



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 03:32 AM UTC

PDB ID : 8E2K / pdb_00008e2k
EMDB ID : EMD-27841
Title : Cryo-EM structure of BIRC6/HtrA2-S306A
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2022-08-15
Resolution : 3.21 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:

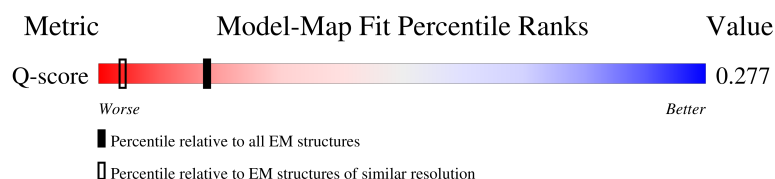
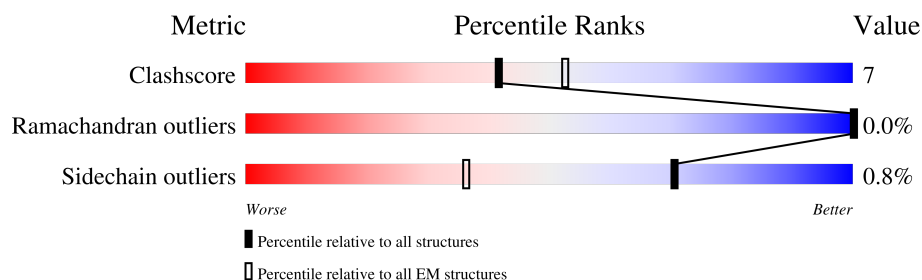
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.21 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	14613 (2.71 - 3.71)

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	4898	
1	B	4898	
2	X	332	
2	Y	332	

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Mol	Chain	Length	Quality of chain
2	Z	332	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 96785 atoms, of which 48882 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2745	Total	C	H	N	O	S	21	0
			43316	13710	21895	3643	3918	150		
1	B	2745	Total	C	H	N	O	S	21	0
			43316	13710	21895	3643	3918	150		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP Q9NR09
A	-39	GLY	-	expression tag	UNP Q9NR09
A	-38	ASP	-	expression tag	UNP Q9NR09
A	-37	TYR	-	expression tag	UNP Q9NR09
A	-36	LYS	-	expression tag	UNP Q9NR09
A	-35	ASP	-	expression tag	UNP Q9NR09
A	-34	HIS	-	expression tag	UNP Q9NR09
A	-33	ASP	-	expression tag	UNP Q9NR09
A	-32	GLY	-	expression tag	UNP Q9NR09
A	-31	ASP	-	expression tag	UNP Q9NR09
A	-30	TYR	-	expression tag	UNP Q9NR09
A	-29	LYS	-	expression tag	UNP Q9NR09
A	-28	ASP	-	expression tag	UNP Q9NR09
A	-27	HIS	-	expression tag	UNP Q9NR09
A	-26	ASP	-	expression tag	UNP Q9NR09
A	-25	ILE	-	expression tag	UNP Q9NR09
A	-24	ASP	-	expression tag	UNP Q9NR09
A	-23	TYR	-	expression tag	UNP Q9NR09
A	-22	LYS	-	expression tag	UNP Q9NR09
A	-21	ASP	-	expression tag	UNP Q9NR09
A	-20	ASP	-	expression tag	UNP Q9NR09
A	-19	ASP	-	expression tag	UNP Q9NR09
A	-18	ASP	-	expression tag	UNP Q9NR09
A	-17	LYS	-	expression tag	UNP Q9NR09
A	-16	GLY	-	expression tag	UNP Q9NR09
A	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	expression tag	UNP Q9NR09
A	-13	SER	-	expression tag	UNP Q9NR09
A	-12	GLY	-	expression tag	UNP Q9NR09
A	-11	GLY	-	expression tag	UNP Q9NR09
A	-10	LEU	-	expression tag	UNP Q9NR09
A	-9	GLU	-	expression tag	UNP Q9NR09
A	-8	VAL	-	expression tag	UNP Q9NR09
A	-7	LEU	-	expression tag	UNP Q9NR09
A	-6	PHE	-	expression tag	UNP Q9NR09
A	-5	GLN	-	expression tag	UNP Q9NR09
A	-4	GLY	-	expression tag	UNP Q9NR09
A	-3	PRO	-	expression tag	UNP Q9NR09
A	-2	SER	-	expression tag	UNP Q9NR09
A	-1	ARG	-	expression tag	UNP Q9NR09
A	0	THR	-	expression tag	UNP Q9NR09
A	1332	VAL	LEU	conflict	UNP Q9NR09
B	-40	MET	-	expression tag	UNP Q9NR09
B	-39	GLY	-	expression tag	UNP Q9NR09
B	-38	ASP	-	expression tag	UNP Q9NR09
B	-37	TYR	-	expression tag	UNP Q9NR09
B	-36	LYS	-	expression tag	UNP Q9NR09
B	-35	ASP	-	expression tag	UNP Q9NR09
B	-34	HIS	-	expression tag	UNP Q9NR09
B	-33	ASP	-	expression tag	UNP Q9NR09
B	-32	GLY	-	expression tag	UNP Q9NR09
B	-31	ASP	-	expression tag	UNP Q9NR09
B	-30	TYR	-	expression tag	UNP Q9NR09
B	-29	LYS	-	expression tag	UNP Q9NR09
B	-28	ASP	-	expression tag	UNP Q9NR09
B	-27	HIS	-	expression tag	UNP Q9NR09
B	-26	ASP	-	expression tag	UNP Q9NR09
B	-25	ILE	-	expression tag	UNP Q9NR09
B	-24	ASP	-	expression tag	UNP Q9NR09
B	-23	TYR	-	expression tag	UNP Q9NR09
B	-22	LYS	-	expression tag	UNP Q9NR09
B	-21	ASP	-	expression tag	UNP Q9NR09
B	-20	ASP	-	expression tag	UNP Q9NR09
B	-19	ASP	-	expression tag	UNP Q9NR09
B	-18	ASP	-	expression tag	UNP Q9NR09
B	-17	LYS	-	expression tag	UNP Q9NR09
B	-16	GLY	-	expression tag	UNP Q9NR09
B	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP Q9NR09
B	-13	SER	-	expression tag	UNP Q9NR09
B	-12	GLY	-	expression tag	UNP Q9NR09
B	-11	GLY	-	expression tag	UNP Q9NR09
B	-10	LEU	-	expression tag	UNP Q9NR09
B	-9	GLU	-	expression tag	UNP Q9NR09
B	-8	VAL	-	expression tag	UNP Q9NR09
B	-7	LEU	-	expression tag	UNP Q9NR09
B	-6	PHE	-	expression tag	UNP Q9NR09
B	-5	GLN	-	expression tag	UNP Q9NR09
B	-4	GLY	-	expression tag	UNP Q9NR09
B	-3	PRO	-	expression tag	UNP Q9NR09
B	-2	SER	-	expression tag	UNP Q9NR09
B	-1	ARG	-	expression tag	UNP Q9NR09
B	0	THR	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09

- Molecule 2 is a protein called Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	X	292	Total	C	H	N	O	S	0	0
			4473	1405	2248	397	418	5		
2	Y	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		
2	Z	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	133	MET	-	initiating methionine	UNP O43464
X	306	ALA	SER	conflict	UNP O43464
X	459	HIS	-	expression tag	UNP O43464
X	460	HIS	-	expression tag	UNP O43464
X	461	HIS	-	expression tag	UNP O43464
X	462	HIS	-	expression tag	UNP O43464
X	463	HIS	-	expression tag	UNP O43464
X	464	HIS	-	expression tag	UNP O43464
Y	133	MET	-	initiating methionine	UNP O43464
Y	306	ALA	SER	conflict	UNP O43464
Y	459	HIS	-	expression tag	UNP O43464
Y	460	HIS	-	expression tag	UNP O43464

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	461	HIS	-	expression tag	UNP O43464
Y	462	HIS	-	expression tag	UNP O43464
Y	463	HIS	-	expression tag	UNP O43464
Y	464	HIS	-	expression tag	UNP O43464
Z	133	MET	-	initiating methionine	UNP O43464
Z	306	ALA	SER	conflict	UNP O43464
Z	459	HIS	-	expression tag	UNP O43464
Z	460	HIS	-	expression tag	UNP O43464
Z	461	HIS	-	expression tag	UNP O43464
Z	462	HIS	-	expression tag	UNP O43464
Z	463	HIS	-	expression tag	UNP O43464
Z	464	HIS	-	expression tag	UNP O43464



