



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:50 PM UTC

PDB ID : 8JQI / pdb_00008jqi
EMDB ID : EMD-36573
Title : Cryo EM map of full length PLC gamma 2 and FGFR1 Kinase Domain
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-06-14
Resolution : 4.10 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

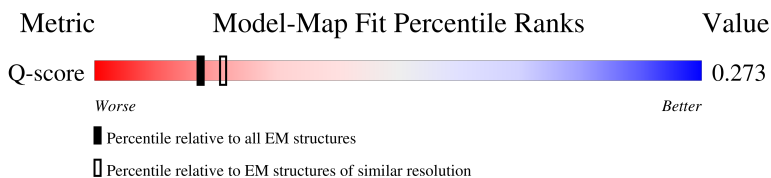
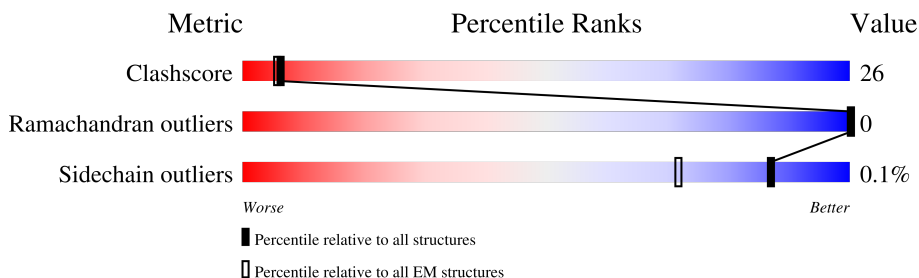
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	1265	
2	B	822	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11180 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 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1062	Total	C	N	O	S	0	0
			8716	5554	1495	1623	44		

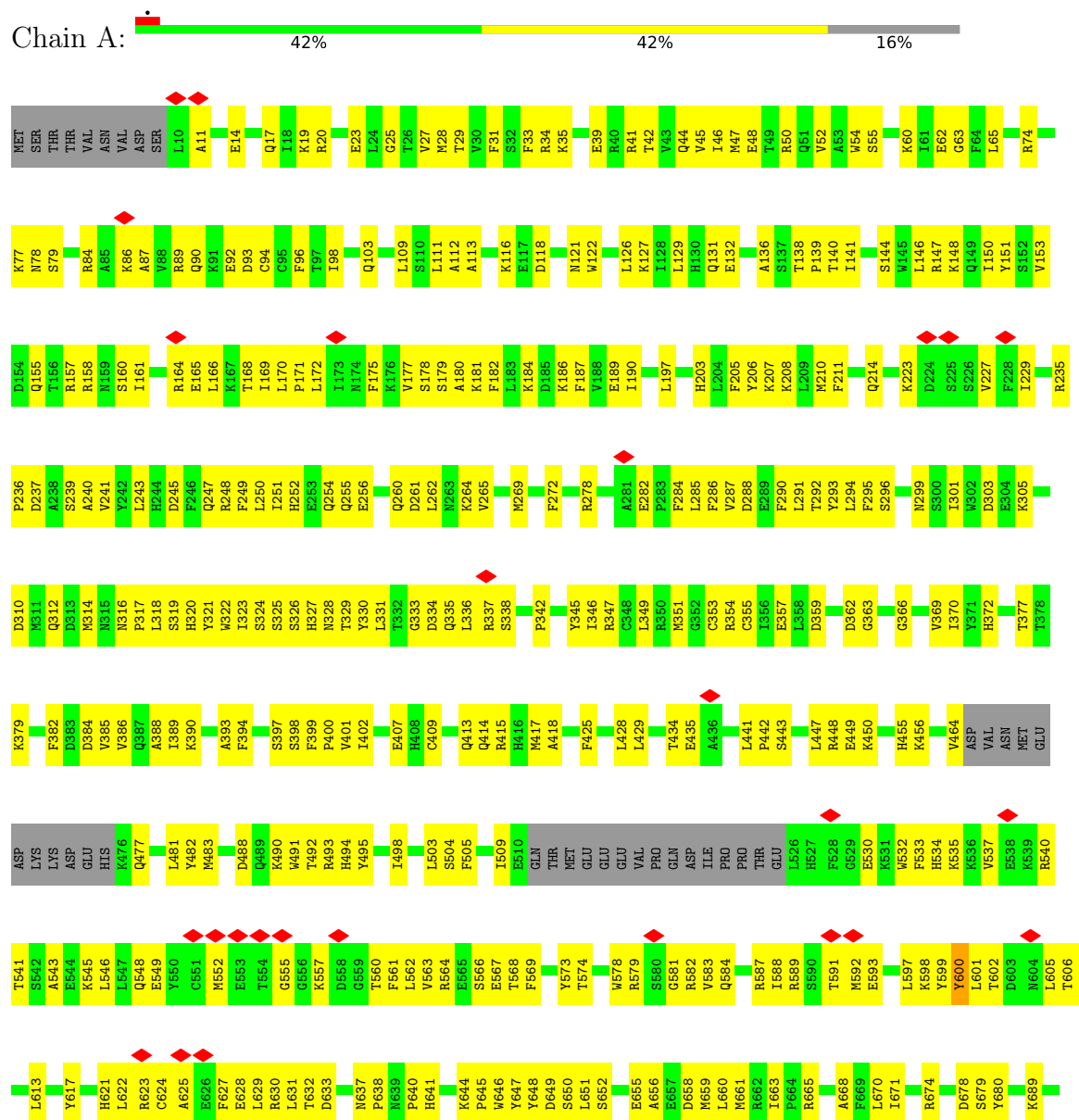
- Molecule 2 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	307	Total	C	N	O	S	0	0
			2464	1567	422	456	19		

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: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2



ILE	PRO	LEU	ARG	ARG	GLN	VAL	THR	VAL	SER	ALA	ASP	SER	SER	ALA	SER	MET	ASN	SER	GLY	VAL	LEU	LEU	VAL	ARG	PRO	SER	ARG	LEU	SER	SER	SER	GLY	THR	PRO	MET	LEU	ALA	GLY	VAL	SER	GLU	Y463	E464	L465	P466	E467	D468	P469	R470	W471	E472	L473	P474	R475	D476	R477	L478	W479	L480
G481	K482	P483	L484	G485	E486	G487	C488	F489	G490	Q491	V492	V493	L494	A495	E496	A497	I498	G499	L500	D501	K502	D503	K504	P505	N506	R507	V508	T509	K510	V511	A512	V513	K514	K517	S518	D519	A520	T521	E522	K523	D524	L525	S526	D527	L528	I529	S530	E531	M532	E533	M534	M535	M536	M537	I538	G539	K540	H541	
K542	N543	I544	I545	N546	L547	L548	G549	A550	C551	T552	Q553	D554	G555	P556	L557	Y558	V559	I560	V561	E562	Y563	A564	S565	K566	G567	N568	L569	R570	E571	Y572	L573	Q574	A575	R576	R577	P578	P579	E582	Y583	C584	Y585	N586	P587	S588	H589	N590	P591	E592	E593	Q594	L595	S596	S597	K598	D599	L600	V601	S602	
C603	A604	Y605	Q606	V607	A608	R609	G610	M611	E612	Y613	L614	A615	S616	K617	K618	C619	I620	H621	R622	D623	L624	A625	A626	R627	N628	V629	L630	V631	T632	E633	D634	N635	V636	M637	K638	I639	A640	D641	F642	G643	L644	A645	R646	D647	I648	H649	H650	I651	D652	Y653	Y654	K655	K656	T657	T658	N659	G660	R661	L662
P663	V664	K665	W666	M667	A668	P669	E670	A671	L672	F673	D674	R675	I676	V677	T678	H679	Q680	S681	W684	S685	F686	G687	V688	L689	L690	W691	E692	I693	F694	T695	L696	G697	G698	S699	P700	Y701	P702	G703	V704	P705	V706	E707	E708	L709	F710	K711	L712	L713	K714	E715	G716	H717	R718	W719	D720	K721	P722	S723	
N724	C725	T726	N727	E728	L729	Y730	N733	R734	W737	H738	A739	V740	P741	S742	Q743	R744	P745	K748	Q749	L750	V751	E752	D753	L754	D755	R756	L760	T761	Q764	L767	D768	L769	MET	PRO	PRO	LEU	ASP	GLN	TYR	SER	PRO	SER	PHE	PRO	ASP	THR	ARG	SER	SER	THR	CYS	SER	SER						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.0932	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.872	Depositor
Minimum map value	-0.889	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	237.6, 237.6, 237.6	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.29	0/8918	0.53	2/12036 (0.0%)
2	B	0.18	0/2520	0.45	1/3410 (0.0%)
All	All	0.27	0/11438	0.51	3/15446 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	648	ILE	N-CA-C	-5.92	106.64	111.91
1	A	223	LYS	CB-CA-C	-5.64	110.05	116.54
1	A	633	ASP	N-CA-C	5.43	118.19	108.47

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	8716	0	8616	487	0
2	B	2464	0	2460	102	0
All	All	11180	0	11076	573	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 26.

