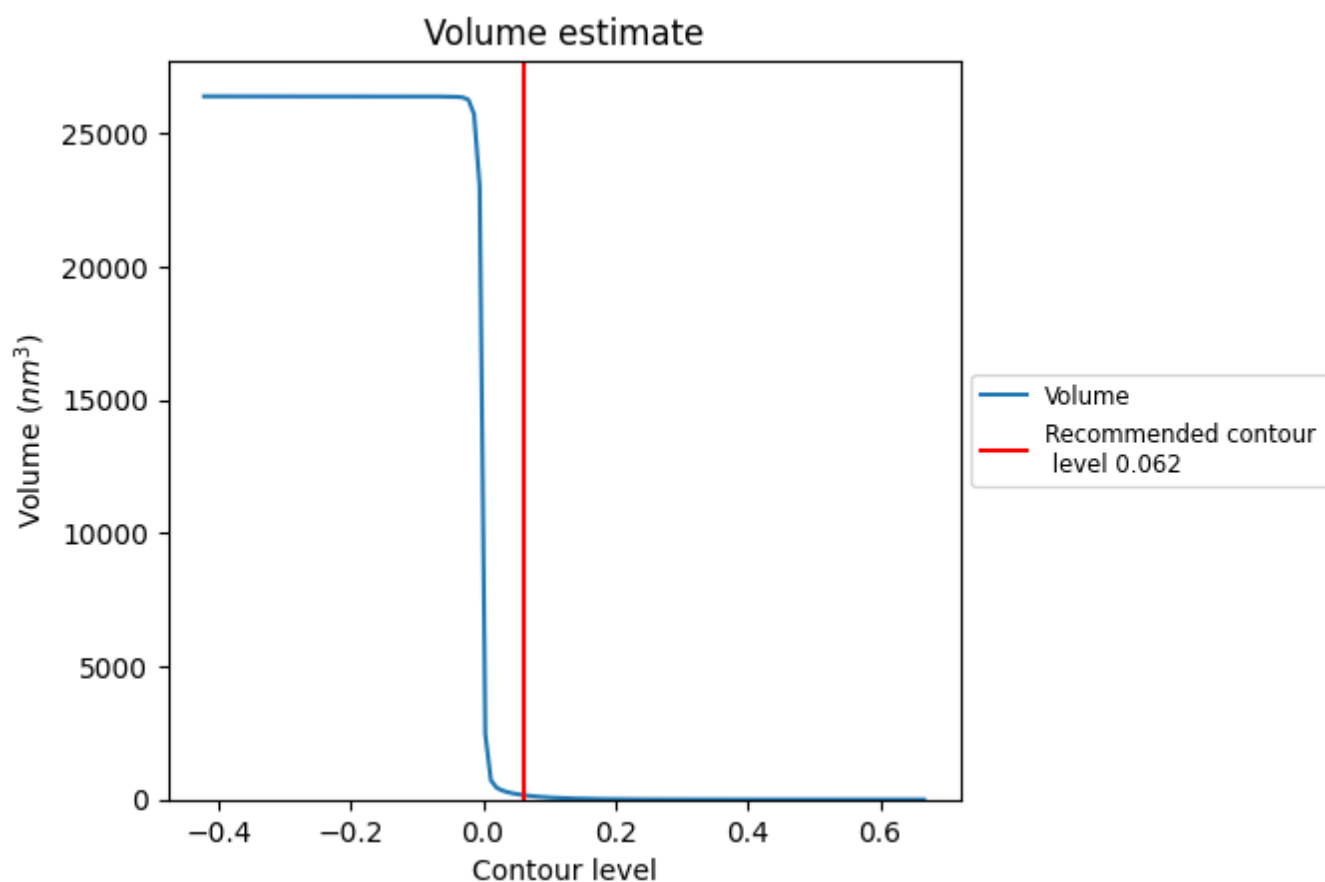
This section contains the results of statistical analysis of the map.

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.