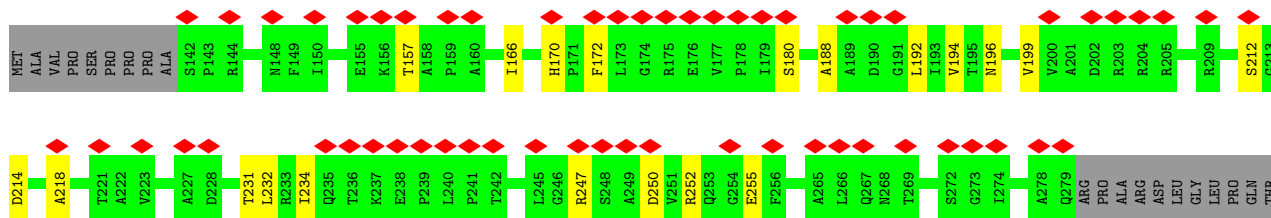


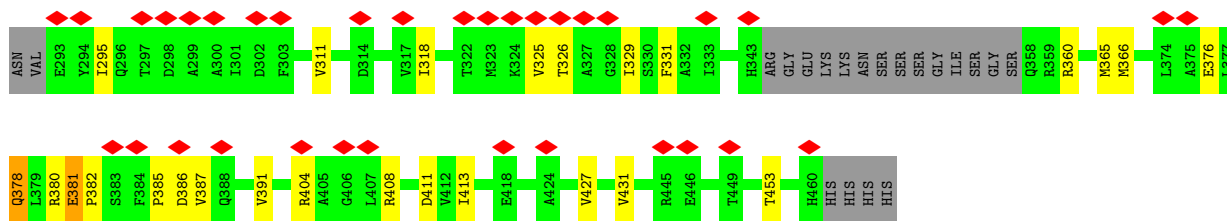




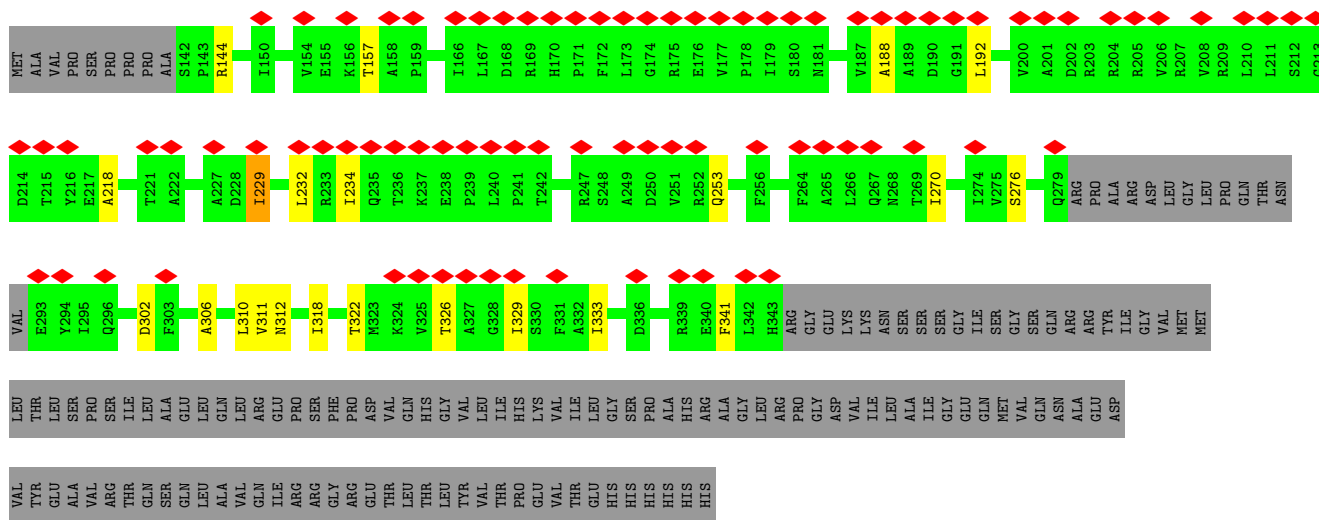




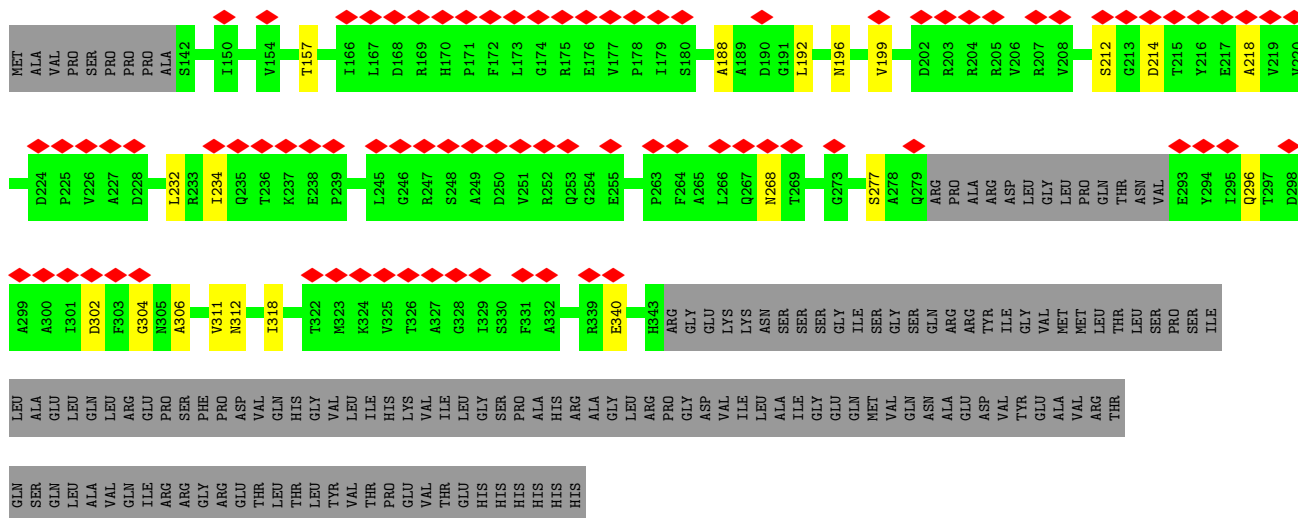




• Molecule 2: Serine protease HTRA2, mitochondrial



• Molecule 2: Serine protease HTRA2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.659	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.384	Depositor
Minimum map value	-0.530	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.18	0/21893	0.33	0/29721
1	B	0.19	0/21893	0.33	0/29721
2	X	0.16	0/2263	0.43	0/3082
2	Y	0.14	0/1442	0.40	0/1967
2	Z	0.13	0/1442	0.40	0/1967
All	All	0.18	0/48933	0.34	0/66458

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	21421	21895	21819	320	0
1	B	21421	21895	21819	294	0
2	X	2225	2248	2250	29	0
2	Y	1418	1422	1424	14	0
2	Z	1418	1422	1424	15	0
All	All	47903	48882	48736	652	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 7.