All (573) 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:602:THR:HG21	2:B:769:LEU:HB2	1.41	1.01
1:A:593:GLU:HB2	1:A:598:LYS:HG3	1.48	0.96
1:A:336:LEU:HD23	1:A:495:TYR:HE2	1.35	0.90
1:A:338:SER:H	1:A:377:THR:HG22	1.37	0.90
1:A:31:PHE:HE2	1:A:86:LYS:HB2	1.36	0.89
2:B:663:PRO:HB2	2:B:666:TRP:HB2	1.54	0.88
1:A:579:ARG:HG3	1:A:582:ARG:HB2	1.55	0.87
1:A:561:PHE:HB3	1:A:631:LEU:HD22	1.58	0.85
1:A:127:LYS:HG2	1:A:131:GLN:HE22	1.42	0.84
1:A:346:ILE:HD11	1:A:388:ALA:HB1	1.58	0.84
1:A:331:LEU:HD13	1:A:335:GLN:HA	1.61	0.83
1:A:94:CYS:HB2	1:A:113:ALA:HB3	1.61	0.82
1:A:602:THR:CG2	2:B:769:LEU:HB2	2.09	0.82
1:A:90:GLN:HG2	1:A:112:ALA:HB1	1.61	0.82
1:A:600:TYR:HB2	1:A:606:THR:OG1	1.79	0.81
1:A:55:SER:HB2	1:A:62:GLU:H	1.44	0.81
1:A:1060:LEU:HD22	1:A:1127:PRO:HG3	1.64	0.80
2:B:631:VAL:HG22	2:B:637:MET:HE1	1.62	0.79
1:A:876:LEU:HD23	1:A:887:GLU:H	1.50	0.77
1:A:1085:VAL:HG22	1:A:1136:VAL:HG12	1.66	0.77
1:A:50:ARG:HH22	1:A:140:THR:HG22	1.50	0.77
1:A:678:ASP:HB2	1:A:697:ARG:HH12	1.50	0.76
1:A:578:TRP:HE1	1:A:581:GLY:H	1.30	0.76
1:A:947:LEU:HA	1:A:956:ARG:HH22	1.49	0.76
2:B:531:GLU:HG2	2:B:535:MET:HE3	1.68	0.76
2:B:529:ILE:HA	2:B:532:MET:HE2	1.68	0.75
1:A:578:TRP:HA	1:A:583:VAL:HA	1.68	0.75
1:A:1014:PHE:HD1	1:A:1021:MET:HE1	1.51	0.75
1:A:415:ARG:HH12	1:A:928:ILE:H	1.33	0.73
1:A:984:ARG:HA	1:A:1009:MET:HB2	1.70	0.73
1:A:394:PHE:HB3	1:A:398:SER:HA	1.72	0.72
1:A:589:ARG:NH2	2:B:755:ASP:OD2	2.23	0.71
1:A:978:ASN:ND2	1:A:1006:GLY:O	2.23	0.71
1:A:938:LYS:HE2	1:A:953:ARG:HB3	1.72	0.71
1:A:464:VAL:HB	1:A:924:GLN:HB2	1.72	0.70
1:A:901:GLN:HA	1:A:904:ARG:HD3	1.73	0.70
1:A:407:GLU:OE1	1:A:455:HIS:NE2	2.24	0.70
1:A:45:VAL:HG22	1:A:52:VAL:HG22	1.74	0.69
2:B:486:GLU:HG3	2:B:491:GLN:HG3	1.74	0.69
1:A:211:PHE:HE2	1:A:236:PRO:HA	1.55	0.69
2:B:755:ASP:OD2	2:B:756:ARG:NH2	2.25	0.69
1:A:855:LEU:HD23	1:A:906:ILE:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:HIS:NE2	1:A:1169:ASN:O	2.25	0.69
1:A:1039:GLN:HE21	1:A:1043:MET:HE1	1.58	0.69
1:A:34:ARG:HG3	1:A:35:LYS:HG2	1.74	0.68
1:A:482:TYR:HB2	1:A:889:ALA:HB3	1.76	0.68
1:A:189:GLU:OE2	1:A:208:LYS:NZ	2.25	0.68
1:A:491:TRP:HZ2	1:A:868:ASN:HB2	1.57	0.68
1:A:170:LEU:HD22	1:A:175:PHE:HD2	1.59	0.67
1:A:211:PHE:CE2	1:A:236:PRO:HA	2.30	0.67
1:A:335:GLN:HE22	1:A:994:SER:HA	1.59	0.67
2:B:623:ASP:OD1	2:B:627:ARG:NH2	2.27	0.67
1:A:1001:ARG:HE	1:A:1051:MET:HE1	1.60	0.67
1:A:369:VAL:HG21	1:A:379:LYS:HD2	1.76	0.67
1:A:651:LEU:HD11	1:A:659:MET:HE1	1.77	0.67
2:B:533:GLU:HB3	2:B:537:MET:HE1	1.75	0.67
2:B:607:VAL:HG12	2:B:611:MET:HE1	1.75	0.67
1:A:301:ILE:HD12	1:A:1163:ARG:HD2	1.76	0.66
1:A:320:HIS:HB3	1:A:1044:ARG:HD3	1.78	0.66
1:A:974:LEU:HD22	1:A:1005:CYS:HB3	1.77	0.66
1:A:602:THR:HG21	2:B:769:LEU:CB	2.23	0.66
1:A:892:ARG:HE	1:A:894:GLU:HG2	1.61	0.66
2:B:568:ASN:HA	2:B:630:LEU:HA	1.78	0.66
1:A:836:GLU:HA	1:A:839:ILE:HD12	1.76	0.66
1:A:229:ILE:HG23	1:A:249:PHE:HB2	1.78	0.65
1:A:409:CYS:SG	1:A:414:GLN:NE2	2.69	0.65
1:A:256:GLU:OE2	1:A:1163:ARG:NH2	2.26	0.65
1:A:362:ASP:OD1	1:A:413:GLN:NE2	2.25	0.65
2:B:614:LEU:HB3	2:B:619:CYS:HB3	1.79	0.65
1:A:31:PHE:CE2	1:A:86:LYS:HB2	2.27	0.65
1:A:245:ASP:OD1	1:A:248:ARG:NH1	2.27	0.65
2:B:528:LEU:HD11	2:B:559:VAL:HG21	1.77	0.65
1:A:214:GLN:HE22	1:A:1071:ARG:HH21	1.44	0.65
1:A:710:PHE:HD2	1:A:716:LEU:HA	1.62	0.65
1:A:295:PHE:HE1	1:A:1181:LEU:HB2	1.61	0.64
1:A:1066:LYS:HB2	1:A:1119:LYS:HG2	1.78	0.64
1:A:118:ASP:HA	1:A:121:ASN:ND2	2.12	0.64
1:A:328:ASN:N	1:A:357:GLU:OE1	2.27	0.64
2:B:644:LEU:HB3	2:B:646:ARG:HG2	1.79	0.64
1:A:251:ILE:HD11	1:A:260:GLN:HA	1.79	0.64
1:A:254:GLN:OE1	1:A:1162:PHE:N	2.31	0.64
1:A:578:TRP:NE1	1:A:581:GLY:H	1.94	0.64
1:A:415:ARG:NH1	1:A:929:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:PHE:CD1	1:A:1021:MET:HE1	2.33	0.63
1:A:858:TYR:HA	1:A:878:PRO:HA	1.81	0.63
1:A:863:ALA:H	1:A:874:PHE:HA	1.64	0.63
1:A:593:GLU:HB2	1:A:598:LYS:CG	2.26	0.63
1:A:623:ARG:NH1	1:A:624:CYS:O	2.31	0.63
1:A:1167:LEU:HB2	1:A:1178:ALA:HB1	1.80	0.62
1:A:214:GLN:NE2	1:A:1071:ARG:HH21	1.98	0.62
2:B:729:LEU:O	2:B:733:MET:HG3	1.99	0.62
1:A:210:MET:O	1:A:214:GLN:HG2	2.00	0.62
1:A:324:SER:HA	1:A:1028:PHE:CE2	2.35	0.62
1:A:89:ARG:HH11	1:A:89:ARG:HA	1.63	0.62
1:A:347:ARG:NH1	1:A:351:MET:HG2	2.14	0.62
1:A:1138:GLU:OE2	1:A:1146:ASN:ND2	2.32	0.61
1:A:329:THR:HB	1:A:345:TYR:HE1	1.65	0.61
1:A:579:ARG:HD2	1:A:584:GLN:HB2	1.82	0.61
1:A:187:PHE:HE1	1:A:197:LEU:HD21	1.64	0.61
1:A:327:HIS:CG	1:A:987:PRO:HD2	2.35	0.61
1:A:997:TYR:O	1:A:999:PRO:HD3	2.00	0.61
2:B:517:LYS:HZ1	2:B:520:ALA:HA	1.65	0.61
2:B:701:TYR:HB3	2:B:704:VAL:HB	1.83	0.61
2:B:478:LEU:HD21	2:B:513:VAL:HG21	1.82	0.61
1:A:214:GLN:HB2	1:A:1112:ILE:HD11	1.82	0.61
1:A:540:ARG:N	1:A:567:GLU:OE2	2.31	0.61
1:A:597:LEU:HD13	1:A:599:TYR:OH	2.01	0.61
1:A:1140:ASP:OD2	1:A:1146:ASN:ND2	2.29	0.61
1:A:214:GLN:HE21	1:A:291:LEU:HD21	1.67	0.60
2:B:528:LEU:O	2:B:532:MET:HG3	2.01	0.60
1:A:483:MET:HA	1:A:483:MET:HE3	1.82	0.60
1:A:214:GLN:CB	1:A:1112:ILE:HD11	2.32	0.60
1:A:29:THR:HB	1:A:112:ALA:HB3	1.81	0.60
1:A:164:ARG:NH2	1:A:165:GLU:OE2	2.35	0.60
2:B:566:LYS:HD3	2:B:572:TYR:HE1	1.65	0.60
1:A:46:ILE:O	1:A:50:ARG:N	2.35	0.60
1:A:456:LYS:HA	1:A:939:PRO:HG2	1.83	0.60
1:A:589:ARG:HG2	1:A:600:TYR:HE1	1.65	0.59
1:A:1088:GLU:HB3	1:A:1098:LYS:HG3	1.84	0.59
1:A:1001:ARG:NH1	1:A:1093:GLU:OE2	2.35	0.59
1:A:857:THR:HA	1:A:879:LYS:HD2	1.85	0.59
1:A:1165:VAL:O	1:A:1179:SER:HA	2.02	0.59
2:B:637:MET:HE3	2:B:637:MET:HA	1.83	0.59
1:A:543:ALA:HB1	1:A:562:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:HD23	1:A:1008:GLN:OE1	2.02	0.59
1:A:153:VAL:HG21	1:A:165:GLU:HB3	1.83	0.58
1:A:241:VAL:N	1:A:285:LEU:O	2.32	0.58
1:A:600:TYR:HB2	1:A:606:THR:CG2	2.32	0.58
1:A:600:TYR:HB2	1:A:606:THR:HG23	1.85	0.58
1:A:158:ARG:HG3	1:A:160:SER:H	1.68	0.58
1:A:187:PHE:CE1	1:A:197:LEU:HD21	2.39	0.58
1:A:845:LEU:HD23	1:A:849:CYS:HA	1.85	0.58
1:A:77:LYS:HE3	1:A:92:GLU:HA	1.85	0.57
1:A:607:PHE:CD1	1:A:613:LEU:HB2	2.40	0.57
1:A:23:GLU:OE2	1:A:47:MET:HG2	2.04	0.57
1:A:1167:LEU:HD21	1:A:1180:LEU:HD13	1.87	0.57
2:B:631:VAL:CG1	2:B:635:ASN:HA	2.34	0.57
1:A:1019:LYS:HG3	1:A:1133:ARG:NE	2.18	0.57
2:B:576:ARG:NH1	2:B:590:ASN:O	2.37	0.57
1:A:310:ASP:OD1	1:A:312:GLN:HG3	2.05	0.57
1:A:680:TYR:CE2	1:A:713:LEU:HD11	2.39	0.57
1:A:464:VAL:HG21	1:A:925:SER:H	1.69	0.57
2:B:692:GLU:O	2:B:697:GLY:N	2.38	0.57
1:A:335:GLN:HB3	1:A:372:HIS:CE1	2.40	0.57
1:A:491:TRP:CZ2	1:A:868:ASN:HB2	2.39	0.57
2:B:547:LEU:HA	2:B:561:VAL:HG12	1.87	0.57
1:A:1068:LEU:HB2	1:A:1181:LEU:HD22	1.86	0.57
1:A:1014:PHE:HA	1:A:1021:MET:CE	2.35	0.56
2:B:602:SER:O	2:B:606:GLN:HG2	2.04	0.56
1:A:17:GLN:HA	1:A:20:ARG:HG2	1.88	0.56
1:A:327:HIS:CD2	1:A:987:PRO:HD2	2.40	0.56
1:A:533:PHE:CE2	1:A:535:LYS:HG3	2.41	0.56
2:B:491:GLN:HE22	2:B:517:LYS:HB3	1.69	0.56
2:B:721:LYS:NZ	2:B:722:PRO:O	2.28	0.56
2:B:625:ALA:HB3	2:B:628:ASN:OD1	2.04	0.56
1:A:1057:ARG:HA	1:A:1125:TYR:CZ	2.41	0.56
1:A:139:PRO:HD3	1:A:272:PHE:CE1	2.41	0.56
1:A:214:GLN:NE2	1:A:291:LEU:HD21	2.21	0.56
1:A:710:PHE:CD2	1:A:716:LEU:HA	2.40	0.56
1:A:1052:PRO:HG2	1:A:1125:TYR:HE2	1.70	0.56
2:B:500:LEU:HD12	2:B:509:THR:HB	1.88	0.56
2:B:566:LYS:HD3	2:B:572:TYR:CE1	2.41	0.56
1:A:336:LEU:HD23	1:A:495:TYR:CE2	2.28	0.55
1:A:337:ARG:HD3	1:A:495:TYR:CG	2.42	0.55
1:A:161:ILE:HG23	1:A:165:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:PRO:HB3	1:A:977:TYR:CD1	2.41	0.55
2:B:577:ARG:HG3	2:B:582:GLU:HG2	1.87	0.55
1:A:74:ARG:NH1	1:A:78:ASN:O	2.39	0.55
1:A:564:ARG:NH2	1:A:574:THR:HG21	2.21	0.55
1:A:84:ARG:HB2	1:A:86:LYS:HG2	1.86	0.55
1:A:573:TYR:HB3	1:A:588:ILE:HD12	1.88	0.55
1:A:600:TYR:CB	1:A:606:THR:HG23	2.36	0.55
2:B:718:ARG:HB3	2:B:734:ARG:HH21	1.72	0.55
1:A:206:TYR:O	1:A:210:MET:HE3	2.06	0.55
1:A:295:PHE:CE1	1:A:1181:LEU:HB2	2.42	0.55
1:A:190:ILE:HD13	1:A:205:PHE:HB2	1.88	0.55
1:A:591:THR:HA	2:B:609:ARG:HH12	1.71	0.55
2:B:577:ARG:HD2	2:B:582:GLU:HA	1.88	0.55
1:A:303:ASP:OD2	1:A:305:LYS:NZ	2.38	0.55
1:A:323:ILE:HD12	1:A:1036:TYR:CD2	2.42	0.55
1:A:1002:LEU:HB3	1:A:1007:SER:OG	2.07	0.55
1:A:1053:PRO:O	1:A:1057:ARG:HG3	2.07	0.55
2:B:556:PRO:HG2	2:B:558:TYR:CZ	2.42	0.55
2:B:726:THR:HG22	2:B:729:LEU:HD12	1.89	0.55
2:B:671:ALA:HA	2:B:676:ILE:N	2.22	0.54
1:A:48:GLU:OE2	1:A:147:ARG:NH2	2.40	0.54
1:A:975:LEU:HD13	1:A:1050:PRO:HG3	1.89	0.54
1:A:1039:GLN:NE2	1:A:1043:MET:HE1	2.22	0.54
1:A:103:GLN:HA	1:A:1171:TYR:HD2	1.72	0.54
1:A:956:ARG:HB3	1:A:958:PHE:CE1	2.43	0.54
1:A:988:LYS:NZ	1:A:990:GLN:HB2	2.22	0.54
1:A:1074:PRO:HG3	1:A:1175:ILE:HG21	1.90	0.54
1:A:17:GLN:HG3	1:A:20:ARG:HE	1.73	0.54