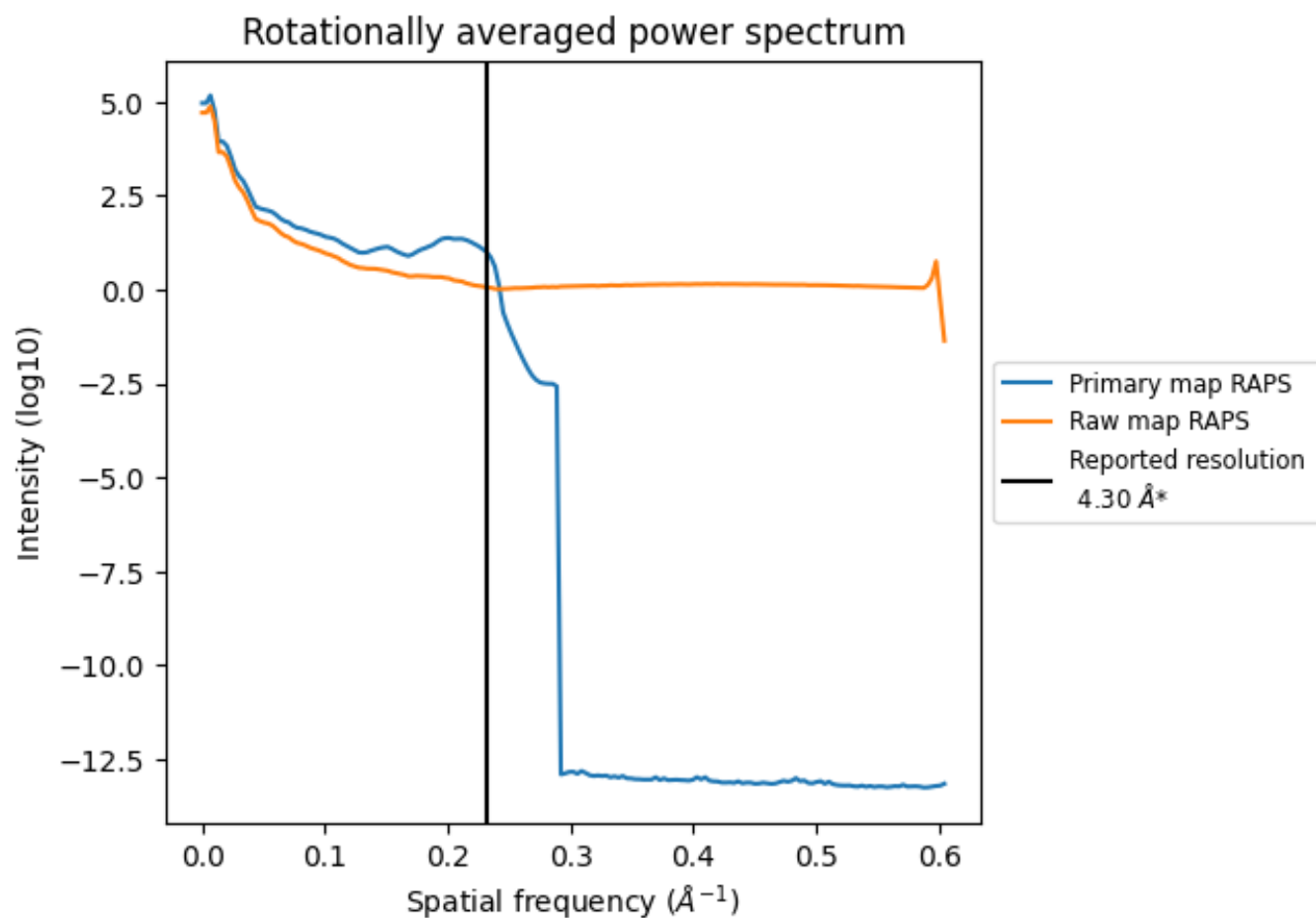
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm^3 ; this corresponds to an approximate mass of 148 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 ⓘ