All (652) 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:3817:LEU:HD11	1:A:4189:LEU:HD12	1.35	1.05
1:B:1194:LEU:HD13	1:B:2565:GLN:N	1.83	0.93
1:A:3813:LEU:HD23	1:A:3817:LEU:HD12	1.52	0.92
1:A:3374:HIS:N	2:X:381:GLU:OE2	2.04	0.90
1:A:3374:HIS:ND1	2:X:381:GLU:OE1	2.05	0.89
1:A:4218:ARG:NH2	1:A:4397:GLU:OE2	2.06	0.88
1:B:822:GLY:N	1:B:849:ILE:O	2.11	0.83
1:A:164:GLU:OE1	1:A:258:ARG:NH2	2.12	0.83
1:A:1406:ARG:NH2	1:A:2580:GLU:OE1	2.12	0.82
1:B:3981:MET:O	1:B:3982:THR:OG1	1.98	0.81
1:A:2784:THR:OG1	1:B:3242:GLU:OE2	1.97	0.81
1:A:3817:LEU:O	1:A:4186:ARG:NH1	2.12	0.81
1:B:1866:SER:N	2:Z:340:GLU:OE2	2.13	0.81
1:A:3242:GLU:OE2	1:B:2784:THR:OG1	1.99	0.80
1:A:3981:MET:O	1:A:3982:THR:OG1	2.00	0.79
1:A:3809:ARG:NH2	1:B:1923:ASP:OD1	2.16	0.79
1:B:1946:PRO:O	1:B:1952:ASN:ND2	2.15	0.79
1:A:137:ARG:NH2	1:A:148:THR:O	2.17	0.78
1:B:1337:ARG:NH1	1:B:1342:GLY:O	2.18	0.77
1:B:378:GLN:NE2	1:B:418:MET:SD	2.59	0.76
1:B:1575:ASP:OD2	1:B:1789:ARG:NH2	2.20	0.75
1:B:2079:GLY:O	1:B:2083:VAL:HG23	1.86	0.75
1:B:3781:MET:HE2	1:B:3815:LEU:HD23	1.67	0.75
1:B:1329:GLU:OE2	1:B:1333:ASN:ND2	2.20	0.74
1:A:2079:GLY:O	1:A:2083:VAL:HG23	1.88	0.74
1:A:4440:MET:O	1:A:4444:VAL:HG23	1.87	0.74
1:A:288:ASN:O	1:A:292:THR:HG23	1.87	0.73
2:Z:157:THR:HG21	2:Z:311:VAL:HG11	1.71	0.73
1:A:857:THR:OG1	1:A:906:THR:O	2.05	0.73
1:B:283:MET:HE3	1:B:283:MET:HA	1.70	0.73
1:A:1318:ARG:HA	1:A:1321:MET:HE2	1.72	0.72
1:B:4181:ALA:O	1:B:4185:LEU:HD12	1.89	0.72
1:A:3771:ILE:HD11	1:A:3815:LEU:HD11	1.71	0.71
1:B:2891:ALA:O	1:B:3031:SER:OG	2.08	0.71
1:A:2781:VAL:HG13	1:A:2832:PRO:HB3	1.72	0.71
1:A:1799:ILE:HD12	1:A:1799:ILE:O	1.91	0.71
1:B:2781:VAL:HG13	1:B:2832:PRO:HB3	1.72	0.70
1:B:1783:MET:HE3	1:B:1783:MET:HA	1.73	0.70
1:B:1797:ARG:NH2	1:B:1882:THR:O	2.25	0.70
1:A:1461:GLU:N	1:A:1461:GLU:OE1	2.24	0.70
1:B:1799:ILE:HD12	1:B:1799:ILE:O	1.92	0.69
1:A:131:ASP:O	1:A:388:ILE:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1783:MET:HE3	1:A:1783:MET:HA	1.73	0.69
1:A:226:HIS:CE1	1:A:227:VAL:HG23	2.28	0.69
1:B:3817:LEU:O	1:B:4186:ARG:NH1	2.24	0.69
1:B:1337:ARG:NH2	1:B:1344:ILE:O	2.25	0.69
1:B:1461:GLU:N	1:B:1461:GLU:OE1	2.24	0.68
1:A:3813:LEU:HD13	1:B:1930:LEU:HD11	1.76	0.68
1:B:3781:MET:HE2	1:B:3815:LEU:CD2	2.22	0.68
1:B:1557:LEU:HB3	1:B:1560:LEU:HD21	1.77	0.67
1:A:1329:GLU:OE2	1:A:1333:ASN:ND2	2.28	0.67
1:B:903:LEU:HD21	1:B:905:ILE:HG23	1.76	0.67
1:A:568:LEU:CD2	1:A:736:ILE:HG21	2.25	0.67
1:B:4440:MET:O	1:B:4444:VAL:HG23	1.94	0.66
1:A:4254:LEU:HD13	1:A:4319:HIS:HB3	1.77	0.66
1:B:4230:ASP:OD1	1:B:4231:GLY:N	2.29	0.66
1:B:2149:LEU:HD21	1:B:2163:LEU:HD11	1.78	0.66
1:B:2872:THR:HG22	1:B:3000:LEU:CD1	2.25	0.66
1:A:2711:TYR:O	1:A:2764:LYS:NZ	2.28	0.66
1:A:228:LEU:HG	1:A:259:LEU:HD11	1.78	0.66
1:B:228:LEU:HG	1:B:259:LEU:HD11	1.77	0.66
1:B:3817:LEU:HD11	1:B:4189:LEU:HD12	1.77	0.66
1:A:3517:LEU:HD12	1:A:3552:VAL:HG11	1.78	0.66
1:A:1575:ASP:OD2	1:A:1789:ARG:NH2	2.28	0.65
1:A:2149:LEU:HD21	1:A:2163:LEU:HD11	1.77	0.65
1:A:3374:HIS:H	2:X:381:GLU:CD	2.05	0.65
1:B:1318:ARG:HA	1:B:1321:MET:HE2	1.78	0.65
1:B:1409:ALA:HB1	1:B:2582:MET:SD	2.36	0.65
1:B:2850:VAL:N	1:B:2941:SER:OG	2.30	0.65
1:A:1054:GLN:NE2	1:A:1298:GLU:OE2	2.27	0.64
1:A:1337:ARG:NH2	1:A:1344:ILE:O	2.30	0.64
1:A:228:LEU:HD23	1:A:259:LEU:HD21	1.80	0.64
1:B:226:HIS:CE1	1:B:227:VAL:HG23	2.32	0.64
1:B:3352:ALA:O	1:B:3355:THR:HG22	1.98	0.64
1:B:568:LEU:CD2	1:B:736:ILE:HG21	2.28	0.63
1:B:1808:THR:OG1	1:B:1841:SER:N	2.31	0.63
1:A:1566:LEU:HD13	1:A:1799:ILE:HD13	1.81	0.63
1:A:4412:LEU:HD13	1:A:4488:VAL:HG13	1.80	0.63
1:A:1353:LEU:HD13	1:A:1403:LYS:HB2	1.79	0.62
1:A:4489:TYR:O	1:A:4493:THR:HG23	1.99	0.62
1:B:232:ALA:O	1:B:236:VAL:HG23	1.99	0.62
1:A:414:VAL:HG22	1:A:418:MET:HE1	1.82	0.62
1:B:3530:MET:HE3	1:B:3530:MET:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3819:ASP:OD2	1:B:3863:SER:OG	2.11	0.62
1:A:2349:ASP:OD1	1:A:2350:LEU:N	2.34	0.61
1:A:3352:ALA:O	1:A:3355:THR:HG22	2.01	0.61
1:B:4063:GLU:OE1	1:B:4063:GLU:N	2.30	0.60
2:Z:188:ALA:HB3	2:Z:192:LEU:HB3	1.82	0.60
1:B:3535:ASN:O	1:B:3540:LYS:NZ	2.28	0.60
1:B:288:ASN:O	1:B:292:THR:HG23	2.01	0.60
1:A:1946:PRO:O	1:A:1952:ASN:ND2	2.33	0.60
1:B:953:CYS:SG	1:B:961:LEU:HD21	2.41	0.60
1:B:3058:LEU:HD12	1:B:3101:MET:HE2	1.83	0.60
2:X:196:ASN:OD1	2:X:199:VAL:HG23	2.02	0.60
1:A:4063:GLU:OE1	1:A:4063:GLU:N	2.29	0.59
1:A:4230:ASP:OD1	1:A:4231:GLY:N	2.34	0.59
1:B:228:LEU:HD23	1:B:259:LEU:HD21	1.84	0.59
1:B:1322:LEU:HD21	1:B:1362:VAL:HG11	1.85	0.59
1:A:953:CYS:SG	1:A:961:LEU:HD21	2.42	0.59
1:A:1337:ARG:NH1	1:A:1342:GLY:O	2.36	0.59
1:B:1105:ASP:OD2	1:B:1304:ARG:NH1	2.36	0.59
1:A:232:ALA:O	1:A:236:VAL:HG23	2.03	0.59
1:B:2083:VAL:HG22	1:B:2124:ILE:HG23	1.83	0.59
1:B:1194:LEU:HD11	1:B:2567:LEU:HG	1.83	0.59
2:X:381:GLU:H	2:X:382:PRO:CD	2.16	0.59
1:A:327:MET:N	1:A:327:MET:HE2	2.18	0.59
1:A:2872:THR:HG22	1:A:3000:LEU:CD1	2.32	0.58
1:B:2349:ASP:OD1	1:B:2350:LEU:N	2.36	0.58
1:A:3530:MET:HE3	1:A:3530:MET:HA	1.85	0.58
1:A:940:PHE:CD1	1:A:956:THR:HG22	2.38	0.58
1:B:1810:GLY:O	1:B:1863:ARG:NH1	2.36	0.58
1:B:3693:VAL:HG23	1:B:3699:MET:HG2	1.85	0.58
1:B:1093:LEU:CD2	1:B:1301:VAL:HG11	2.33	0.58
1:B:280:ARG:NH2	1:B:328:CYS:O	2.37	0.57
1:A:2325:HIS:N	1:A:2326:GLU:OE1	2.38	0.57
1:A:283:MET:HE3	1:A:283:MET:HA	1.86	0.57
1:A:2804:CYS:SG	1:A:2807:ILE:HG23	2.44	0.57
1:A:736:ILE:HG23	1:A:747:VAL:HG22	1.86	0.57
1:B:3229:LEU:H	1:B:3229:LEU:HD22	1.69	0.57
1:B:2325:HIS:N	1:B:2326:GLU:OE1	2.37	0.57
1:A:1042:VAL:HG12	1:A:1091:PHE:CD2	2.39	0.56
1:B:961:LEU:HD23	1:B:962:HIS:N	2.20	0.56
1:A:2891:ALA:O	1:A:3031:SER:OG	2.19	0.56
1:B:1385:LEU:HD11	1:B:1408:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2804:CYS:SG	1:B:2807:ILE:HG23	2.45	0.56
1:A:3837:ILE:HG22	1:A:3839:ALA:H	1.70	0.56
1:B:1085:SER:O	1:B:1089:HIS:NE2	2.38	0.56
1:A:1808:THR:OG1	1:A:1841:SER:N	2.39	0.56
1:A:3377:ASN:OD1	2:X:381:GLU:HG2	2.05	0.56
1:A:736:ILE:CG2	1:A:745:LEU:HD11	2.35	0.56
1:A:1053:GLN:O	1:A:1056:ARG:NE	2.38	0.56
1:B:2711:TYR:O	1:B:2764:LYS:NZ	2.35	0.56
1:B:176:ALA:O	1:B:181:VAL:HG22	2.06	0.56
1:A:1813:ALA:N	1:A:1861:ILE:O	2.39	0.56
1:B:4364:LEU:HB2	1:B:4411:LEU:HD11	1.87	0.56
2:X:360:ARG:NE	2:X:431:VAL:O	2.38	0.56
1:A:1322:LEU:CD2	1:A:1362:VAL:HG11	2.36	0.55
1:A:4233:LEU:HD12	1:A:4237:MET:CE	2.36	0.55
1:B:2013:ASP:OD1	1:B:2013:ASP:N	2.39	0.55
1:B:4438:ALA:O	1:B:4442:THR:HG23	2.05	0.55
1:A:1085:SER:O	1:A:1089:HIS:NE2	2.33	0.55
1:B:1093:LEU:HD21	1:B:1301:VAL:HG11	1.88	0.55
1:A:961:LEU:HD23	1:A:962:HIS:N	2.21	0.55
1:A:3811:LEU:C	1:A:3811:LEU:HD23	2.31	0.55
1:B:3771:ILE:HD11	1:B:3815:LEU:HD11	1.89	0.55
1:A:822:GLY:N	1:A:849:ILE:O	2.39	0.55
1:A:4361:LEU:O	1:A:4365:SER:N	2.40	0.55
1:B:1042:VAL:HG12	1:B:1091:PHE:CD2	2.41	0.55
1:B:4233:LEU:HD12	1:B:4237:MET:CE	2.37	0.55
1:A:2326:GLU:OE1	1:A:2326:GLU:N	2.38	0.55
1:A:3624:LYS:NZ	1:A:3628:ASP:OD2	2.36	0.55
1:A:1193:ASP:OD1	1:A:1194:LEU:N	2.38	0.54
1:A:1194:LEU:HD12	1:A:2565:GLN:N	2.23	0.54
1:B:4217:LEU:HD11	1:B:4221:PHE:CZ	2.42	0.54
1:B:4254:LEU:HD13	1:B:4319:HIS:HB3	1.89	0.54
1:A:1958:ARG:O	1:A:1958:ARG:NE	2.32	0.54
1:A:2998:LEU:HD22	1:A:3040:LEU:HD12	1.90	0.54
1:B:1193:ASP:OD1	1:B:1194:LEU:N	2.31	0.54
1:B:1054:GLN:NE2	1:B:1298:GLU:OE2	2.33	0.54
1:B:2326:GLU:OE1	1:B:2326:GLU:N	2.37	0.54
1:B:4489:TYR:O	1:B:4493:THR:HG23	2.07	0.54
1:A:1849:PRO:O	1:A:2570:ARG:NH1	2.37	0.54
1:B:3811:LEU:C	1:B:3811:LEU:HD23	2.33	0.54