1:A:103:GLN:HA	1:A:1171:TYR:CD2	2.42	0.54
1:A:203:HIS:CE1	1:A:207:LYS:HE3	2.42	0.54
1:A:52:VAL:HG21	1:A:126:LEU:HD11	1.88	0.54
1:A:269:MET:SD	1:A:269:MET:N	2.80	0.54
1:A:328:ASN:HD22	1:A:330:TYR:HE1	1.56	0.54
1:A:325:SER:HB3	1:A:355:CYS:HB3	1.90	0.54
1:A:334:ASP:HA	1:A:994:SER:OG	2.08	0.54
1:A:602:THR:HG21	2:B:769:LEU:H	1.73	0.54
1:A:658:ASP:HA	1:A:661:MET:HE2	1.89	0.54
2:B:665:LYS:HB3	2:B:700:PRO:HB2	1.90	0.54
1:A:533:PHE:HD2	1:A:535:LYS:HE3	1.72	0.54
2:B:631:VAL:HG12	2:B:635:ASN:HA	1.89	0.54
1:A:943:THR:OG1	1:A:946:ASN:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:O	1:A:351:MET:HG3	2.07	0.53
1:A:328:ASN:ND2	1:A:359:ASP:OD2	2.39	0.53
1:A:549:GLU:HA	1:A:552:MET:HG3	1.90	0.53
1:A:641:HIS:HA	1:A:644:LYS:HG2	1.90	0.53
2:B:623:ASP:OD1	2:B:663:PRO:HG3	2.08	0.53
1:A:482:TYR:HB3	1:A:491:TRP:HE3	1.74	0.53
1:A:1023:MET:HE3	1:A:1090:CYS:HB3	1.90	0.53
1:A:323:ILE:HD12	1:A:1036:TYR:CE2	2.43	0.53
1:A:165:GLU:O	1:A:169:ILE:HG12	2.08	0.53
1:A:347:ARG:NH2	1:A:1173:GLU:OE2	2.42	0.53
1:A:170:LEU:HD22	1:A:175:PHE:CD2	2.41	0.53
1:A:229:ILE:HD12	1:A:249:PHE:HA	1.90	0.53
1:A:624:CYS:HB2	2:B:767:LEU:HD21	1.90	0.53
1:A:370:ILE:HD12	1:A:385:VAL:HG21	1.90	0.52
1:A:1107:ASN:ND2	1:A:1111:PRO:HA	2.24	0.52
1:A:649:ASP:OD1	1:A:650:SER:N	2.39	0.52
1:A:418:ALA:HB2	1:A:930:LEU:HB2	1.92	0.52
1:A:660:LEU:HD13	1:A:663:ILE:HD11	1.91	0.52
1:A:600:TYR:HB2	1:A:606:THR:CB	2.40	0.52
1:A:1019:LYS:HG3	1:A:1133:ARG:CZ	2.40	0.52
1:A:294:LEU:O	1:A:1164:SER:HB3	2.09	0.52
1:A:564:ARG:HG3	1:A:574:THR:HB	1.91	0.52
1:A:874:PHE:CZ	1:A:888:PHE:HB2	2.45	0.52
1:A:409:CYS:HB2	1:A:413:GLN:OE1	2.10	0.52
1:A:899:TRP:O	1:A:903:ILE:HD12	2.10	0.51
2:B:517:LYS:HG2	2:B:520:ALA:HB2	1.91	0.51
1:A:483:MET:HE1	1:A:888:PHE:CE1	2.46	0.51
1:A:589:ARG:HH22	2:B:756:ARG:HH22	1.58	0.51
1:A:400:PRO:HG3	1:A:447:LEU:HB2	1.93	0.51
1:A:505:PHE:CZ	1:A:851:GLY:HA3	2.46	0.51
1:A:602:THR:CB	2:B:769:LEU:HB2	2.40	0.51
2:B:574:GLN:HG2	2:B:577:ARG:NH2	2.26	0.51
1:A:170:LEU:HB3	1:A:175:PHE:O	2.10	0.51
1:A:415:ARG:HH12	1:A:928:ILE:N	2.05	0.51
1:A:488:ASP:HB3	1:A:490:LYS:HZ3	1.75	0.51
1:A:858:TYR:HD2	1:A:876:LEU:HB3	1.76	0.51
1:A:873:VAL:HG22	1:A:889:ALA:HB2	1.93	0.50
1:A:938:LYS:HE2	1:A:953:ARG:CB	2.41	0.50
2:B:483:PRO:HA	2:B:493:VAL:HA	1.92	0.50
1:A:170:LEU:CD1	1:A:177:VAL:HB	2.41	0.50
1:A:483:MET:HE1	1:A:888:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:TYR:CD2	1:A:713:LEU:HD11	2.46	0.50
1:A:239:SER:O	1:A:287:VAL:N	2.44	0.50
1:A:329:THR:HB	1:A:345:TYR:CE1	2.44	0.50
1:A:975:LEU:CD1	1:A:1050:PRO:HG3	2.41	0.50
1:A:434:THR:HG23	1:A:435:GLU:HG2	1.93	0.50
1:A:1141:MET:SD	1:A:1141:MET:N	2.84	0.50
1:A:862:LYS:HE3	1:A:900:PHE:CD2	2.47	0.50
1:A:1053:PRO:HG2	1:A:1056:GLN:HG2	1.92	0.50
1:A:129:LEU:O	1:A:132:GLU:HG3	2.12	0.50
1:A:1089:ILE:HD11	1:A:1122:PHE:CD2	2.46	0.50
1:A:1130:ALA:HB3	1:A:1155:ILE:HD12	1.94	0.50
1:A:310:ASP:O	1:A:314:MET:HG2	2.12	0.50
1:A:541:THR:O	1:A:545:LYS:HG2	2.12	0.50
2:B:678:THR:O	2:B:681:SER:OG	2.24	0.50
1:A:249:PHE:HD2	1:A:250:LEU:HD12	1.77	0.49
1:A:286:PHE:O	1:A:290:PHE:N	2.42	0.49
1:A:347:ARG:HH12	1:A:351:MET:HG2	1.76	0.49
1:A:385:VAL:O	1:A:389:ILE:HG13	2.12	0.49
1:A:161:ILE:O	1:A:197:LEU:N	2.45	0.49
1:A:319:SER:OG	1:A:978:ASN:O	2.30	0.49
1:A:648:TYR:HE1	1:A:670:LEU:HB2	1.76	0.49
1:A:726:TYR:O	1:A:729:MET:HG3	2.11	0.49
1:A:861:VAL:HG23	1:A:875:ILE:HB	1.94	0.49
1:A:840:ILE:HA	1:A:843:ASN:HD21	1.75	0.49
1:A:876:LEU:HD21	1:A:888:PHE:CE2	2.47	0.49
1:A:597:LEU:HD13	1:A:599:TYR:CZ	2.47	0.49
1:A:837:LYS:HA	1:A:840:ILE:HD12	1.95	0.49
1:A:855:LEU:HD21	1:A:903:ILE:HG13	1.94	0.49
1:A:1087:VAL:HG22	1:A:1134:PHE:HD1	1.78	0.49
1:A:1136:VAL:HG23	1:A:1148:LEU:HB2	1.93	0.49
1:A:725:LEU:HG	1:A:1142:PHE:CE2	2.46	0.49
2:B:745:PRO:HG2	2:B:750:LEU:HD11	1.95	0.49
1:A:121:ASN:OD1	1:A:122:TRP:N	2.46	0.49
1:A:566:SER:OG	1:A:569:PHE:O	2.30	0.49
1:A:630:ARG:CZ	1:A:632:THR:HG22	2.42	0.49
1:A:644:LYS:HB3	1:A:646:TRP:NE1	2.27	0.49
1:A:652:SER:N	1:A:655:GLU:OE2	2.41	0.49
2:B:482:LYS:HD3	2:B:483:PRO:O	2.13	0.49
1:A:249:PHE:CD2	1:A:250:LEU:HD12	2.48	0.49
1:A:659:MET:O	1:A:663:ILE:HG12	2.13	0.49
1:A:863:ALA:HB2	1:A:875:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ARG:HE	1:A:1051:MET:CE	2.24	0.49
1:A:1168:LYS:HD3	1:A:1172:SER:HA	1.95	0.49
2:B:496:GLU:OE2	2:B:510:LYS:NZ	2.46	0.49
2:B:734:ARG:HG2	2:B:734:ARG:HH11	1.78	0.49
1:A:60:LYS:HB2	1:A:155:GLN:HG3	1.94	0.48
1:A:146:LEU:HD11	1:A:206:TYR:CD2	2.48	0.48
1:A:181:LYS:HA	1:A:184:LYS:NZ	2.28	0.48
1:A:574:THR:HA	1:A:587:ARG:HA	1.94	0.48
1:A:988:LYS:NZ	1:A:991:ARG:HG3	2.28	0.48
1:A:738:GLU:OE1	1:A:738:GLU:N	2.25	0.48
1:A:872:PHE:HB3	1:A:896:LEU:HD22	1.95	0.48
2:B:600:LEU:HD22	2:B:693:ILE:HG23	1.95	0.48
1:A:592:MET:HE1	2:B:613:TYR:HA	1.95	0.48
1:A:316:ASN:OD1	1:A:1044:ARG:NH1	2.46	0.48
1:A:600:TYR:CD1	1:A:600:TYR:C	2.91	0.48
1:A:14:GLU:HA	1:A:17:GLN:NE2	2.28	0.48
1:A:574:THR:HA	1:A:588:ILE:H	1.78	0.48
1:A:960:GLU:OE2	1:A:988:LYS:HE3	2.13	0.48
1:A:349:LEU:HA	1:A:353:CYS:SG	2.53	0.48
1:A:622:LEU:HG	1:A:629:LEU:O	2.14	0.48
1:A:627:PHE:CE2	2:B:767:LEU:HD11	2.49	0.48
1:A:349:LEU:HD22	1:A:354:ARG:HH21	1.78	0.48
1:A:564:ARG:NH1	1:A:567:GLU:OE1	2.46	0.48
1:A:938:LYS:O	1:A:955:ILE:N	2.42	0.48
2:B:577:ARG:CD	2:B:582:GLU:HA	2.43	0.48
1:A:996:ASN:HD21	1:A:1021:MET:HE2	1.79	0.48
1:A:1017:ALA:HB2	1:A:1171:TYR:CD1	2.49	0.48
2:B:471:TRP:CE2	2:B:536:LYS:HG2	2.49	0.48
1:A:1050:PRO:O	1:A:1052:PRO:HD3	2.14	0.48
2:B:655:LYS:HE3	2:B:659:ASN:HB3	1.96	0.48
1:A:876:LEU:HD21	1:A:888:PHE:CD2	2.49	0.48
1:A:178:SER:HB3	1:A:182:PHE:HE2	1.79	0.47
1:A:985:VAL:HG11	1:A:1002:LEU:HD21	1.95	0.47
1:A:355:CYS:HA	1:A:402:ILE:O	2.14	0.47
1:A:448:ARG:HG3	1:A:449:GLU:OE1	2.14	0.47
1:A:875:ILE:HG12	1:A:887:GLU:OE2	2.14	0.47
2:B:576:ARG:HD3	2:B:594:GLN:HA	1.95	0.47
2:B:612:GLU:OE2	2:B:748:LYS:HD3	2.14	0.47
1:A:74:ARG:NH1	1:A:79:SER:OG	2.46	0.47
1:A:354:ARG:HA	1:A:401:VAL:HG23	1.96	0.47
1:A:488:ASP:HB3	1:A:490:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:GLU:O	1:A:982:LEU:HB2	2.14	0.47
1:A:39:GLU:HG3	1:A:41:ARG:CZ	2.44	0.47
1:A:177:VAL:HG22	1:A:180:ALA:H	1.79	0.47
2:B:624:LEU:HB3	2:B:685:SER:HB3	1.96	0.47
1:A:17:GLN:HA	1:A:20:ARG:NE	2.30	0.47
1:A:122:TRP:O	1:A:126:LEU:HD23	2.14	0.47
1:A:342:PRO:HG2	1:A:384:ASP:OD2	2.14	0.47
1:A:1014:PHE:HA	1:A:1021:MET:HE3	1.97	0.47
2:B:657:THR:C	2:B:659:ASN:H	2.20	0.47
1:A:235:ARG:HH11	1:A:237:ASP:CG	2.23	0.47
2:B:545:ILE:HG22	2:B:642:PHE:CE1	2.49	0.47
1:A:627:PHE:CE1	1:A:629:LEU:HB2	2.50	0.47
1:A:988:LYS:HD2	1:A:990:GLN:HB2	1.96	0.47
1:A:349:LEU:HD23	1:A:353:CYS:SG	2.54	0.47
1:A:386:VAL:HA	1:A:389:ILE:HD12	1.96	0.47
1:A:488:ASP:CG	1:A:665:ARG:HH12	2.22	0.47
1:A:892:ARG:HG3	1:A:894:GLU:H	1.80	0.47
2:B:484:LEU:HD11	2:B:494:LEU:HB2	1.97	0.47
1:A:859:ASN:O	1:A:877:GLU:HB3	2.13	0.47
1:A:854:ASP:OD2	1:A:856:ASN:HB3	2.15	0.46
1:A:954:GLU:OE1	1:A:954:GLU:N	2.47	0.46
1:A:1069:GLY:HA2	1:A:1113:TRP:CE3	2.49	0.46
1:A:48:GLU:HG2	1:A:147:ARG:HE	1.79	0.46
1:A:533:PHE:CD2	1:A:535:LYS:HE3	2.50	0.46
2:B:545:ILE:HG22	2:B:642:PHE:HE1	1.80	0.46
1:A:150:ILE:HG12	1:A:161:ILE:HD11	1.96	0.46
1:A:151:TYR:CE2	1:A:157:ARG:HB2	2.50	0.46
1:A:11:ALA:HB3	1:A:14:GLU:HG3	1.96	0.46
1:A:165:GLU:HA	1:A:168:THR:HG22	1.98	0.46
1:A:481:LEU:HD21	1:A:899:TRP:CZ2	2.51	0.46
1:A:293:TYR:O	1:A:296:SER:OG	2.32	0.46
1:A:952:PHE:HB3	1:A:980:LYS:HD2	1.96	0.46
1:A:27:VAL:HA	1:A:42:THR:HA	1.97	0.46
1:A:354:ARG:NH1	1:A:397:SER:O	2.48	0.46
1:A:382:PHE:CE2	1:A:417:MET:HG3	2.51	0.46
1:A:1111:PRO:HG2	1:A:1113:TRP:CZ3	2.51	0.46
1:A:211:PHE:HB2	1:A:288:ASP:CG	2.41	0.46
1:A:464:VAL:HG11	1:A:925:SER:OG	2.16	0.46
1:A:545:LYS:O	1:A:548:GLN:N	2.49	0.46
1:A:600:TYR:HA	1:A:606:THR:HA	1.98	0.46
1:A:579:ARG:N	1:A:582:ARG:O	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ALA:HA	1:A:733:TYR:O	2.16	0.46
1:A:166:LEU:HD11	1:A:205:PHE:CE2	2.51	0.46
1:A:54:TRP:CZ2	1:A:63:GLY:HA3	2.51	0.45
1:A:278:ARG:HH21	1:A:286:PHE:HE2	1.64	0.45
1:A:316:ASN:O	1:A:443:SER:HA	2.16	0.45
1:A:28:MET:CE	1:A:111:LEU:HB3	2.46	0.45
1:A:93:ASP:OD1	1:A:94:CYS:N	2.48	0.45
1:A:503:LEU:O	1:A:853:LEU:HD23	2.16	0.45
1:A:530:GLU:HG2	1:A:532:TRP:NE1	2.32	0.45
1:A:605:LEU:HD13	1:A:617:TYR:CE1	2.52	0.45
1:A:901:GLN:O	1:A:904:ARG:HB2	2.16	0.45
1:A:1031:ASN:O	1:A:1034:THR:OG1	2.31	0.45
1:A:1168:LYS:HG3	1:A:1173:GLU:C	2.42	0.45
2:B:749:GLN:O	2:B:752:GLU:HG3	2.16	0.45
1:A:65:LEU:HD22	1:A:109:LEU:HD13	1.98	0.45
1:A:150:ILE:O	1:A:153:VAL:HG12	2.16	0.45
1:A:184:LYS:HB3	1:A:184:LYS:HE3	1.79	0.45
1:A:637:ASN:O	1:A:640:PRO:HD3	2.16	0.45