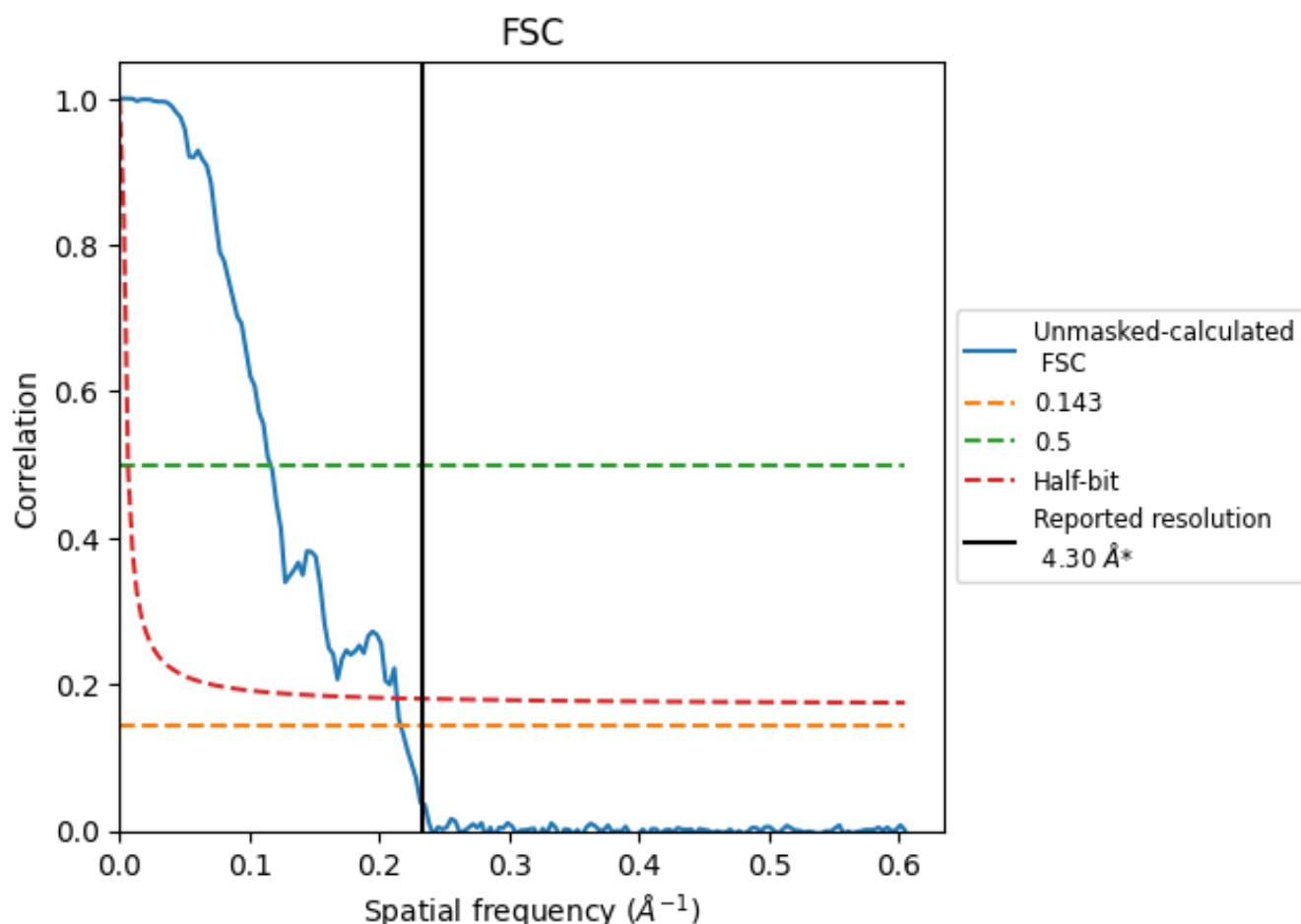


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

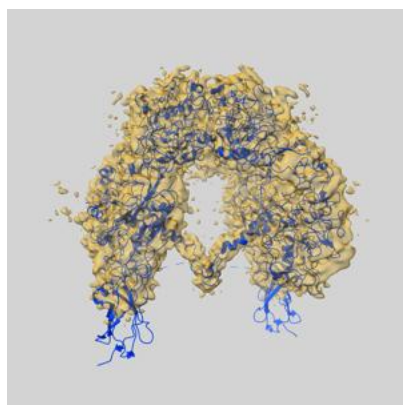
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	4.30
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	4.62	8.61	4.68	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

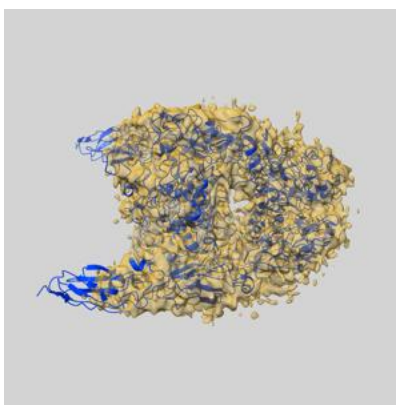
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34065 and PDB model 7YRR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