1:B:736:ILE:CG2	1:B:745:LEU:HD11	2.37	0.54
1:B:823:GLY:O	1:B:848:HIS:ND1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1801:LEU:HD11	1:B:1804:VAL:HG23	1.89	0.54
1:A:2850:VAL:N	1:A:2941:SER:OG	2.41	0.54
1:B:740:ALA:HB2	1:B:861:LEU:CD1	2.38	0.54
1:A:513:LEU:HD21	1:A:568:LEU:HB2	1.90	0.54
1:B:280:ARG:NH1	1:B:329:PHE:O	2.41	0.54
2:X:408:ARG:N	2:X:411:ASP:OD2	2.38	0.54
1:A:511:SER:O	1:A:568:LEU:N	2.34	0.54
1:B:298:HIS:NE2	1:B:324:ASP:OD2	2.34	0.54
1:B:3837:ILE:HG22	1:B:3839:ALA:H	1.73	0.54
1:A:903:LEU:HD21	1:A:905:ILE:HG23	1.90	0.54
1:A:2762:LEU:HD12	1:A:2811:PHE:HZ	1.72	0.54
1:A:1029:THR:OG1	1:A:1030:ARG:NH2	2.38	0.53
1:B:2868:HIS:O	1:B:2872:THR:HG23	2.08	0.53
2:X:170:HIS:O	2:X:172:PHE:N	2.38	0.53
1:B:1484:ARG:NH1	1:B:2018:SER:O	2.41	0.53
1:A:736:ILE:HG22	1:A:745:LEU:HD11	1.91	0.53
1:B:1808:THR:N	1:B:1841:SER:OG	2.39	0.53
1:A:414:VAL:HG22	1:A:418:MET:CE	2.39	0.53
1:A:1067:HIS:ND1	1:A:1072:GLN:OE1	2.39	0.53
1:A:1031:PHE:CE2	1:A:2575:LEU:HD21	2.44	0.53
1:A:89:GLY:O	1:A:115:VAL:HG21	2.09	0.53
1:A:2868:HIS:O	1:A:2872:THR:HG23	2.08	0.53
1:B:110:LYS:HD3	1:B:110:LYS:N	2.24	0.53
1:B:3679:THR:OG1	1:B:3681:ASP:OD1	2.15	0.53
1:A:740:ALA:HB2	1:A:861:LEU:CD1	2.38	0.53
1:A:2332:VAL:HG13	1:A:2358:LEU:HD21	1.90	0.52
1:B:567:LEU:HB2	1:B:635:ILE:HD11	1.92	0.52
1:B:722:LEU:HD11	1:B:733:ILE:HD11	1.91	0.52
1:B:1092:GLU:OE2	1:B:1094:VAL:HG23	2.08	0.52
1:A:1844:LEU:HD22	1:A:2568:ASP:HB3	1.91	0.52
1:B:826:VAL:HG12	1:B:846:ILE:CD1	2.40	0.52
1:B:1866:SER:C	2:Z:340:GLU:OE2	2.53	0.52
1:B:4224:THR:O	1:B:4235:ARG:NH1	2.41	0.52
1:A:1477:VAL:HG13	1:A:2023:LEU:HD22	1.89	0.52
1:A:289:ARG:O	1:A:292:THR:OG1	2.21	0.52
1:A:3988:THR:OG1	1:A:4067:ILE:N	2.43	0.52
1:B:1193:ASP:HB2	1:B:1199:GLY:HA2	1.92	0.52
1:A:165:LEU:HD12	1:A:221:PHE:HE2	1.75	0.52
1:A:412:TRP:CD1	1:A:420:VAL:HG22	2.45	0.51
1:A:1042:VAL:HG12	1:A:1091:PHE:HD2	1.75	0.51
1:A:1409:ALA:HB1	1:A:2582:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4437:LEU:HD22	1:A:4485:ALA:HB2	1.92	0.51
1:B:95:ASP:OD2	1:B:212:LYS:NZ	2.28	0.51
1:A:110:LYS:HD3	1:A:110:LYS:N	2.25	0.51
1:A:4205:SER:O	1:A:4208:VAL:HG22	2.11	0.51
1:A:3781:MET:HE2	1:A:3815:LEU:CD2	2.41	0.51
1:A:1030:ARG:HD3	1:A:1895:HIS:NE2	2.26	0.51
1:A:2914:THR:HG23	1:A:2917:GLN:H	1.77	0.50
1:B:1094:VAL:HG22	1:B:1219:SER:HB2	1.92	0.50
1:A:1393:PHE:O	1:A:1447:SER:OG	2.24	0.50
1:B:3817:LEU:CD1	1:B:4189:LEU:HD12	2.40	0.50
1:A:926:VAL:HG21	1:A:964:LEU:HD13	1.94	0.50
1:A:2049:VAL:HG22	1:A:2050:LEU:H	1.75	0.50
1:B:1813:ALA:N	1:B:1861:ILE:O	2.42	0.50
1:B:1335:LEU:HB2	1:B:1352:VAL:HG11	1.94	0.50
1:A:1940:GLN:HA	1:A:1940:GLN:OE1	2.12	0.50
1:A:1314:GLU:OE1	1:A:1318:ARG:NH2	2.43	0.50
1:B:1783:MET:HE1	1:B:1789:ARG:HG3	1.94	0.50
2:X:188:ALA:HB3	2:X:192:LEU:HB3	1.93	0.50
1:A:1092:GLU:OE2	1:A:1094:VAL:HG23	2.12	0.49
1:A:1321:MET:HE3	1:A:1358:TRP:CZ3	2.48	0.49
1:B:2599:THR:HG22	1:B:2599:THR:O	2.12	0.49
1:A:566:CYS:SG	1:A:632:LEU:HD12	2.53	0.49
1:A:1322:LEU:HD21	1:A:1362:VAL:HG11	1.93	0.49
1:B:1322:LEU:CD2	1:B:1362:VAL:HG11	2.41	0.49
1:B:3789:PHE:CE2	1:B:4083:ILE:HD11	2.47	0.49
1:B:289:ARG:NH2	1:B:310:ALA:O	2.38	0.49
1:B:4364:LEU:CB	1:B:4411:LEU:HD11	2.42	0.49
2:X:325:VAL:HG21	2:X:331:PHE:CE2	2.47	0.49
1:B:1776:GLN:HB3	1:B:1875:LEU:HD12	1.95	0.49
1:B:3813:LEU:HD23	1:B:3817:LEU:HD12	1.95	0.49
1:A:129:VAL:HG11	1:A:388:ILE:HG21	1.94	0.49
1:A:1353:LEU:HD13	1:A:1403:LYS:CB	2.42	0.49
1:A:3251:LEU:HD23	1:B:2717:ARG:CG	2.43	0.49
1:B:1404:CYS:O	1:B:1408:LEU:HD23	2.12	0.49
1:B:1958:ARG:O	1:B:1958:ARG:NE	2.34	0.49
1:A:2391:ASP:OD1	1:A:2391:ASP:N	2.44	0.49
1:B:2049:VAL:HG22	1:B:2050:LEU:H	1.78	0.49
1:B:2391:ASP:OD1	1:B:2391:ASP:N	2.46	0.49
2:Z:277:SER:HB3	2:Z:296:GLN:HB3	1.95	0.49
1:A:3709:ASN:OD1	1:A:3709:ASN:C	2.56	0.49
1:A:3817:LEU:HB3	1:A:4186:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1867:THR:O	1:B:1867:THR:HG22	2.13	0.49
1:A:4377:LEU:HB3	1:A:4436:LEU:HB3	1.94	0.49
1:A:4495:LEU:C	1:A:4495:LEU:HD23	2.37	0.49
1:B:1852:VAL:CG1	1:B:1884:ILE:HD13	2.43	0.49
1:B:2180:ASP:OD1	1:B:2180:ASP:C	2.56	0.49
1:A:4224:THR:O	1:A:4235:ARG:NH1	2.45	0.48
1:B:1067:HIS:ND1	1:B:1072:GLN:OE1	2.46	0.48
1:B:1393:PHE:O	1:B:1447:SER:OG	2.29	0.48
1:B:1406:ARG:NH2	1:B:2580:GLU:OE1	2.46	0.48
1:B:1925:GLN:HG2	1:B:1984:LEU:HD21	1.95	0.48
2:X:212:SER:OG	2:X:214:ASP:OD2	2.22	0.48
1:B:2046:VAL:N	1:B:2047:PRO:CD	2.76	0.48
1:A:176:ALA:O	1:A:181:VAL:HG22	2.14	0.48
1:A:736:ILE:HG12	1:A:747:VAL:HG13	1.94	0.48
1:A:3846:HIS:CE1	1:A:3848:MET:HE2	2.48	0.48
2:X:318:ILE:C	2:X:318:ILE:HD12	2.39	0.48
1:A:2180:ASP:C	1:A:2180:ASP:OD1	2.56	0.48
1:A:2878:MET:HE1	1:A:2880:ARG:NE	2.29	0.48
1:A:3058:LEU:HD12	1:A:3101:MET:HE2	1.94	0.48
1:B:1820:TRP:CZ3	1:B:1857:LYS:HB2	2.48	0.48
1:B:2998:LEU:HD22	1:B:3040:LEU:HD12	1.95	0.48
2:X:376:GLU:O	2:X:380:ARG:HB2	2.13	0.48
1:A:3989:LEU:HD23	1:A:4064:THR:HG21	1.96	0.48
1:B:2763:VAL:HG21	1:B:2818:ILE:HG21	1.95	0.48
1:B:568:LEU:HD22	1:B:736:ILE:HG21	1.95	0.48
1:A:356:PRO:HB2	1:A:363:THR:HG22	1.95	0.48
1:A:632:LEU:O	1:A:717:VAL:N	2.46	0.48
1:A:1557:LEU:HB3	1:A:1560:LEU:HD21	1.96	0.48
1:B:1824:GLU:O	1:B:1828:GLY:HA3	2.14	0.48
1:A:3281:ARG:HD2	1:B:2783:PRO:HG2	1.95	0.48
1:A:1127:ASN:ND2	1:A:1221:LEU:HD21	2.29	0.48
1:A:2180:ASP:OD1	1:A:2181:TYR:N	2.46	0.48
1:A:4364:LEU:HB2	1:A:4411:LEU:HD11	1.95	0.47
1:B:744:HIS:CD2	1:B:827:LEU:HD11	2.49	0.47
1:A:4369:LEU:HG	1:A:4373:MET:HE2	1.96	0.47
1:B:289:ARG:O	1:B:292:THR:OG1	2.27	0.47
1:B:1813:ALA:HB2	1:B:1863:ARG:HA	1.95	0.47
1:B:4442:THR:O	1:B:4446:THR:HG23	2.14	0.47
1:A:2763:VAL:HG21	1:A:2818:ILE:HG21	1.96	0.47
1:B:566:CYS:SG	1:B:632:LEU:HD12	2.55	0.47
1:B:1471:ALA:O	1:B:1475:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2833:LEU:HD21	1:B:2914:THR:C	2.39	0.47
1:A:513:LEU:HD23	1:A:566:CYS:SG	2.54	0.47
1:A:2336:VAL:HG23	1:A:2358:LEU:HD11	1.95	0.47
1:B:3867:SER:HB3	1:B:3979:ALA:HB1	1.95	0.47
1:A:1471:ALA:O	1:A:1475:THR:HG23	2.14	0.47
1:B:1194:LEU:HD21	1:B:2581:LEU:HD23	1.96	0.47
1:B:1512:MET:O	1:B:1513:SER:OG	2.23	0.47
1:B:3867:SER:N	1:B:3979:ALA:O	2.45	0.47
1:B:4437:LEU:HD22	1:B:4485:ALA:HB2	1.95	0.47
1:A:1832:VAL:HG23	1:A:2567:LEU:O	2.15	0.47
1:A:1842:LEU:CD2	1:A:2566:ALA:HB1	2.45	0.47
1:A:1914:LEU:C	1:A:1914:LEU:HD23	2.39	0.47
1:A:2167:MET:HE2	1:A:2171:VAL:HG23	1.96	0.47
1:A:3244:SER:OG	1:A:3246:ASP:OD1	2.32	0.47
1:B:1042:VAL:HG12	1:B:1091:PHE:HD2	1.78	0.47
1:B:2878:MET:HE1	1:B:2880:ARG:NE	2.30	0.47
1:B:3364:ALA:O	1:B:3368[A]:SER:OG	2.29	0.47
1:A:3639:LEU:HD11	1:A:3683:VAL:HG13	1.97	0.47
1:A:1817:ILE:HB	1:A:1832:VAL:HG12	1.96	0.47
1:A:4409:VAL:N	1:A:4410:PRO:HD2	2.30	0.47
1:B:85:VAL:HG12	1:B:86:THR:N	2.30	0.47
1:A:91:ILE:HD11	1:A:117:CYS:HB3	1.97	0.47
1:A:3709:ASN:N	1:A:3710:PRO:CD	2.78	0.47
1:B:1790:PHE:CD1	1:B:1790:PHE:C	2.92	0.47
1:A:85:VAL:HG12	1:A:86:THR:N	2.30	0.46
1:A:2083:VAL:HG22	1:A:2124:ILE:HG23	1.97	0.46
1:B:826:VAL:HG12	1:B:846:ILE:HD11	1.98	0.46
1:B:1867:THR:OG1	2:Z:340:GLU:OE1	2.32	0.46
2:Y:318:ILE:HD12	2:Y:318:ILE:C	2.40	0.46
1:A:1117:ILE:CG2	1:A:1192:LEU:HD11	2.45	0.46
1:A:3111:MET:HE2	1:A:3331:LEU:HA	1.97	0.46
1:B:2870:TYR:OH	1:B:2916:ASP:OD1	2.24	0.46
1:A:568:LEU:HD21	1:A:736:ILE:HG21	1.98	0.46
1:A:568:LEU:HD22	1:A:736:ILE:HG21	1.97	0.46
1:A:1797:ARG:NH2	1:A:1882:THR:O	2.48	0.46
1:A:1830:ARG:HD3	1:A:1833:VAL:HG23	1.96	0.46
1:B:2336:VAL:HG23	1:B:2358:LEU:HD11	1.97	0.46
2:Y:302:ASP:O	2:Y:306:ALA:N	2.45	0.46