1:A:720:TYR:CZ	1:A:725:LEU:HD13	2.51	0.45
1:A:860:VAL:HG13	1:A:900:PHE:CE1	2.52	0.45
1:A:1027:LEU:HB2	1:A:1131:PHE:HZ	1.81	0.45
1:A:1054:GLU:HA	1:A:1057:ARG:CZ	2.46	0.45
2:B:686:PHE:CD1	2:B:689:LEU:HD23	2.51	0.45
1:A:144:SER:O	1:A:148:LYS:HG3	2.15	0.45
1:A:602:THR:OG1	2:B:769:LEU:HB2	2.16	0.45
2:B:595:LEU:HD22	2:B:599:ASP:HB3	1.97	0.45
1:A:337:ARG:HD3	1:A:495:TYR:CD2	2.51	0.45
1:A:429:LEU:HD21	1:A:933:LEU:HD12	1.97	0.45
1:A:697:ARG:HG3	1:A:702:PHE:HD1	1.81	0.45
1:A:839:ILE:O	1:A:843:ASN:ND2	2.49	0.45
1:A:955:ILE:HD12	1:A:982:LEU:C	2.42	0.45
1:A:996:ASN:ND2	1:A:1021:MET:HB2	2.32	0.45
1:A:240:ALA:HB1	1:A:284:PHE:HB2	1.99	0.45
1:A:874:PHE:CE1	1:A:888:PHE:HB2	2.51	0.45
1:A:996:ASN:HD22	1:A:1021:MET:HB2	1.80	0.45
1:A:1136:VAL:HG11	1:A:1180:LEU:HD11	1.99	0.45
1:A:442:PRO:HG2	1:A:447:LEU:HD11	1.98	0.45
1:A:179:SER:OG	1:A:181:LYS:HG2	2.17	0.45
1:A:252:HIS:O	1:A:255:GLN:NE2	2.36	0.45
1:A:345:TYR:OH	1:A:357:GLU:O	2.33	0.45
1:A:624:CYS:HB2	2:B:769:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:ALA:O	2:B:675:ARG:HA	2.17	0.45
1:A:327:HIS:HD2	1:A:986:TYR:HB2	1.82	0.44
1:A:560:THR:HG22	1:A:578:TRP:HB3	1.99	0.44
1:A:1000:PHE:HA	1:A:1003:TRP:HE3	1.82	0.44
2:B:624:LEU:HB3	2:B:685:SER:CB	2.47	0.44
2:B:655:LYS:O	2:B:661:ARG:HB2	2.16	0.44
1:A:39:GLU:HG3	1:A:41:ARG:NE	2.33	0.44
1:A:211:PHE:HB2	1:A:288:ASP:OD2	2.18	0.44
1:A:546:LEU:HD21	1:A:638:PRO:HG3	1.99	0.44
1:A:621:HIS:HB2	1:A:628:GLU:HG3	1.99	0.44
1:A:627:PHE:CD1	1:A:629:LEU:HB2	2.52	0.44
1:A:845:LEU:HB3	1:A:849:CYS:HB2	2.00	0.44
2:B:603:CYS:O	2:B:607:VAL:HG23	2.17	0.44
1:A:150:ILE:CG1	1:A:161:ILE:HD11	2.47	0.44
2:B:691:TRP:HB2	2:B:737:TRP:HH2	1.82	0.44
1:A:265:VAL:O	1:A:269:MET:HG2	2.17	0.44
1:A:390:LYS:HB2	1:A:425:PHE:HE1	1.82	0.44
1:A:1138:GLU:HB3	1:A:1148:LEU:HD11	2.00	0.44
2:B:496:GLU:HB3	2:B:510:LYS:NZ	2.33	0.44
2:B:576:ARG:HH11	2:B:593:GLU:HB2	1.83	0.44
1:A:477:GLN:H	1:A:498:ILE:CG1	2.30	0.44
1:A:537:VAL:HG11	1:A:543:ALA:HB2	2.00	0.44
1:A:624:CYS:SG	1:A:625:ALA:N	2.90	0.44
2:B:576:ARG:O	2:B:576:ARG:HG3	2.18	0.44
1:A:1136:VAL:O	1:A:1148:LEU:HB2	2.17	0.44
1:A:138:THR:O	1:A:141:ILE:HG22	2.18	0.44
1:A:158:ARG:NH2	1:A:165:GLU:HG3	2.33	0.44
1:A:322:TRP:CH2	1:A:1129:LEU:HD22	2.53	0.44
1:A:1069:GLY:HA2	1:A:1113:TRP:HE3	1.82	0.44
1:A:261:ASP:OD2	1:A:264:LYS:HG2	2.17	0.44
1:A:321:TYR:CZ	1:A:1038:LEU:HD13	2.52	0.44
1:A:19:LYS:HE2	1:A:129:LEU:HG	2.00	0.44
1:A:327:HIS:O	1:A:1013:ASN:ND2	2.51	0.44
1:A:621:HIS:HB2	1:A:628:GLU:OE2	2.18	0.44
1:A:247:GLN:NE2	1:A:262:LEU:HD12	2.32	0.43
1:A:394:PHE:HA	1:A:397:SER:O	2.17	0.43
1:A:449:GLU:O	1:A:450:LYS:HD2	2.18	0.43
1:A:621:HIS:ND1	1:A:630:ARG:HB3	2.32	0.43
1:A:1057:ARG:HG2	1:A:1125:TYR:CE2	2.53	0.43
1:A:573:TYR:HB2	1:A:588:ILE:HB	2.01	0.43
1:A:1174:ASP:OD1	1:A:1174:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:HIS:ND1	1:A:563:VAL:O	2.52	0.43
1:A:648:TYR:CE1	1:A:670:LEU:HB2	2.52	0.43
1:A:1084:PHE:CZ	1:A:1137:TYR:HB2	2.54	0.43
1:A:160:SER:HA	1:A:197:LEU:O	2.19	0.43
1:A:161:ILE:HB	1:A:197:LEU:HB2	1.99	0.43
1:A:180:ALA:O	1:A:184:LYS:NZ	2.46	0.43
1:A:227:VAL:HG13	1:A:229:ILE:HD11	1.99	0.43
1:A:1159:LYS:HE3	1:A:1163:ARG:NH1	2.33	0.43
1:A:567:GLU:H	1:A:567:GLU:CD	2.27	0.43
1:A:568:THR:HG21	2:B:764:GLN:NE2	2.34	0.43
1:A:646:TRP:CD1	1:A:646:TRP:H	2.36	0.43
1:A:674:ARG:HD3	1:A:679:SER:OG	2.19	0.43
1:A:726:TYR:O	1:A:727:ARG:C	2.60	0.43
1:A:901:GLN:O	1:A:905:GLU:OE1	2.36	0.43
1:A:1067:VAL:HG21	1:A:1180:LEU:HD23	2.00	0.43
1:A:170:LEU:HB2	1:A:171:PRO:HD3	2.00	0.43
1:A:645:PRO:HB2	1:A:736:THR:HG21	2.00	0.43
1:A:743:TYR:O	1:A:747:ARG:HG3	2.18	0.43
1:A:978:ASN:OD1	1:A:1008:GLN:NE2	2.52	0.43
2:B:513:VAL:HA	2:B:559:VAL:O	2.18	0.43
1:A:33:PHE:HB3	1:A:84:ARG:HH21	1.83	0.43
1:A:132:GLU:O	1:A:136:ALA:N	2.52	0.43
1:A:591:THR:HG22	1:A:592:MET:N	2.34	0.43
1:A:988:LYS:HZ1	1:A:991:ARG:HG3	1.82	0.43
2:B:567:GLY:O	2:B:631:VAL:N	2.35	0.43
2:B:597:SER:O	2:B:601:VAL:HG23	2.19	0.43
2:B:684:TRP:CE3	2:B:737:TRP:HA	2.54	0.43
1:A:48:GLU:HG2	1:A:147:ARG:HG2	2.00	0.43
1:A:999:PRO:HG2	1:A:1003:TRP:CZ3	2.53	0.43
2:B:740:VAL:O	2:B:744:ARG:HG3	2.19	0.43
1:A:1139:GLU:HG3	1:A:1143:SER:HA	2.00	0.42
1:A:25:GLY:HA3	1:A:44:GLN:HB3	2.00	0.42
1:A:316:ASN:CG	1:A:1044:ARG:HH12	2.27	0.42
1:A:533:PHE:HE1	1:A:573:TYR:CE2	2.37	0.42
1:A:728:LYS:HD2	1:A:728:LYS:HA	1.72	0.42
2:B:569:LEU:HD22	2:B:637:MET:HE2	2.01	0.42
1:A:349:LEU:HD22	1:A:354:ARG:NH2	2.34	0.42
1:A:366:GLY:O	1:A:413:GLN:HG2	2.19	0.42
1:A:678:ASP:O	1:A:697:ARG:NH2	2.52	0.42
1:A:689:LYS:HB3	1:A:689:LYS:HE3	1.81	0.42
1:A:702:PHE:HE2	1:A:712:SER:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:LYS:HD3	1:A:870:LYS:HA	1.86	0.42
1:A:251:ILE:O	1:A:255:GLN:NE2	2.52	0.42
1:A:353:CYS:O	1:A:354:ARG:NE	2.36	0.42
1:A:702:PHE:CE2	1:A:712:SER:HA	2.54	0.42
1:A:727:ARG:NH1	1:A:1144:ASP:OD2	2.52	0.42
1:A:892:ARG:HG3	1:A:894:GLU:N	2.34	0.42
1:A:903:ILE:HA	1:A:906:ILE:HD12	2.00	0.42
2:B:542:LYS:O	2:B:638:LYS:HG2	2.20	0.42
1:A:647:TYR:HD1	1:A:671:ILE:HG23	1.84	0.42
1:A:836:GLU:O	1:A:840:ILE:HG13	2.19	0.42
1:A:1114:ALA:HB3	1:A:1117:GLN:HB3	2.00	0.42
1:A:299:ASN:OD1	1:A:1163:ARG:HG2	2.20	0.42
1:A:600:TYR:CG	1:A:601:LEU:N	2.88	0.42
1:A:670:LEU:HB3	1:A:735:VAL:HB	2.01	0.42
1:A:206:TYR:CZ	1:A:210:MET:HE1	2.54	0.42
1:A:317:PRO:HB3	1:A:441:LEU:O	2.19	0.42
1:A:589:ARG:HG2	1:A:600:TYR:CE1	2.51	0.42
1:A:592:MET:HE1	2:B:613:TYR:CA	2.50	0.42
1:A:252:HIS:C	1:A:255:GLN:HE21	2.25	0.42
1:A:903:ILE:O	1:A:907:THR:HG23	2.19	0.42
2:B:686:PHE:CE1	2:B:689:LEU:HD23	2.54	0.42
1:A:838:GLN:O	1:A:841:GLU:HG3	2.20	0.42
1:A:876:LEU:HD23	1:A:887:GLU:N	2.28	0.42
1:A:182:PHE:O	1:A:186:LYS:HG2	2.20	0.42
1:A:428:LEU:HA	1:A:428:LEU:HD12	1.77	0.42
1:A:335:GLN:HB3	1:A:372:HIS:ND1	2.34	0.41
1:A:858:TYR:CD2	1:A:876:LEU:HB3	2.54	0.41
2:B:480:LEU:H	2:B:480:LEU:HD23	1.85	0.41
1:A:168:THR:O	1:A:172:LEU:HD23	2.20	0.41
1:A:318:LEU:HB3	1:A:441:LEU:HB3	2.01	0.41
1:A:333:GLY:N	1:A:338:SER:OG	2.53	0.41
1:A:555:GLY:O	1:A:557:LYS:HG2	2.19	0.41
1:A:656:ALA:O	1:A:660:LEU:HD23	2.20	0.41
1:A:987:PRO:HG3	1:A:997:TYR:CD1	2.55	0.41
2:B:692:GLU:HG2	2:B:698:GLY:O	2.20	0.41
1:A:354:ARG:NH2	1:A:393:ALA:O	2.41	0.41
1:A:455:HIS:ND1	1:A:456:LYS:O	2.53	0.41
1:A:697:ARG:HG3	1:A:702:PHE:CD1	2.54	0.41
1:A:988:LYS:HZ3	1:A:990:GLN:HB2	1.85	0.41
1:A:187:PHE:CZ	1:A:197:LEU:HD11	2.56	0.41
1:A:644:LYS:HB3	1:A:646:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:O	1:A:172:LEU:HB2	2.21	0.41
1:A:976:LYS:HD2	1:A:976:LYS:HA	1.84	0.41
1:A:400:PRO:HG2	1:A:1036:TYR:OH	2.21	0.41
1:A:243:LEU:N	1:A:282:GLU:OE2	2.48	0.41
1:A:855:LEU:HD21	1:A:903:ILE:CG1	2.50	0.41
2:B:644:LEU:HB3	2:B:646:ARG:CG	2.47	0.41
2:B:730:TYR:O	2:B:734:ARG:HG2	2.20	0.41
1:A:327:HIS:CD2	1:A:986:TYR:HB2	2.56	0.41
2:B:576:ARG:NH1	2:B:593:GLU:HB2	2.36	0.41
1:A:399:PHE:HD1	1:A:400:PRO:HD2	1.85	0.41
1:A:493:ARG:HB2	1:A:509:ILE:CG2	2.50	0.41
1:A:493:ARG:HH22	1:A:891:ASP:CG	2.29	0.41
1:A:568:THR:HG22	2:B:598:LYS:NZ	2.35	0.41
1:A:987:PRO:HG3	1:A:997:TYR:CE1	2.55	0.41
2:B:573:LEU:HD11	2:B:693:ILE:HG12	2.02	0.41
2:B:673:PHE:CZ	2:B:714:LYS:HG3	2.56	0.41
1:A:96:PHE:HE2	1:A:98:ILE:HD11	1.86	0.41
1:A:303:ASP:HA	1:A:1159:LYS:NZ	2.36	0.41
1:A:456:LYS:CA	1:A:939:PRO:HG2	2.51	0.41
1:A:483:MET:HG2	1:A:494:HIS:CD2	2.56	0.41
1:A:678:ASP:HB2	1:A:697:ARG:NH1	2.28	0.41
1:A:326:SER:HA	1:A:1012:LEU:H	1.85	0.40
1:A:482:TYR:HB3	1:A:491:TRP:CE3	2.55	0.40
1:A:884:PRO:HA	1:A:885:PRO:HD3	1.96	0.40
1:A:1167:LEU:HB2	1:A:1178:ALA:CB	2.49	0.40
1:A:34:ARG:O	1:A:35:LYS:HD3	2.21	0.40
1:A:206:TYR:OH	1:A:1072:HIS:HE1	2.04	0.40
1:A:272:PHE:HZ	1:A:292:THR:HG22	1.86	0.40
1:A:483:MET:HB2	1:A:492:THR:OG1	2.20	0.40
1:A:503:LEU:HD23	1:A:504:SER:N	2.37	0.40
1:A:87:ALA:HA	1:A:90:GLN:OE1	2.21	0.40
1:A:186:LYS:O	1:A:190:ILE:HG12	2.21	0.40
1:A:187:PHE:HZ	1:A:197:LEU:HD11	1.86	0.40
1:A:963:ALA:O	1:A:967:ILE:HG13	2.20	0.40
2:B:551:CYS:HB2	2:B:558:TYR:HB2	2.02	0.40
2:B:656:LYS:HD2	2:B:661:ARG:NH2	2.37	0.40
1:A:362:ASP:OD1	1:A:363:GLY:N	2.55	0.40
1:A:656:ALA:HA	1:A:659:MET:HE3	2.03	0.40
1:A:116:LYS:HE3	1:A:116:LYS:HB3	1.96	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	1052/1265 (83%)	997 (95%)	55 (5%)	0	100	100
2	B	305/822 (37%)	290 (95%)	15 (5%)	0	100	100
All	All	1357/2087 (65%)	1287 (95%)	70 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	966/1158 (83%)	965 (100%)	1 (0%)	88	89
2	B	271/726 (37%)	271 (100%)	0	100	100
All	All	1237/1884 (66%)	1236 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	600	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	135	ASN