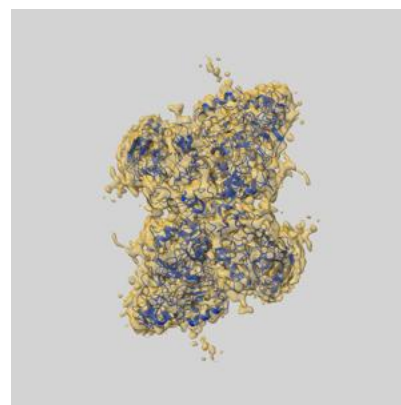
9.1 Map-model overlay [i](#)



X



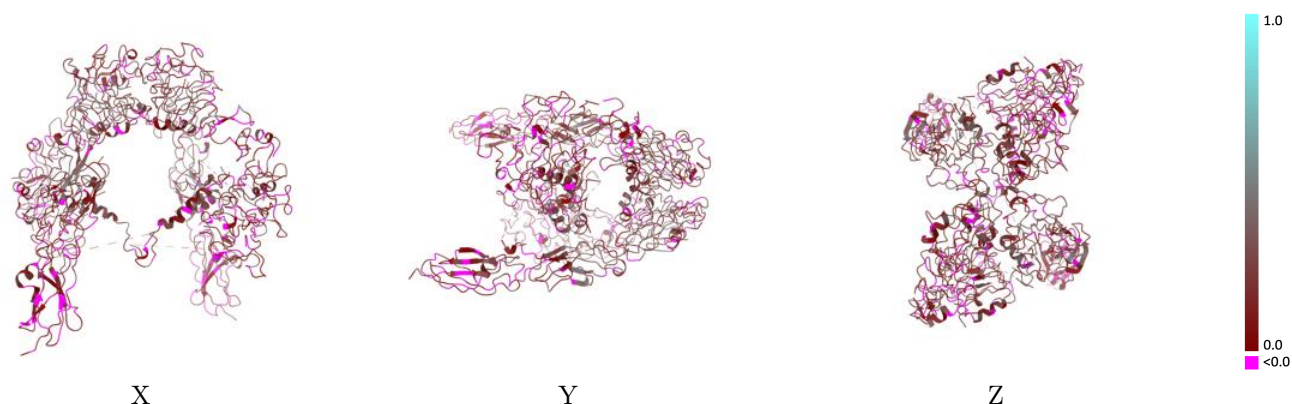
Y



Z

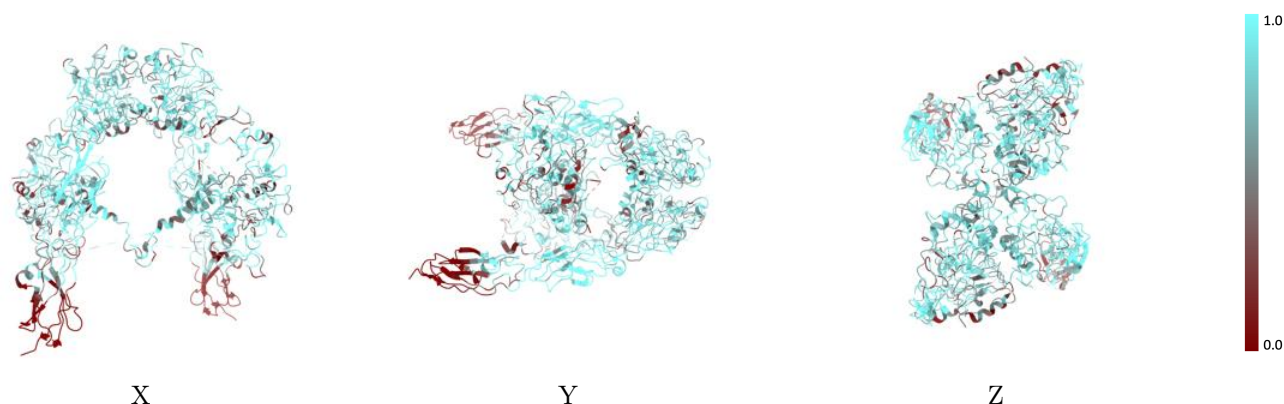
The images above show the 3D surface view of the map at the recommended contour level 0.062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