1:A:568:LEU:HD12	1:A:632:LEU:HD21	1.98	0.46
1:A:1209:VAL:HG13	1:A:1306:PHE:CE2	2.50	0.46
1:A:1804:VAL:HG13	1:A:1878:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1361:GLY:HA3	1:B:2575:LEU:HD13	1.98	0.46
1:B:1390:ARG:HB2	1:B:1390:ARG:NH1	2.30	0.46
1:A:226:HIS:ND1	1:A:227:VAL:HG23	2.31	0.46
1:A:567:LEU:HB2	1:A:635:ILE:HD11	1.97	0.46
1:B:2878:MET:HE1	1:B:2880:ARG:HE	1.80	0.46
1:A:129:VAL:CG1	1:A:388:ILE:HG21	2.46	0.46
1:A:1117:ILE:HG21	1:A:1192:LEU:HD11	1.97	0.46
1:B:1561:LEU:HB3	1:B:1989:ASN:OD1	2.16	0.46
1:B:2025:THR:HG22	1:B:2029:TYR:CE2	2.51	0.46
1:A:1867:THR:HG22	1:A:1867:THR:O	2.14	0.46
1:A:2813:LEU:HD12	1:A:2851:VAL:HG11	1.98	0.46
1:A:3246:ASP:OD1	1:A:3247:GLY:N	2.48	0.46
1:A:4311:THR:OG1	1:A:4314:ARG:NH1	2.48	0.46
1:B:1804:VAL:HG13	1:B:1878:TYR:CD1	2.50	0.46
1:A:156:LYS:N	1:A:159:ASP:OD2	2.42	0.46
1:A:1842:LEU:HD23	1:A:2566:ALA:HB1	1.98	0.46
1:A:1957:LEU:HD21	1:B:3128:THR:HA	1.97	0.46
1:B:72:SER:O	1:B:73:LEU:HD12	2.16	0.46
1:A:2046:VAL:N	1:A:2047:PRO:CD	2.79	0.46
1:A:3813:LEU:HD22	1:A:4191:VAL:HG21	1.98	0.46
2:Y:270:ILE:HD12	2:Y:270:ILE:H	1.81	0.46
2:Z:318:ILE:C	2:Z:318:ILE:HD12	2.41	0.46
1:A:739:CYS:SG	1:A:741:ASP:N	2.87	0.45
1:A:2833:LEU:HD21	1:A:2914:THR:C	2.41	0.45
1:B:4217:LEU:HG	1:B:4221:PHE:CE2	2.50	0.45
1:A:3227:PRO:HD2	1:A:3263:THR:O	2.16	0.45
1:A:4364:LEU:CB	1:A:4411:LEU:HD11	2.46	0.45
1:B:131:ASP:O	1:B:388:ILE:N	2.47	0.45
1:B:1484:ARG:NH2	1:B:2016:GLN:O	2.49	0.45
1:B:4478:VAL:N	1:B:4479:PRO:CD	2.79	0.45
1:A:4224:THR:HG22	1:A:4231:GLY:HA2	1.97	0.45
1:B:239:LEU:HD22	1:B:246:VAL:CG1	2.46	0.45
1:B:1830:ARG:HD3	1:B:1833:VAL:HG23	1.97	0.45
1:B:2332:VAL:HG13	1:B:2358:LEU:HD21	1.98	0.45
1:B:3388:GLN:HG3	1:B:3392[B]:ILE:HD11	1.97	0.45
1:A:2582:MET:HE2	1:A:2586:MET:HE3	1.97	0.45
1:B:513:LEU:HD21	1:B:568:LEU:HB2	1.99	0.45
1:B:2177:ARG:O	1:B:2180:ASP:OD1	2.34	0.45
1:B:3846:HIS:CE1	1:B:3848:MET:HE2	2.51	0.45
2:X:194:VAL:HG22	2:X:231:THR:HG22	1.98	0.45
1:B:129:VAL:HG11	1:B:388:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:ALA:HB3	1:B:901:GLY:HA3	1.98	0.45
1:B:2813:LEU:HD12	1:B:2851:VAL:HG11	1.98	0.45
1:B:4196:GLU:O	1:B:4196:GLU:HG2	2.15	0.45
1:A:291:GLU:O	1:A:294:THR:HG23	2.16	0.45
1:A:1098:ALA:HB1	1:A:1212:MET:SD	2.57	0.45
2:X:378:GLN:NE2	2:X:386:ASP:HA	2.32	0.45
1:A:740:ALA:HB1	1:A:863:PRO:HA	1.98	0.45
1:A:1436:MET:HG3	1:A:1439:LEU:HD12	1.99	0.45
1:A:1450:TRP:HZ2	1:A:1845:HIS:CE1	2.34	0.45
1:A:2080:LEU:HD12	1:A:2598:LEU:HD22	1.99	0.45
1:B:4444:VAL:HG21	1:B:4481:ILE:HD13	1.97	0.45
1:A:1930:LEU:HD11	1:B:3813:LEU:HD13	1.99	0.45
1:B:861:LEU:HD12	1:B:902:HIS:O	2.16	0.45
1:B:4409:VAL:N	1:B:4410:PRO:HD2	2.32	0.45
1:A:1790:PHE:CD1	1:A:1790:PHE:C	2.94	0.45
1:A:3789:PHE:O	1:A:4086:ARG:NH2	2.46	0.45
1:B:2180:ASP:OD1	1:B:2181:TYR:N	2.50	0.45
1:A:357:PHE:CA	1:A:363:THR:HG21	2.47	0.45
1:A:120:ILE:HD12	1:A:120:ILE:N	2.32	0.44
1:A:1114:ILE:HD11	1:A:1118:PRO:HD3	1.98	0.44
1:B:174:LEU:HD22	1:B:200:LEU:HD12	2.00	0.44
1:B:1505:PRO:O	1:B:1985:ASN:ND2	2.38	0.44
2:X:157:THR:HG21	2:X:311:VAL:HG11	1.99	0.44
1:A:123:VAL:HG21	1:A:414:VAL:HG11	1.99	0.44
1:A:129:VAL:HG21	1:A:391:PHE:CB	2.48	0.44
1:A:226:HIS:ND1	1:A:227:VAL:N	2.65	0.44
1:A:3225:ILE:HD11	1:A:3280:LEU:HD13	1.99	0.44
1:A:4224:THR:HG22	1:A:4231:GLY:CA	2.48	0.44
1:B:848:HIS:HD1	1:B:849:ILE:N	2.16	0.44
1:B:1867:THR:HG1	2:Z:340:GLU:CD	2.25	0.44
1:B:3227:PRO:HD2	1:B:3263:THR:O	2.18	0.44
1:B:3343:ASP:OD1	1:B:3343:ASP:N	2.48	0.44
1:B:3709:ASN:C	1:B:3709:ASN:OD1	2.59	0.44
1:B:4235:ARG:O	1:B:4330:TYR:OH	2.31	0.44
1:B:4412:LEU:HD13	1:B:4488:VAL:HG13	1.99	0.44
1:A:1330:LYS:O	1:A:1334:THR:HG22	2.17	0.44
1:A:1335:LEU:HB2	1:A:1352:VAL:HG11	1.99	0.44
1:B:1816:SER:HB2	1:B:1833:VAL:HG22	1.99	0.44
1:B:2106:SER:OG	1:B:2164:ASP:OD1	2.35	0.44
1:B:3388:GLN:HG3	1:B:3392[A]:ILE:HD11	1.97	0.44
1:A:2876:LYS:NZ	1:A:3273:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3236:PRO:HD3	1:A:3291:LEU:HD21	2.00	0.44
1:B:4369:LEU:HG	1:B:4373:MET:HE2	1.99	0.44
2:X:391:VAL:O	2:X:413:ILE:N	2.47	0.44
2:Z:312:ASN:OD1	2:Z:312:ASN:C	2.60	0.44
1:A:4251:LEU:HD11	1:A:4320:VAL:HG13	1.99	0.44
1:B:632:LEU:O	1:B:717:VAL:N	2.50	0.44
1:A:1209:VAL:HG22	1:A:1306:PHE:CZ	2.52	0.44
1:A:1776:GLN:HB3	1:A:1875:LEU:HD12	2.00	0.44
1:A:1798:PRO:O	1:A:1884:ILE:HD11	2.18	0.44
1:A:3343:ASP:OD1	1:A:3343:ASP:N	2.49	0.44
1:A:3518:ASP:OD1	1:A:3518:ASP:N	2.48	0.44
1:A:3760:GLU:O	1:A:3764:VAL:HG23	2.17	0.44
1:A:3989:LEU:CD2	1:A:4064:THR:HG21	2.47	0.44
2:X:404:ARG:NH2	2:X:453:THR:O	2.48	0.44
1:B:119:TYR:C	1:B:120:ILE:HD12	2.43	0.44
1:A:1345:THR:HG22	1:A:1346:GLU:N	2.33	0.44
1:A:3251:LEU:HD23	1:B:2717:ARG:HG3	2.00	0.44
1:A:1805:LEU:O	1:A:1877:PHE:N	2.41	0.44
1:A:3443:ASP:OD1	1:A:3445:GLY:N	2.51	0.44
1:A:3679:THR:OG1	1:A:3681:ASP:OD1	2.20	0.44
1:B:151:GLN:NE2	1:B:162:GLN:O	2.48	0.44
1:A:410:CYS:SG	1:A:420:VAL:HG13	2.58	0.43
1:A:1925:GLN:HG2	1:A:1984:LEU:HD21	1.99	0.43
1:A:2051:GLN:HA	1:A:2051:GLN:OE1	2.17	0.43
1:A:2870:TYR:OH	1:A:2916:ASP:OD1	2.27	0.43
1:A:4438:ALA:O	1:A:4442:THR:HG23	2.18	0.43
1:B:740:ALA:HB1	1:B:863:PRO:HA	2.00	0.43
1:B:1570:CYS:HB2	1:B:1579:ILE:HD13	2.00	0.43
1:B:4209:LEU:N	1:B:4210:PRO:HD2	2.33	0.43
1:B:4495:LEU:C	1:B:4495:LEU:HD23	2.43	0.43
1:A:4217:LEU:HD11	1:A:4221:PHE:CZ	2.53	0.43
1:B:1914:LEU:HD23	1:B:1914:LEU:C	2.43	0.43
2:Y:157:THR:HG21	2:Y:311:VAL:HG11	2.00	0.43
2:Z:302:ASP:O	2:Z:306:ALA:N	2.44	0.43
1:B:740:ALA:HB2	1:B:861:LEU:HD12	2.00	0.43
1:B:2167:MET:HE2	1:B:2171:VAL:HG23	1.99	0.43
1:B:3760:GLU:O	1:B:3764:VAL:HG23	2.19	0.43
1:A:2685:LEU:HD12	1:A:2686:TYR:N	2.34	0.43
1:B:1410:LEU:HG	1:B:2579:ALA:HB2	2.00	0.43
1:A:381:CYS:SG	1:A:408:LYS:NZ	2.81	0.43
1:B:309:MET:HE1	1:B:338:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1801:LEU:HD11	1:B:1804:VAL:CG2	2.49	0.43
1:A:1091:PHE:CD1	1:A:1091:PHE:N	2.87	0.43
1:B:164:GLU:OE1	1:B:258:ARG:NH2	2.52	0.43
2:Y:188:ALA:HB3	2:Y:192:LEU:HB3	2.00	0.43
1:A:3180:GLU:OE1	1:A:3180:GLU:N	2.42	0.43
1:B:1849:PRO:HG2	1:B:2570:ARG:HE	1.84	0.43
2:Z:212:SER:OG	2:Z:214:ASP:OD2	2.34	0.43
1:A:70:LEU:HD22	1:A:84:ALA:HB1	2.01	0.43
1:A:2390:THR:HG22	1:A:2656:GLN:HG3	2.01	0.43
1:B:93:VAL:HG11	1:B:216:TRP:CZ3	2.53	0.43
1:B:120:ILE:HD12	1:B:120:ILE:N	2.33	0.43
1:A:1093:LEU:HD21	1:A:1301:VAL:HG11	2.00	0.43
1:A:1209:VAL:HG22	1:A:1306:PHE:HZ	1.84	0.43
1:B:2991:MET:HE3	1:B:2991:MET:HA	2.00	0.43
1:A:3387:LEU:HD22	1:A:3441:THR:HG21	2.00	0.43
1:B:2051:GLN:OE1	1:B:2051:GLN:HA	2.19	0.43
1:B:2984:VAL:HG13	1:B:2990:ILE:HG21	2.01	0.43
2:X:381:GLU:H	2:X:382:PRO:HD2	1.84	0.43
1:A:70:LEU:HA	1:A:85:VAL:O	2.19	0.42
1:A:4478:VAL:N	1:A:4479:PRO:CD	2.82	0.42
1:B:409:ILE:HB	1:B:424:PHE:CE1	2.53	0.42
1:B:902:HIS:CD2	1:B:923:LEU:HD11	2.53	0.42
1:B:3981:MET:HG3	1:B:3985:GLN:HB2	2.01	0.42
2:X:218:ALA:HB2	2:X:234:ILE:CG2	2.49	0.42
1:A:1406:ARG:NH1	1:A:2576:GLU:HB3	2.34	0.42
1:B:827:LEU:O	1:B:844:ILE:N	2.48	0.42
1:B:857:THR:OG1	1:B:906:THR:O	2.32	0.42
1:B:1566:LEU:HD13	1:B:1799:ILE:HD13	2.00	0.42
1:B:4311:THR:OG1	1:B:4314:ARG:NH1	2.52	0.42
2:X:218:ALA:HB2	2:X:234:ILE:HG22	2.02	0.42
1:A:409:ILE:HD12	1:A:426:ILE:CD1	2.50	0.42
1:A:3684:ALA:HB3	1:A:3685:PRO:HD3	2.01	0.42
1:A:4413:LEU:CD2	1:A:4495:LEU:HD22	2.49	0.42
1:B:940:PHE:HA	1:B:956:THR:HA	2.01	0.42
1:B:1345:THR:HG22	1:B:1346:GLU:N	2.34	0.42
2:Z:218:ALA:HB2	2:Z:234:ILE:CG2	2.49	0.42
1:A:1029:THR:HG22	1:A:1358:TRP:CD2	2.53	0.42
1:A:4209:LEU:N	1:A:4210:PRO:HD2	2.34	0.42