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Mol	Chain	Res	Type
1	A	203	HIS
1	A	214	GLN
1	A	252	HIS
1	A	255	GLN
1	A	260	GLN
1	A	387	GLN
1	A	414	GLN
1	A	604	ASN
1	A	990	GLN
1	A	996	ASN
1	A	1013	ASN
1	A	1031	ASN
1	A	1039	GLN
2	B	491	GLN
2	B	659	ASN
2	B	764	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 ⓘ

There are no chain breaks in this entry.

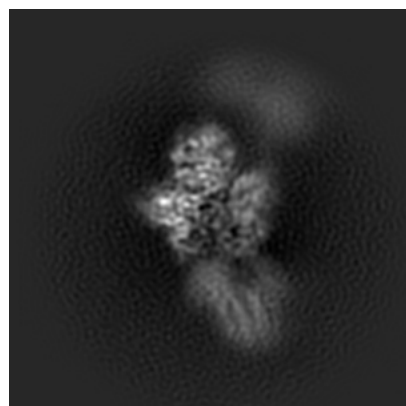
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36573. These allow visual inspection of the internal detail of the map and identification of artifacts.

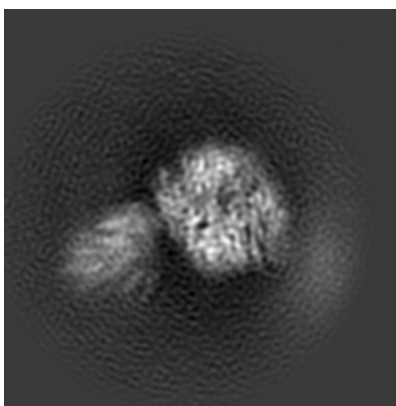
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

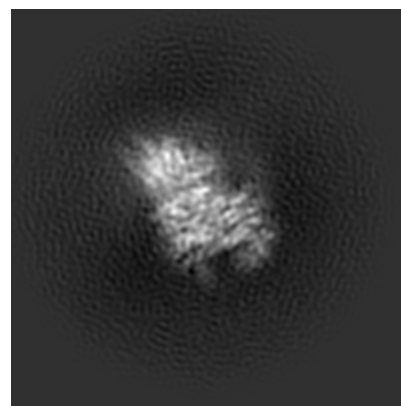
6.1.1 Primary map



X

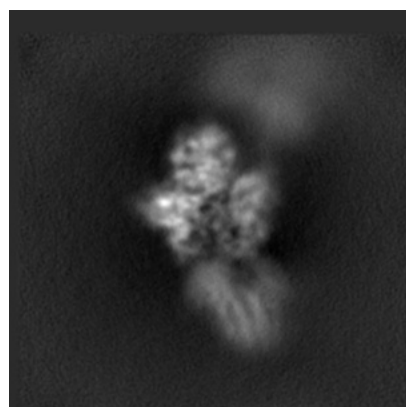


Y

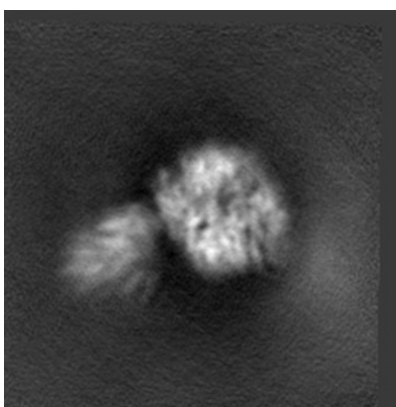


Z

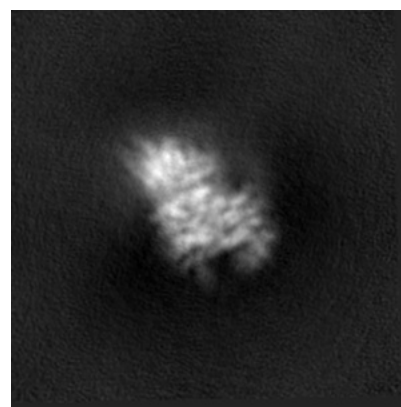
6.1.2 Raw map



X



Y

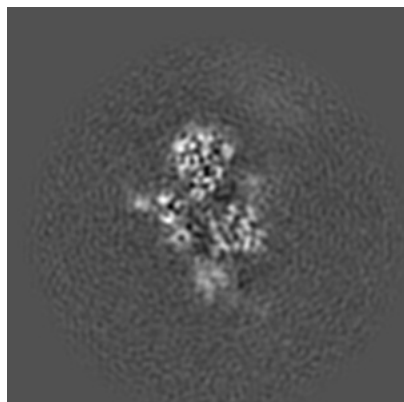


Z

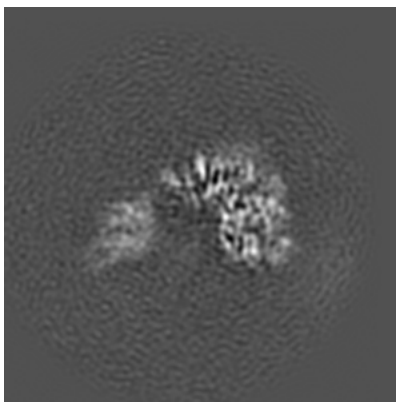
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