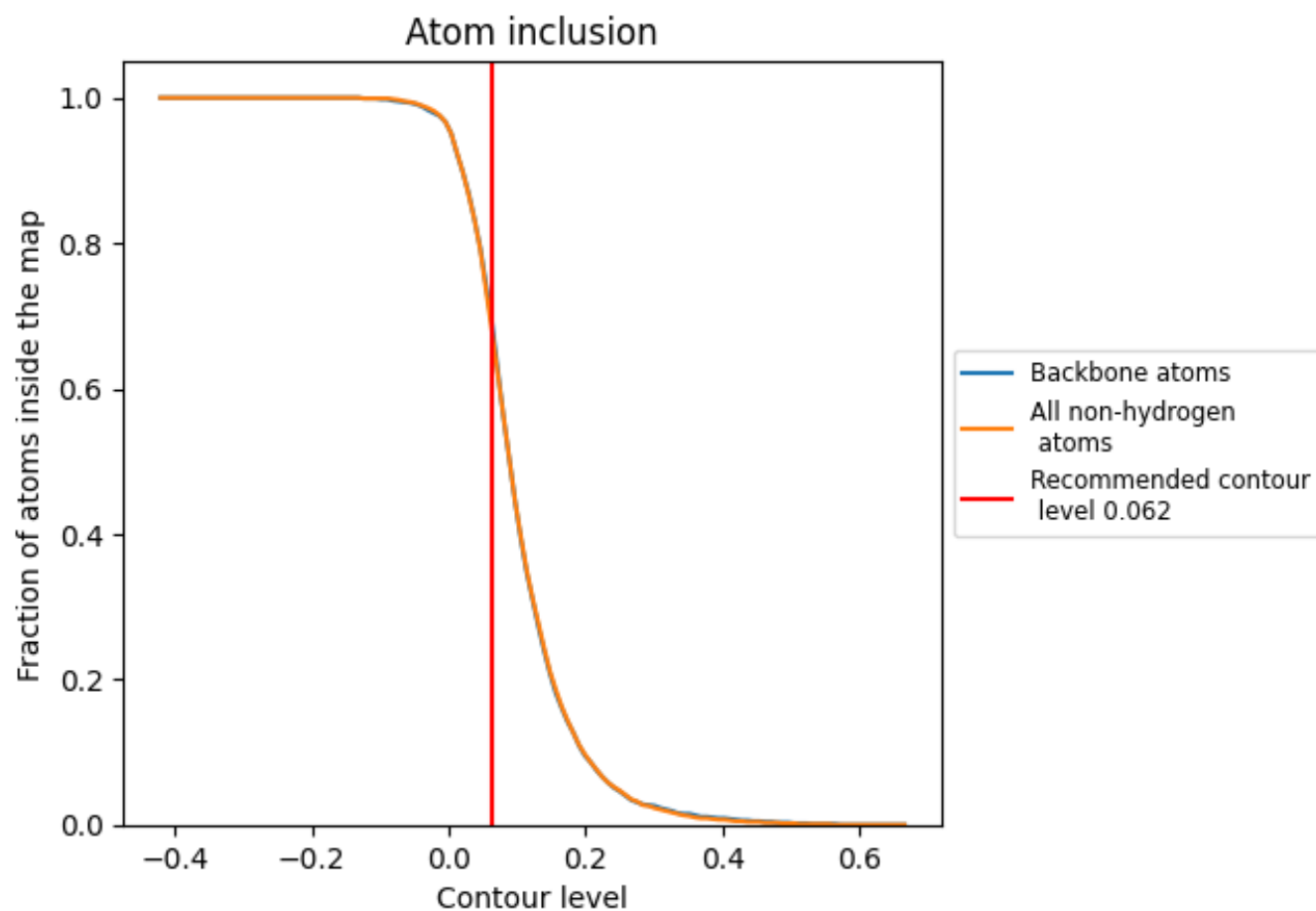
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.062).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6870	<div></div> 0.1750
A	<div></div> 0.6910	<div></div> 0.1730
B	<div></div> 0.6910	<div></div> 0.1670
C	<div></div> 0.7680	<div></div> 0.2800
D	<div></div> 0.7320	<div></div> 0.2640