2:X:250:ASP:O	2:Y:144:ARG:NH2	2.48	0.42
1:A:296:TRP:NE1	1:A:304:ALA:O	2.53	0.42
1:A:1799:ILE:HD12	1:A:1799:ILE:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3817:LEU:HD13	1:A:4186:ARG:HA	2.00	0.42
1:B:1223:HIS:CE1	1:B:1225:LYS:HB2	2.55	0.42
1:B:2670:ASN:OD1	1:B:2670:ASN:C	2.63	0.42
1:B:3291:LEU:HD23	1:B:3292:GLY:N	2.35	0.42
1:A:412:TRP:NE1	1:A:420:VAL:HG22	2.34	0.42
1:A:2687:ASN:OD1	1:A:2688:ALA:N	2.52	0.42
1:A:4233:LEU:HD12	1:A:4237:MET:HE2	2.00	0.42
1:B:854:ASP:HA	1:B:907:THR:HB	2.01	0.42
1:B:1812:LEU:HD23	1:B:1873:ILE:HG12	2.02	0.42
1:B:2892:CYS:N	1:B:3003:SER:O	2.49	0.42
1:A:119:TYR:C	1:A:120:ILE:HD12	2.44	0.42
1:A:189:TYR:HA	1:A:231:ILE:HD11	2.01	0.42
1:A:1446:GLY:O	1:A:1450:TRP:CD1	2.73	0.42
1:A:2853:VAL:HG23	1:A:2939:GLU:C	2.45	0.42
1:B:73:LEU:HD13	1:B:955:CYS:SG	2.60	0.42
1:B:226:HIS:ND1	1:B:227:VAL:N	2.67	0.42
1:B:3684:ALA:HB3	1:B:3685:PRO:HD3	2.01	0.42
1:B:4221:PHE:HE1	1:B:4234:LEU:HG	1.84	0.42
1:A:426:ILE:CG2	1:A:505:LEU:HD23	2.50	0.42
1:A:902:HIS:CD2	1:A:923:LEU:HD11	2.55	0.42
1:A:1782:ARG:HB3	1:A:1784:HIS:NE2	2.34	0.42
1:A:2351:LEU:C	1:A:2351:LEU:HD23	2.45	0.42
1:A:3229:LEU:HD22	1:A:3229:LEU:H	1.85	0.42
1:A:3388:GLN:HG3	1:A:3392[B]:ILE:HD11	2.02	0.42
1:A:3965:PHE:CE2	2:X:385:PRO:HB3	2.55	0.42
1:B:137:ARG:NH2	1:B:148:THR:O	2.53	0.42
1:B:2806:GLN:NE2	1:B:2806:GLN:H	2.18	0.42
1:B:3689:PHE:O	1:B:3693:VAL:HG22	2.20	0.42
2:X:326:THR:HG22	2:X:329:ILE:HB	2.02	0.42
2:Y:326:THR:HG22	2:Y:329:ILE:HB	2.02	0.42
1:A:4442:THR:O	1:A:4446:THR:HG23	2.20	0.42
1:A:3824:MET:SD	1:A:4004:LEU:HD12	2.60	0.41
1:A:4260:ARG:HG3	1:A:4261:VAL:HG23	2.00	0.41
1:B:827:LEU:HD21	1:B:900:LEU:HD21	2.02	0.41
1:B:1334:THR:O	1:B:1344:ILE:HD13	2.20	0.41
1:B:4226:LEU:HD22	1:B:4226:LEU:N	2.35	0.41
1:A:1820:TRP:CZ3	1:A:1857:LYS:HB2	2.55	0.41
1:A:2049:VAL:HG22	1:A:2050:LEU:N	2.35	0.41
1:B:903:LEU:C	1:B:903:LEU:HD23	2.45	0.41
1:B:1798:PRO:O	1:B:1884:ILE:HD11	2.20	0.41
1:B:2332:VAL:HG12	1:B:2374:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.52	0.41
1:A:317:GLN:HB3	1:A:327:MET:HE3	2.03	0.41
1:A:2806:GLN:NE2	1:A:2806:GLN:H	2.19	0.41
1:A:3355:THR:HG23	1:A:3358:LEU:HB2	2.02	0.41
1:A:4080:LEU:HD12	1:A:4171:ALA:HB1	2.01	0.41
1:B:156:LYS:N	1:B:159:ASP:OD2	2.45	0.41
1:B:564:PHE:N	1:B:565:PRO:CD	2.83	0.41
1:B:1114:ILE:HG23	1:B:1114:ILE:O	2.20	0.41
1:A:1322:LEU:HD22	1:A:1362:VAL:HG11	2.02	0.41
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.51	0.41
1:A:3824:MET:HE2	1:A:3824:MET:HB2	1.95	0.41
2:Z:302:ASP:O	2:Z:306:ALA:HB2	2.20	0.41
1:A:4226:LEU:N	1:A:4226:LEU:HD22	2.36	0.41
1:B:70:LEU:O	1:B:71:HIS:HB3	2.20	0.41
1:B:135:GLY:HA2	1:B:377:ALA:HA	2.02	0.41
1:B:289:ARG:O	1:B:293:PHE:CD2	2.73	0.41
1:B:736:ILE:HG22	1:B:745:LEU:HD11	2.01	0.41
1:B:4441:LYS:O	1:B:4445:ASP:OD1	2.39	0.41
2:Y:322:THR:CG2	2:Y:333:ILE:HG12	2.50	0.41
1:A:3566:ILE:HD12	1:A:3566:ILE:N	2.36	0.41
1:B:912:VAL:HG13	1:B:940:PHE:HD2	1.86	0.41
1:B:940:PHE:CD1	1:B:956:THR:HG22	2.55	0.41
1:B:1042:VAL:HG11	1:B:1077:TRP:CE2	2.55	0.41
1:B:1992:GLN:O	1:B:1996:VAL:HG23	2.20	0.41
1:B:2655:VAL:HG11	1:B:2660:LEU:HD22	2.02	0.41
1:B:3712:TRP:CD1	1:B:3712:TRP:N	2.89	0.41
1:B:3824:MET:HE2	1:B:3824:MET:HB2	1.95	0.41
2:X:366:MET:HE1	2:X:427:VAL:CG1	2.51	0.41
1:A:283:MET:O	1:A:289:ARG:NH1	2.43	0.41
1:A:1450:TRP:CZ2	1:A:1845:HIS:HE1	2.39	0.41
1:A:1500:SER:HB3	1:A:1974:TYR:OH	2.20	0.41
1:A:2177:ARG:O	1:A:2180:ASP:OD1	2.38	0.41
1:A:2687:ASN:OD1	1:A:2687:ASN:C	2.63	0.41
1:A:2868:HIS:CE1	1:A:2872:THR:HG21	2.56	0.41
1:A:4152:PRO:HA	1:A:4201:LEU:HD21	2.03	0.41
1:B:414:VAL:HA	1:B:418:MET:HA	2.02	0.41
1:B:2567:LEU:HD21	1:B:2584:LYS:HD3	2.03	0.41
1:B:3058:LEU:CD1	1:B:3101:MET:HE2	2.49	0.41
1:B:4153:ILE:O	1:B:4153:ILE:HG23	2.21	0.41
1:A:1974:TYR:O	1:A:1978:ILE:HG12	2.21	0.41
1:A:2149:LEU:CD2	1:A:2163:LEU:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1799:ILE:HD12	1:B:1799:ILE:C	2.45	0.41
1:B:2687:ASN:OD1	1:B:2687:ASN:C	2.64	0.41
1:B:2826:PHE:HB3	1:B:2866:LEU:HD21	2.03	0.41
1:B:3985:GLN:O	1:B:3989:LEU:HG	2.21	0.41
2:Z:196:ASN:OD1	2:Z:199:VAL:HG23	2.20	0.41
1:A:280:ARG:NH2	1:A:328:CYS:O	2.53	0.41
1:A:744:HIS:HB3	1:A:827:LEU:HD11	2.02	0.41
1:A:1102:GLY:H	1:A:1305:ARG:HA	1.85	0.41
1:A:1126:LYS:HG2	1:A:1180:ASP:O	2.21	0.41
1:A:1785:SER:HB2	1:A:1866:SER:O	2.21	0.41
1:A:1812:LEU:HA	1:A:1862:GLY:HA2	2.02	0.41
1:B:307:ASP:HB3	1:B:308:PRO:HD3	2.03	0.41
1:B:1095:LEU:CD2	1:B:1303:ILE:HD13	2.51	0.41
1:B:3429:ASP:OD2	1:B:3836:ARG:NH1	2.52	0.41
1:B:3865:THR:OG1	1:B:3979:ALA:O	2.38	0.41
2:X:166:ILE:N	2:X:180:SER:O	2.40	0.41
2:X:295:ILE:O	2:X:331:PHE:HA	2.21	0.41
2:Y:229:ILE:HD12	2:Y:341:PHE:CB	2.50	0.41
2:Y:322:THR:HG21	2:Y:333:ILE:HG12	2.03	0.41
2:Z:268:ASN:HB2	2:Z:304:GLY:HA3	2.03	0.41
1:A:1863:ARG:O	1:A:1866:SER:OG	2.29	0.41
1:A:2692:PRO:HG3	1:A:2728:LEU:HB3	2.03	0.41
1:A:3689:PHE:O	1:A:3693:VAL:HG22	2.20	0.41
1:B:226:HIS:ND1	1:B:227:VAL:HG23	2.36	0.41
1:B:575:TYR:N	1:B:575:TYR:CD1	2.88	0.41
1:B:2327:ARG:HD2	1:B:2328:CYS:N	2.36	0.41
1:B:3443:ASP:OD1	1:B:3445:GLY:N	2.54	0.41
1:B:4187:LEU:HG	1:B:4200:ILE:HD13	2.03	0.41
1:A:151:GLN:NE2	1:A:162:GLN:O	2.55	0.40
1:A:299:VAL:O	1:A:305:GLN:NE2	2.54	0.40
1:A:1801:LEU:HD11	1:A:1804:VAL:HG23	2.03	0.40
1:A:4259:PRO:HB3	1:A:4366:GLN:O	2.21	0.40
1:B:1511:GLU:HA	1:B:1557:LEU:O	2.21	0.40
1:B:4008:LEU:HD23	1:B:4008:LEU:N	2.36	0.40
1:A:1114:ILE:O	1:A:1114:ILE:HG23	2.21	0.40
1:A:1317:GLN:O	1:A:1321:MET:HG3	2.21	0.40
1:A:2567:LEU:HD11	1:A:2581:LEU:HG	2.04	0.40
1:A:3560:LEU:O	1:A:3564:MET:HG3	2.22	0.40
1:A:4435:THR:O	1:A:4439:LYS:HG3	2.20	0.40
1:B:296:TRP:CZ2	1:B:309:MET:HE2	2.57	0.40
1:B:1501:SER:OG	1:B:2024:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2049:VAL:HG22	1:B:2050:LEU:N	2.36	0.40
1:B:3355:THR:HG23	1:B:3358:LEU:HB2	2.02	0.40
2:Y:253:GLN:NE2	2:Y:276:SER:O	2.49	0.40
2:Y:310:LEU:HG	2:Y:318:ILE:HD11	2.04	0.40
2:Y:312:ASN:OD1	2:Y:312:ASN:C	2.64	0.40
1:A:508:THR:O	1:A:508:THR:HG22	2.21	0.40
1:A:1051:GLN:O	1:A:1055:GLN:N	2.44	0.40
1:A:1852:VAL:CG1	1:A:1884:ILE:HD13	2.52	0.40
1:A:2073:LYS:HE3	1:A:2077:HIS:CE1	2.56	0.40
1:A:3058:LEU:CD1	1:A:3101:MET:HE2	2.50	0.40
1:A:4380:ASP:OD1	1:A:4380:ASP:N	2.45	0.40
1:B:1209:VAL:HG11	1:B:1322:LEU:HD11	2.03	0.40
1:B:1511:GLU:HG3	1:B:1557:LEU:O	2.22	0.40
2:X:252:ARG:N	2:X:255:GLU:OE2	2.44	0.40
2:Y:218:ALA:HB2	2:Y:234:ILE:CG2	2.51	0.40
1:A:85:VAL:CG1	1:A:86:THR:N	2.85	0.40
1:A:1036:PRO:O	1:A:1096:PRO:HG2	2.22	0.40
1:A:1484:ARG:NH2	1:A:2015:ILE:O	2.54	0.40
1:A:1505:PRO:O	1:A:1985:ASN:ND2	2.50	0.40
1:A:2783:PRO:HG2	1:B:3281:ARG:CD	2.52	0.40
1:A:2991:MET:HE3	1:A:2991:MET:HA	2.02	0.40
1:A:4186:ARG:NE	1:A:4193:ASP:O	2.45	0.40
1:A:4217:LEU:HG	1:A:4221:PHE:CE2	2.57	0.40
1:B:961:LEU:HD23	1:B:961:LEU:C	2.46	0.40
1:B:1192:LEU:HA	1:B:1198:ALA:O	2.21	0.40
1:B:4235:ARG:HE	1:B:4330:TYR:HA	1.87	0.40
1:A:3388:GLN:HG3	1:A:3392[A]:ILE:HD11	2.02	0.40
1:A:3867:SER:N	1:A:3979:ALA:O	2.47	0.40
1:B:4072:GLN:HG2	1:B:4175:LEU:HD13	2.04	0.40
1:B:4445:ASP:OD1	1:B:4482:GLN:NE2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2668/4898 (54%)	2615 (98%)	53 (2%)	0	100	100
1	B	2668/4898 (54%)	2616 (98%)	52 (2%)	0	100	100
2	X	286/332 (86%)	270 (94%)	15 (5%)	1 (0%)	36	67
2	Y	185/332 (56%)	178 (96%)	7 (4%)	0	100	100
2	Z	185/332 (56%)	178 (96%)	7 (4%)	0	100	100
All	All	5992/10792 (56%)	5857 (98%)	134 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	381	GLU