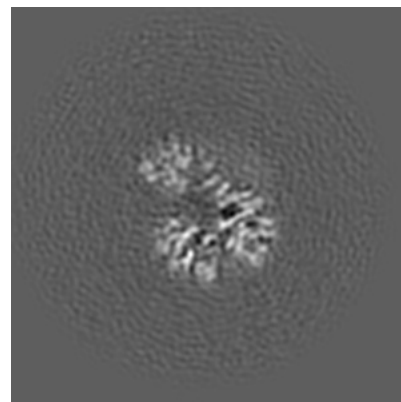
6.2.1 Primary map



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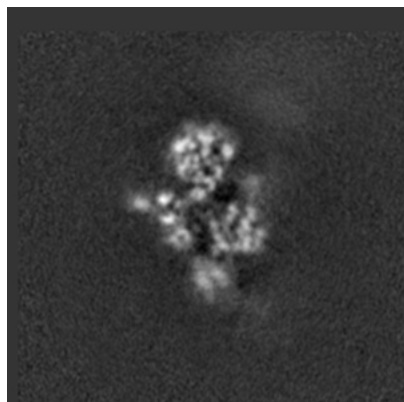


Y Index: 108

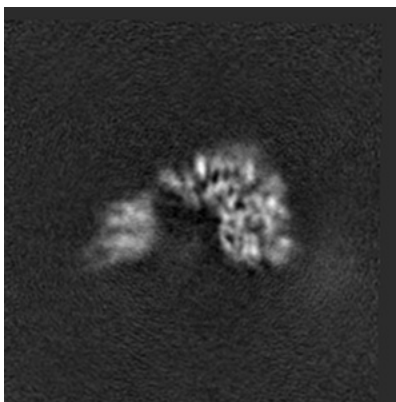


Z Index: 108

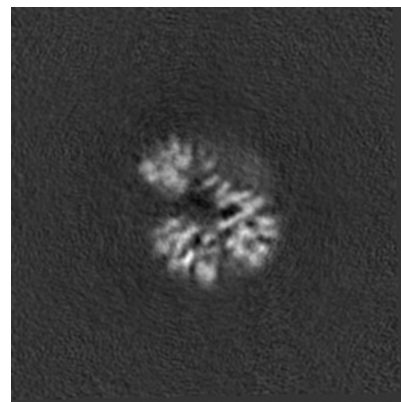
6.2.2 Raw map



X Index: 108



Y Index: 108

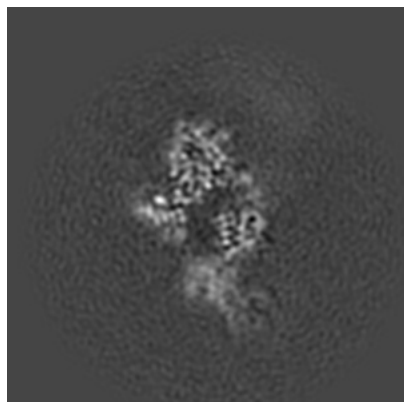


Z Index: 108

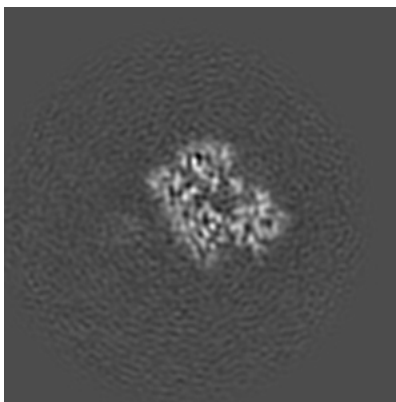
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

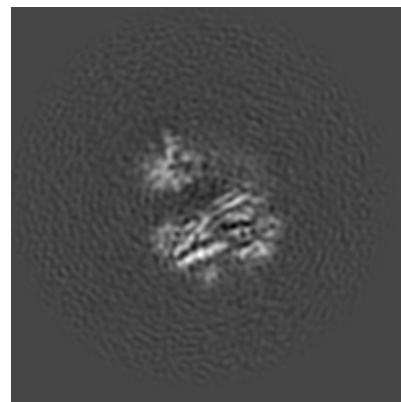
6.3.1 Primary map



X Index: 102

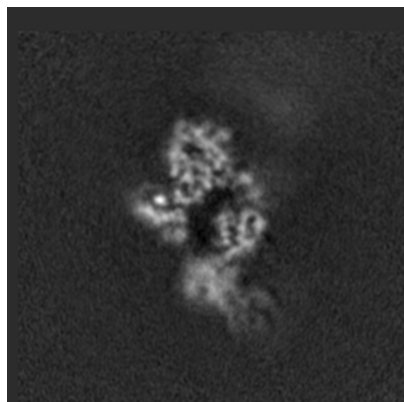


Y Index: 92

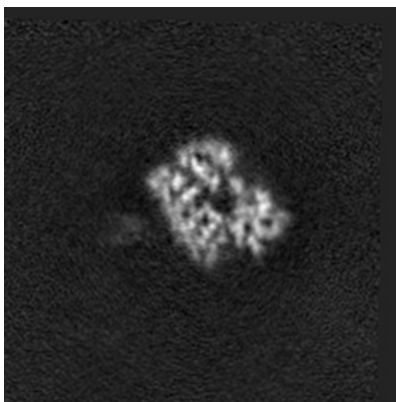


Z Index: 111

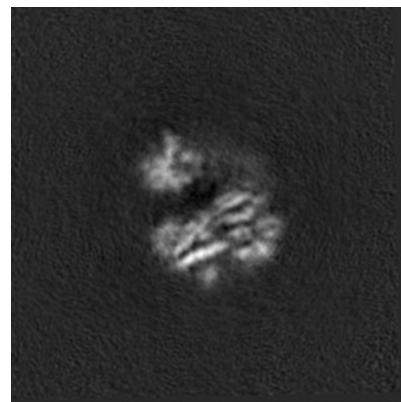
6.3.2 Raw map



X Index: 102



Y Index: 92

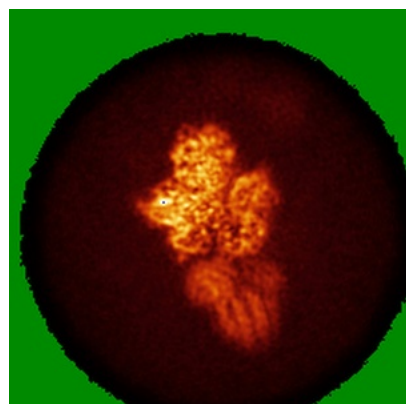


Z Index: 111

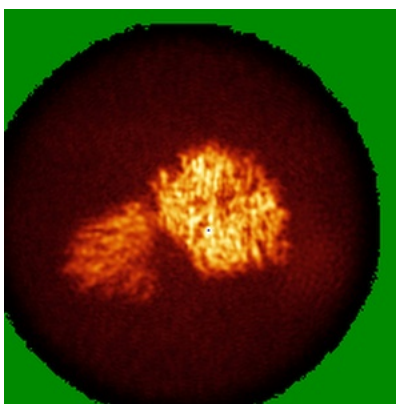
The images above show the largest variance slices of the map in three orthogonal directions.

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

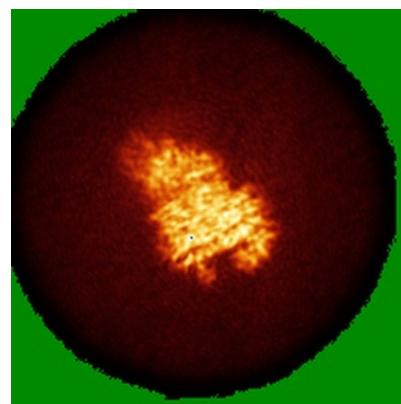
6.4.1 Primary map



X

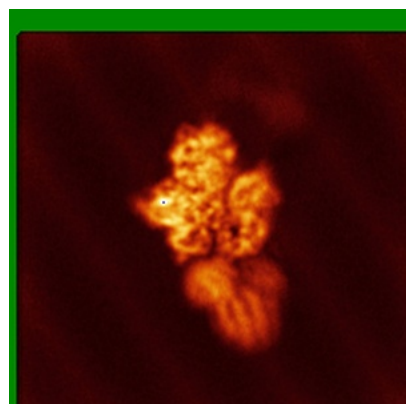


Y

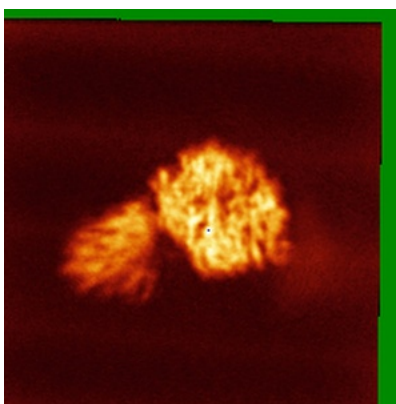


Z

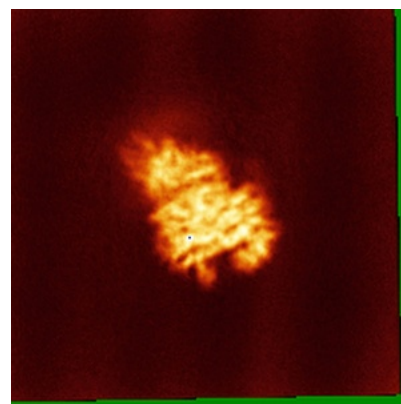
6.4.2 Raw map



X



Y

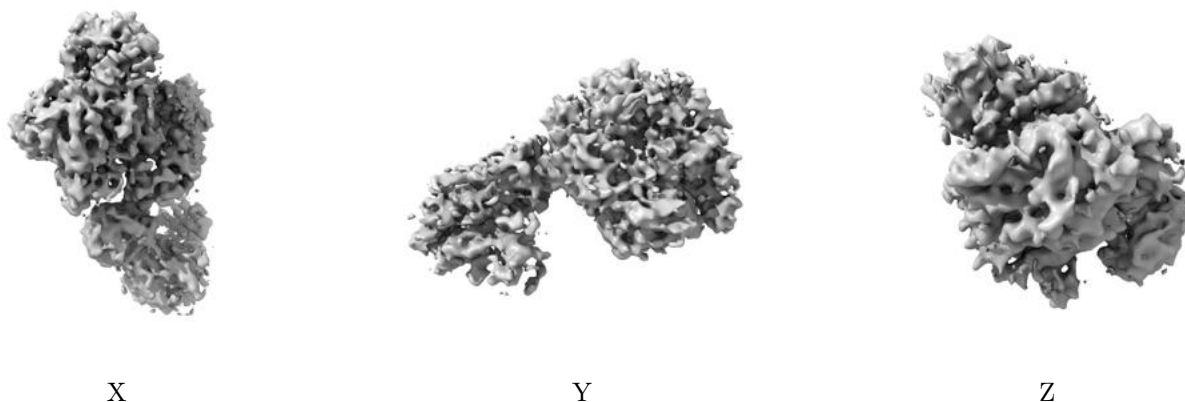


Z

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.

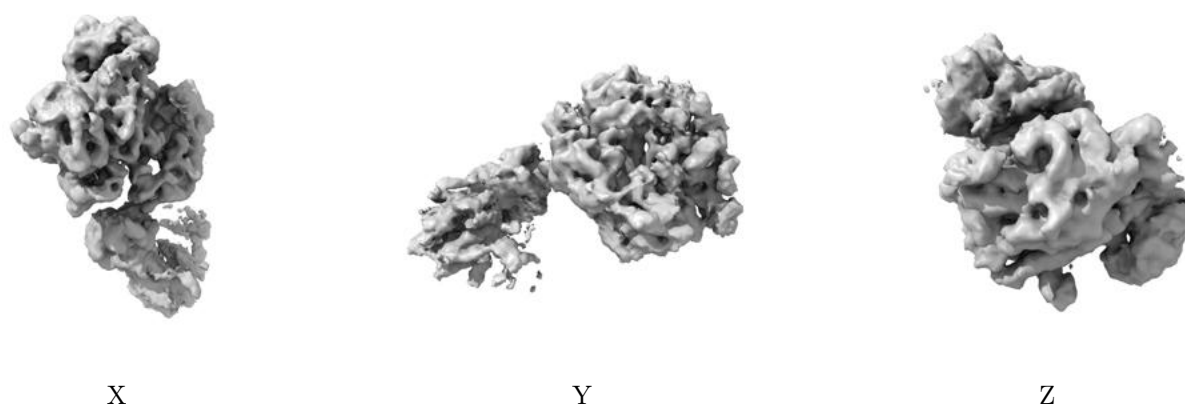
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

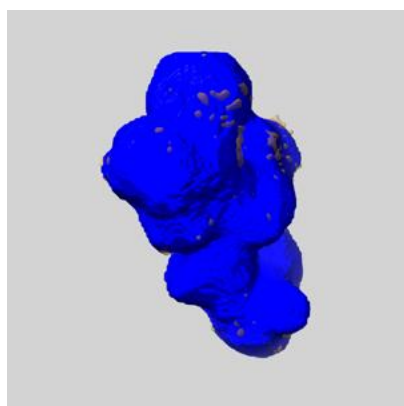
6.6 Mask visualisation [i](#)

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

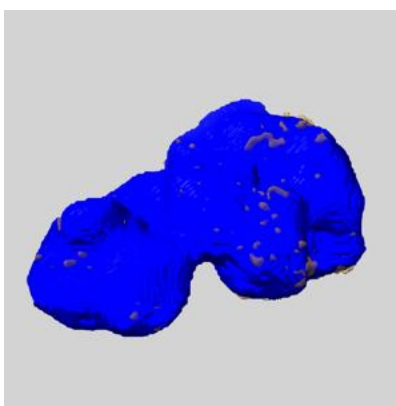
A mask typically either:

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

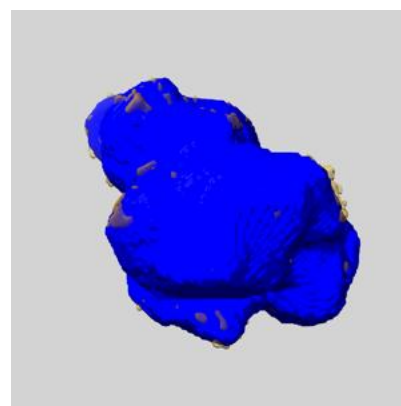
6.6.1 emd_36573_msk_1.map [i](#)



X



Y

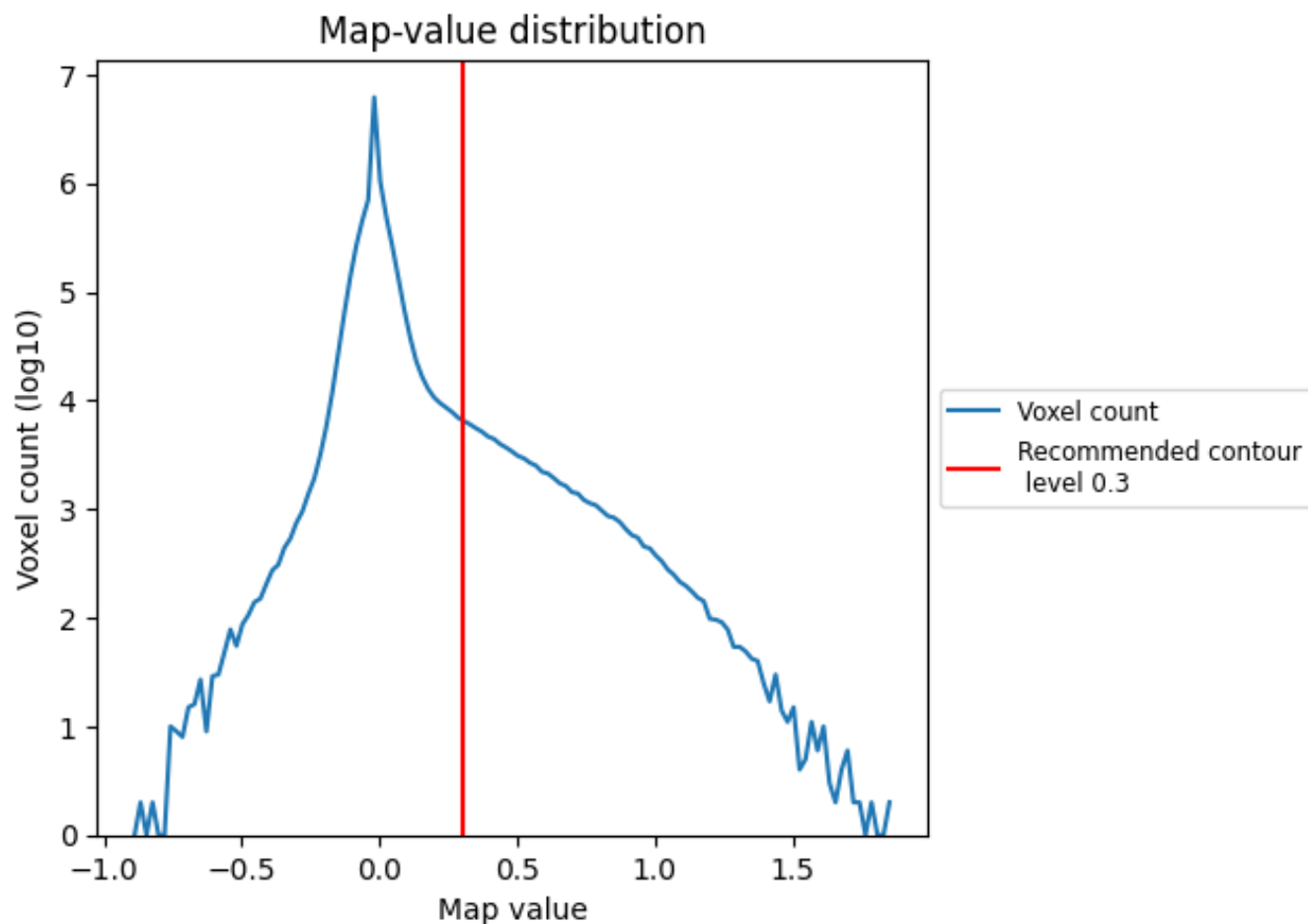


Z

7 Map analysis [i](#)

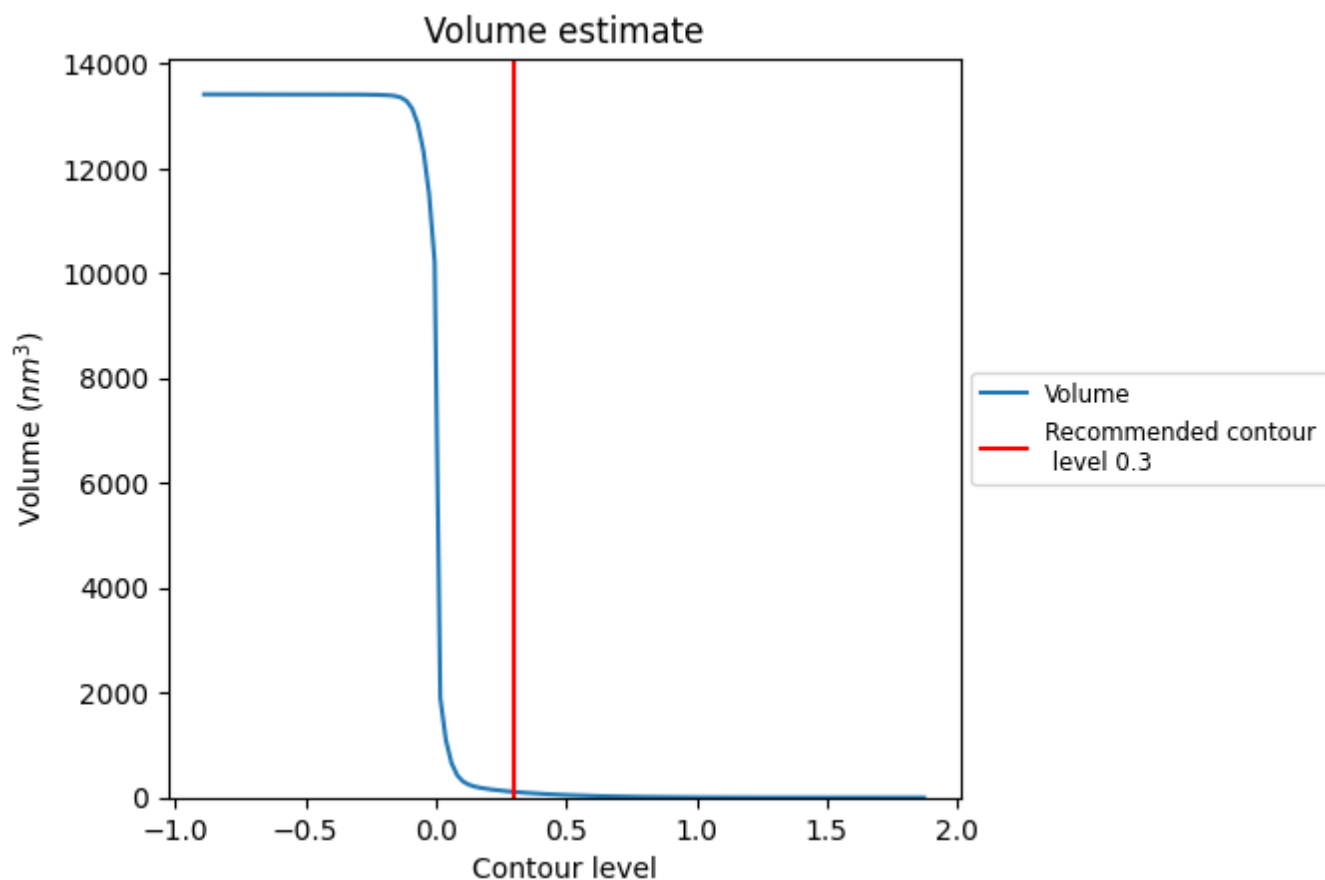
This section contains the results of statistical analysis of the map.

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.

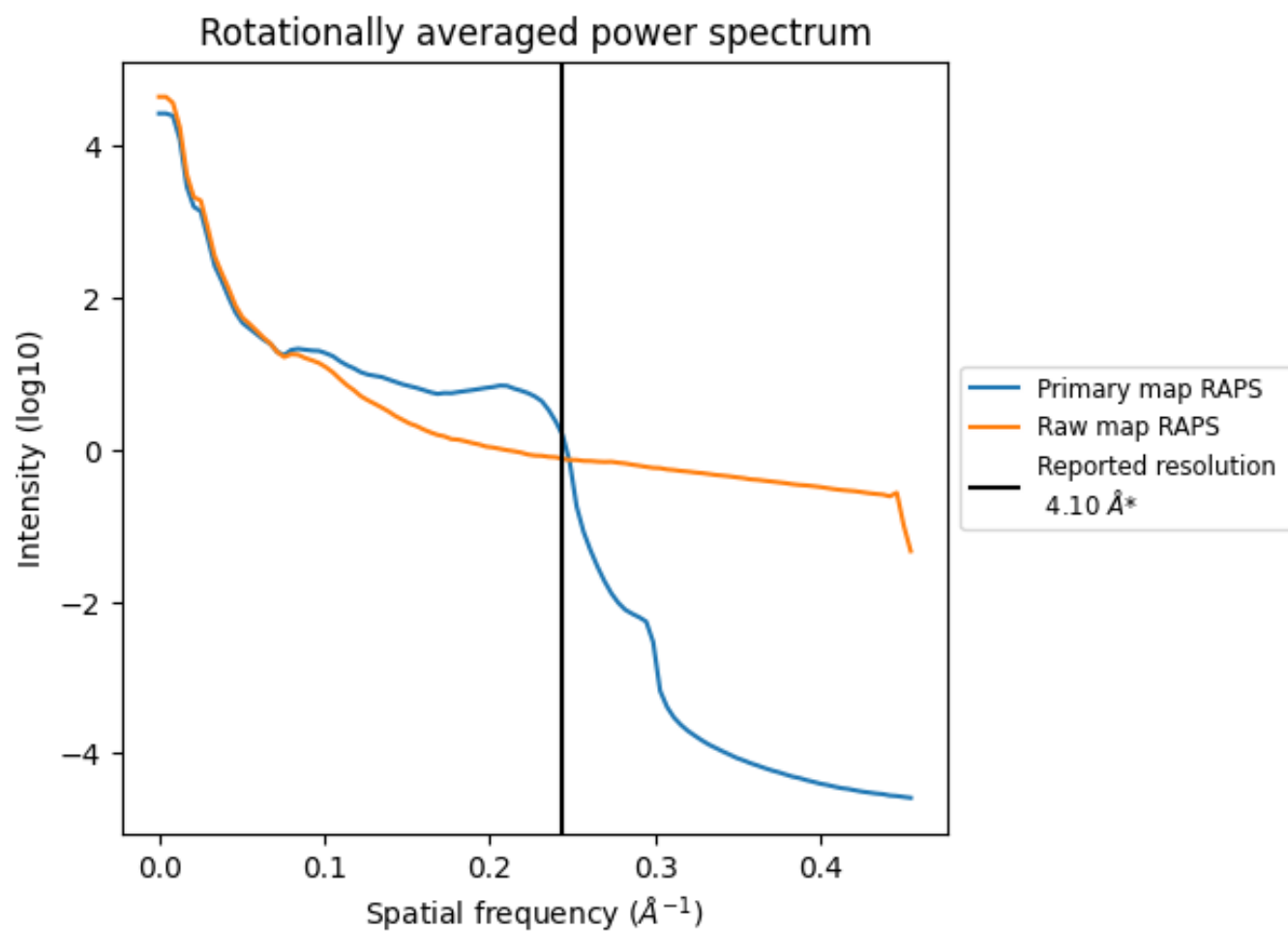
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 98 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 ⓘ