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	2440/4249 (57%)	2422 (99%)	18 (1%)	76	81
1	B	2440/4249 (57%)	2421 (99%)	19 (1%)	73	80
2	X	241/276 (87%)	236 (98%)	5 (2%)	47	69
2	Y	153/276 (55%)	151 (99%)	2 (1%)	61	75
2	Z	153/276 (55%)	152 (99%)	1 (1%)	76	81
All	All	5427/9326 (58%)	5382 (99%)	45 (1%)	70	80

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	HIS
1	A	903	LEU
1	A	1112	SER
1	A	1205	SER

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Mol	Chain	Res	Type
1	A	1399	SER
1	A	1506	VAL
1	A	1996	VAL
1	A	2084	GLN
1	A	2776	GLN
1	A	2806	GLN
1	A	3251	LEU
1	A	3355	THR
1	A	3375	SER
1	A	3392[A]	ILE
1	A	3392[B]	ILE
1	A	3441	THR
1	A	3826	LEU
1	A	4224	THR
1	B	73	LEU
1	B	196	LEU
1	B	1112	SER
1	B	1205	SER
1	B	1296	LEU
1	B	1399	SER
1	B	1506	VAL
1	B	2368	THR
1	B	2806	GLN
1	B	3232	LEU
1	B	3251	LEU
1	B	3355	THR
1	B	3375	SER
1	B	3392[A]	ILE
1	B	3392[B]	ILE
1	B	3441	THR
1	B	3826	LEU
1	B	4185	LEU
1	B	4201	LEU
2	X	232	LEU
2	X	247	ARG
2	X	365	MET
2	X	378	GLN
2	X	387	VAL
2	Y	229	ILE
2	Y	232	LEU
2	Z	232	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	902	HIS
1	A	1050	GLN
1	A	1066	HIS
1	A	1376	ASN
1	A	1840	HIS
1	A	1845	HIS
1	A	2077	HIS
1	A	2084	GLN
1	A	2600	ASN
1	A	2653	HIS
1	A	2662	GLN
1	A	2733	GLN
1	A	2797	GLN
1	A	2868	HIS
1	A	3002	ASN
1	A	3213	HIS
1	A	3403	ASN
1	A	3551	HIS
1	A	3769	GLN
1	A	4308	GLN
1	A	4332	ASN
1	B	76	HIS
1	B	103	GLN
1	B	222	HIS
1	B	244	GLN
1	B	288	ASN
1	B	1015	GLN
1	B	1050	GLN
1	B	1066	HIS
1	B	1347	HIS
1	B	1349	GLN
1	B	1376	ASN
1	B	1895	HIS
1	B	1979	GLN
1	B	2565	GLN
1	B	2662	GLN
1	B	2713	ASN
1	B	2733	GLN
1	B	2806	GLN
1	B	2927	ASN
1	B	3213	HIS
1	B	3374	HIS