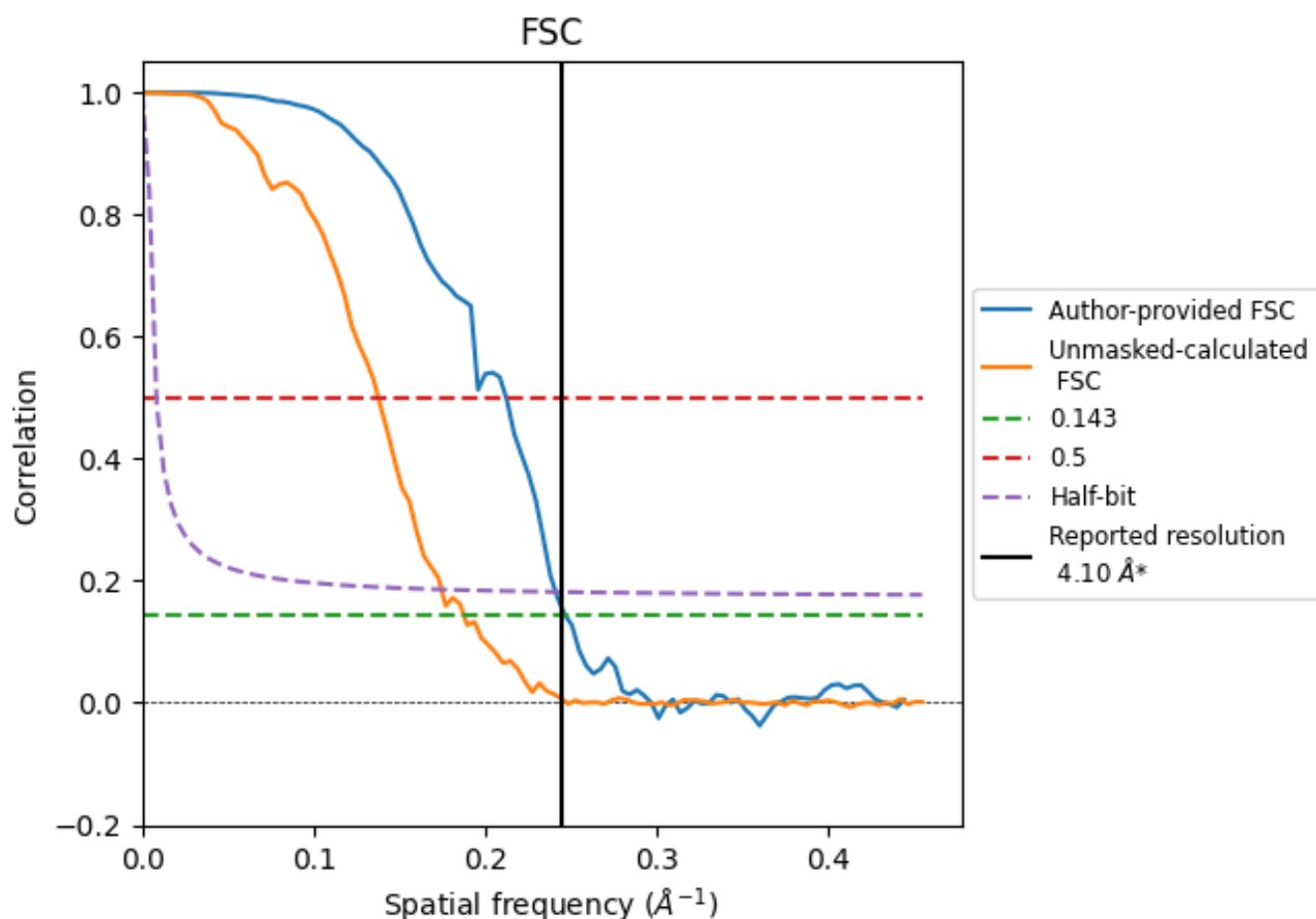


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

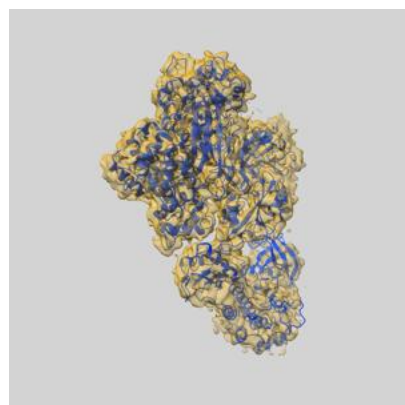
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.06	4.71	4.15
Unmasked-calculated*	5.33	7.27	5.74

*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 5.33 differs from the reported value 4.1 by more than 10 %

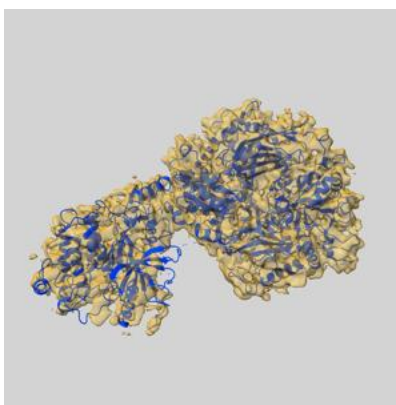
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36573 and PDB model 8JQI. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

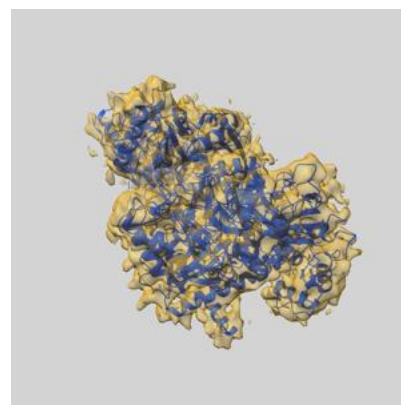
9.1 Map-model overlay [i](#)



X



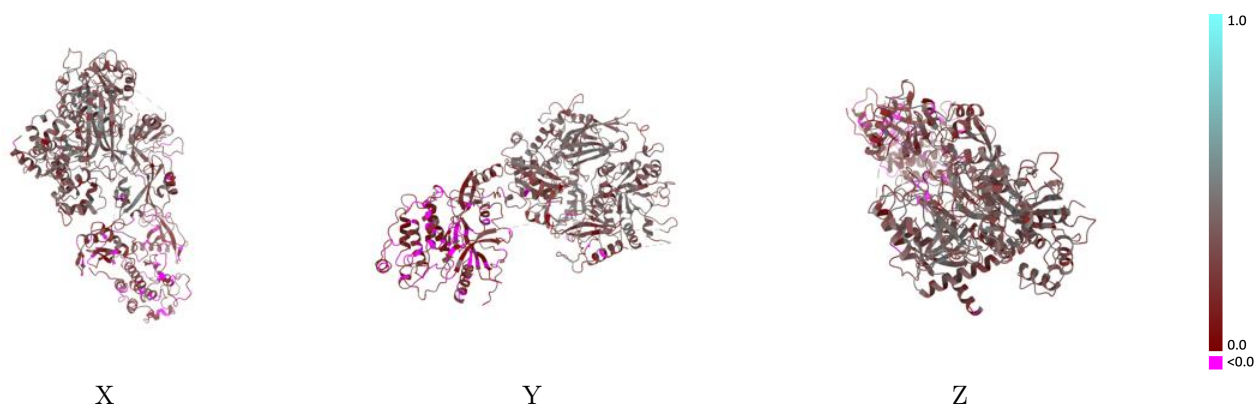
Y



Z

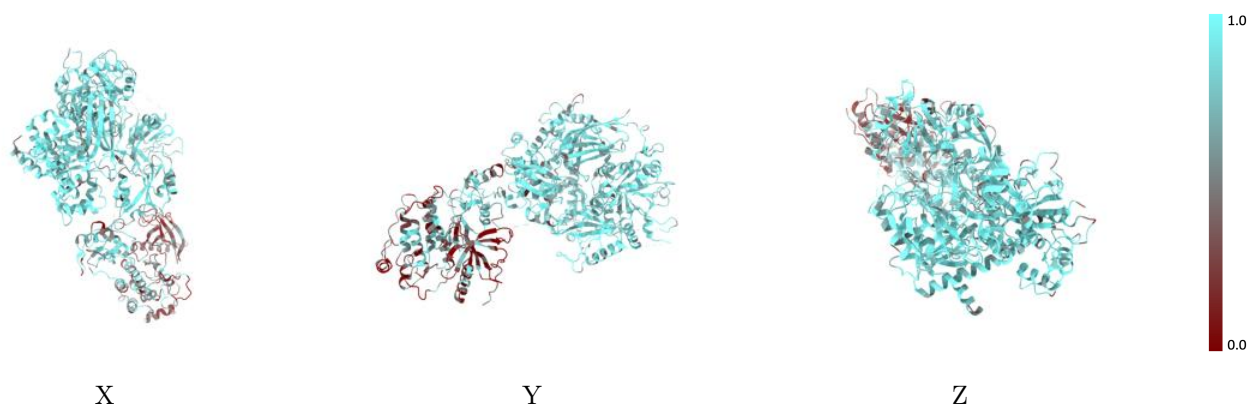
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



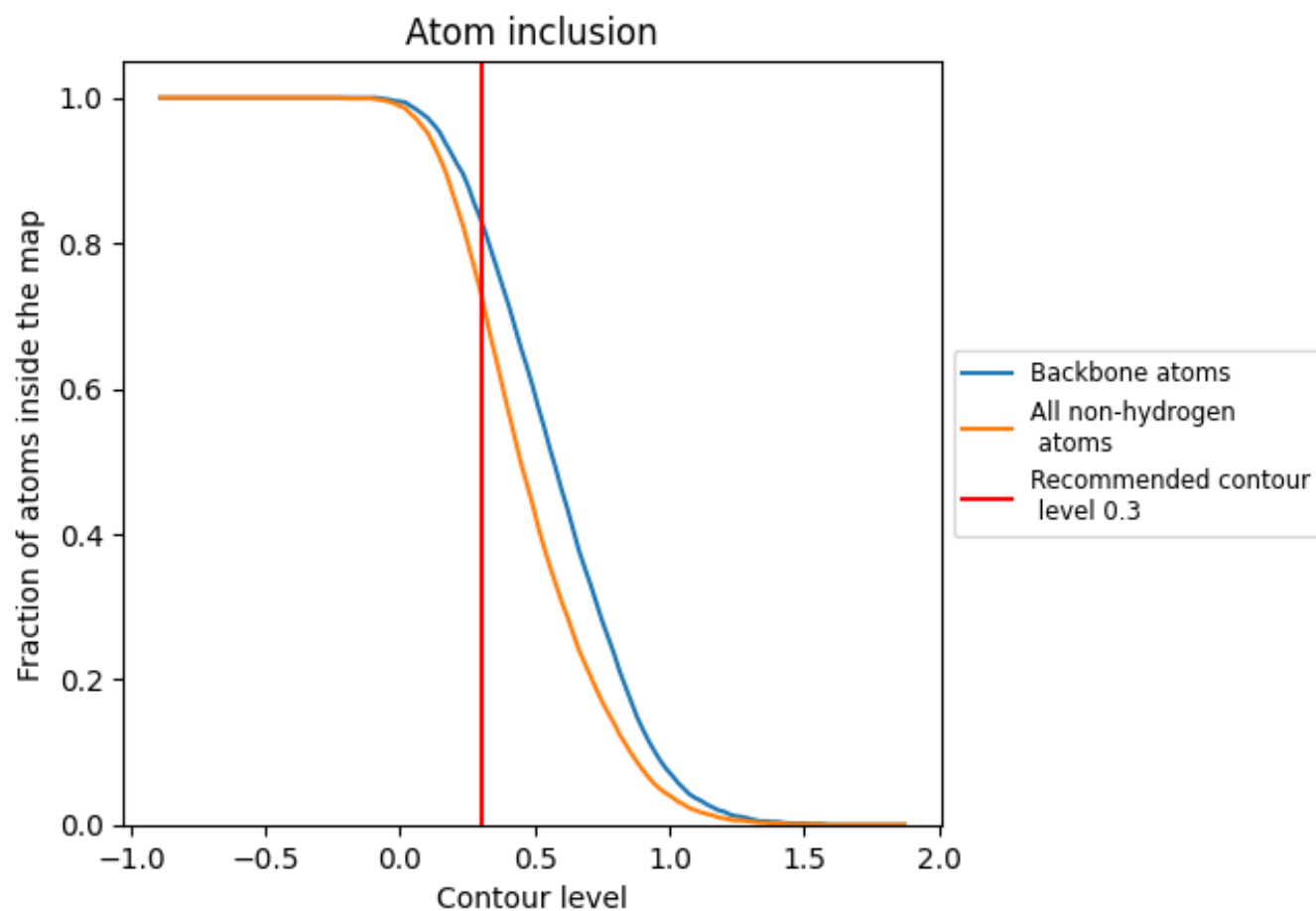
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.2730
A	0.8270	0.3150
B	0.3930	0.1230