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Mol	Chain	Res	Type
1	B	3403	ASN
1	B	4256	HIS
1	B	4332	ASN
1	B	4366	GLN
2	X	378	GLN
2	X	389	HIS
2	Y	235	GLN
2	Z	235	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

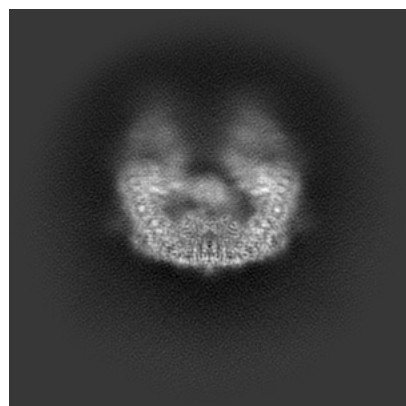
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27841. These allow visual inspection of the internal detail of the map and identification of artifacts.

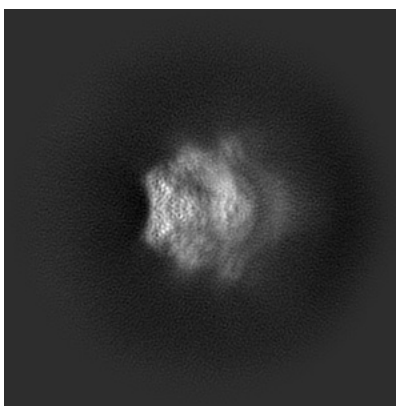
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

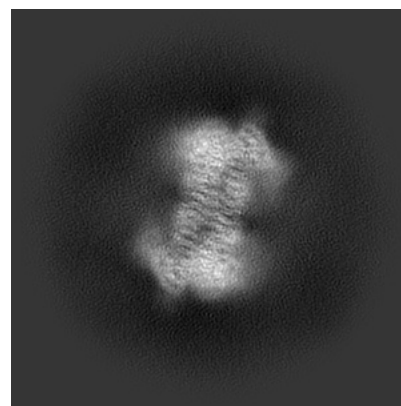
6.1.1 Primary map



X

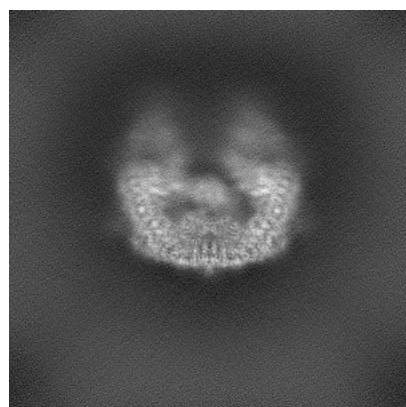


Y

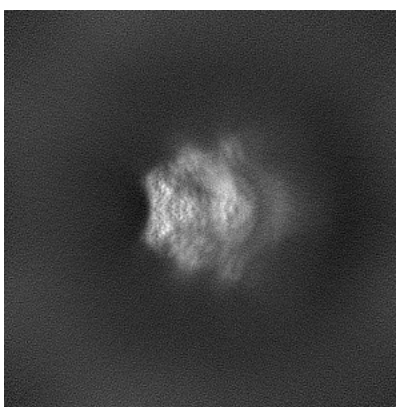


Z

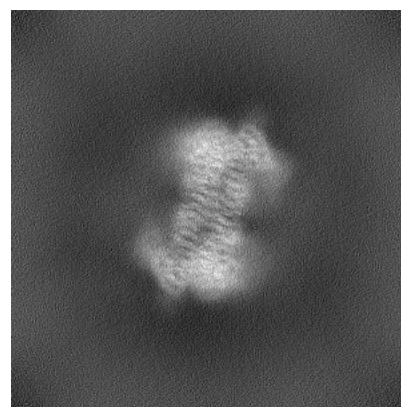
6.1.2 Raw map



X



Y

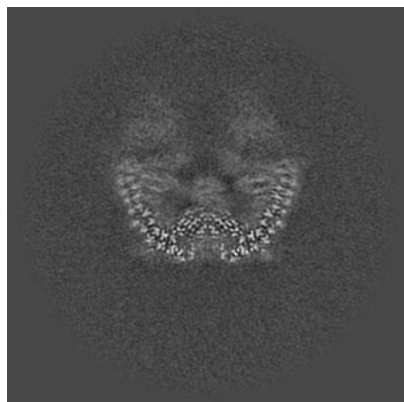


Z

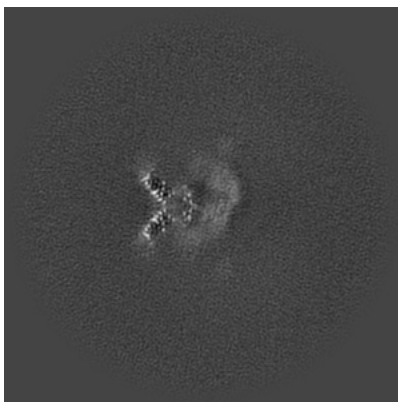
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

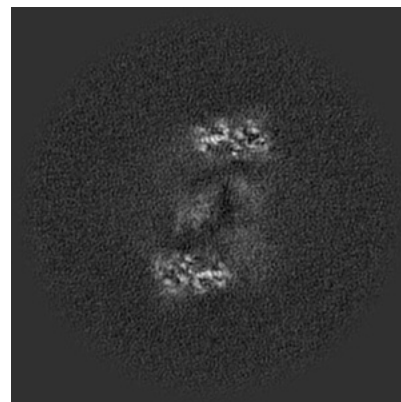
6.2.1 Primary map



X Index: 176

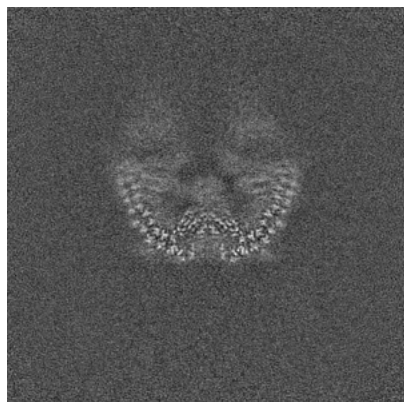


Y Index: 176

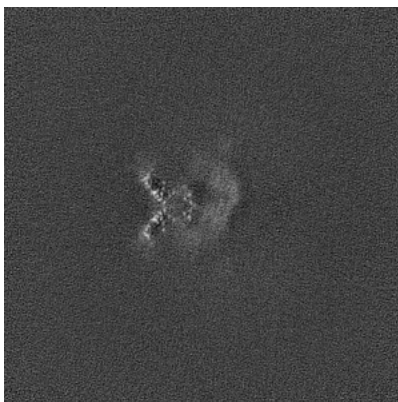


Z Index: 176

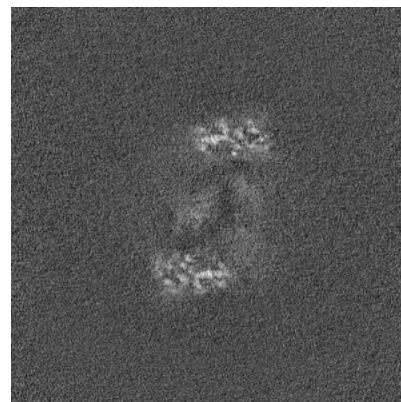
6.2.2 Raw map



X Index: 176



Y Index: 176

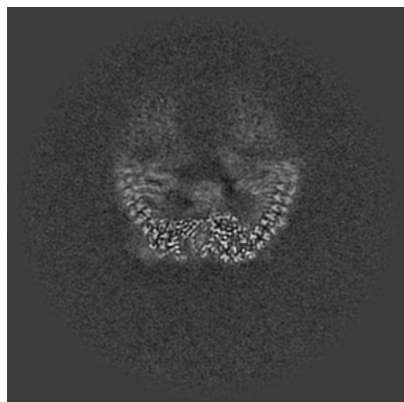


Z Index: 176

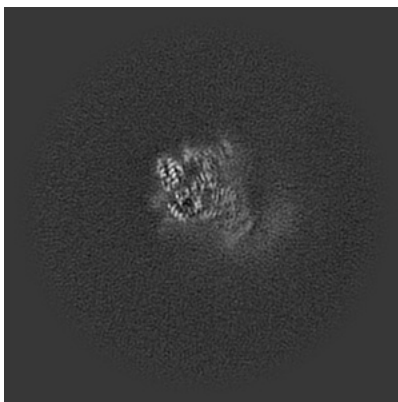
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

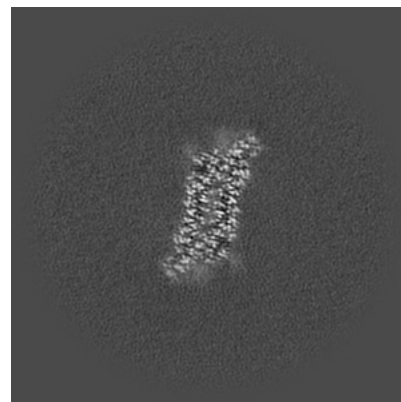
6.3.1 Primary map



X Index: 172

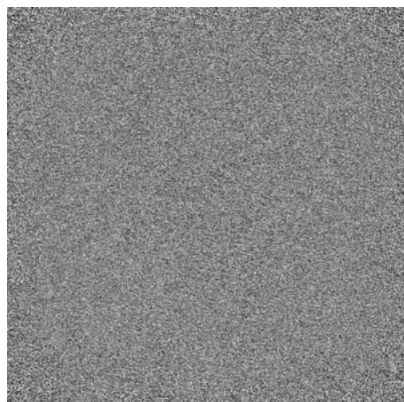


Y Index: 229

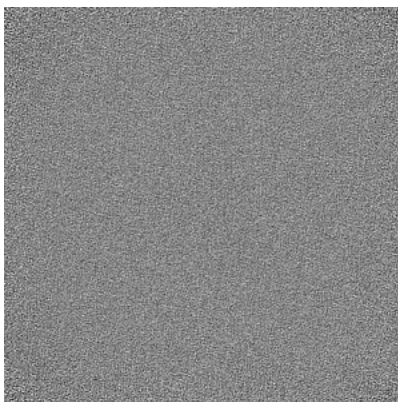


Z Index: 139

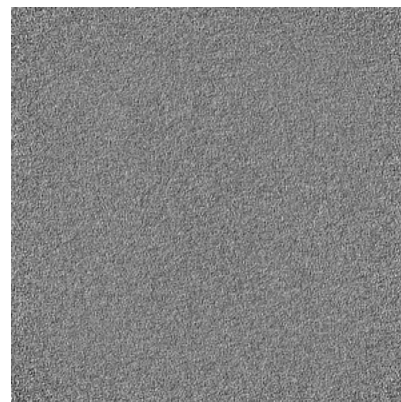
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

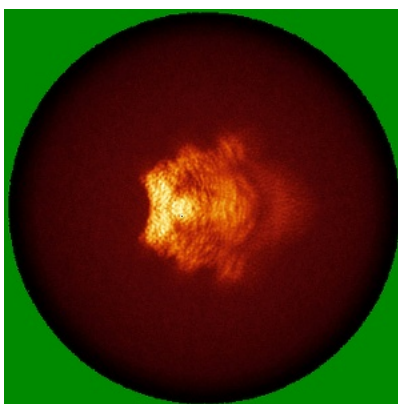
The images above show the largest variance slices of the map in three orthogonal directions.

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

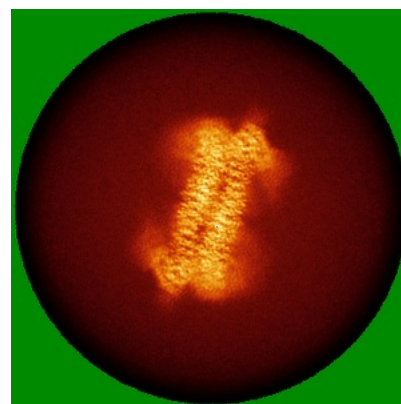
6.4.1 Primary map



X

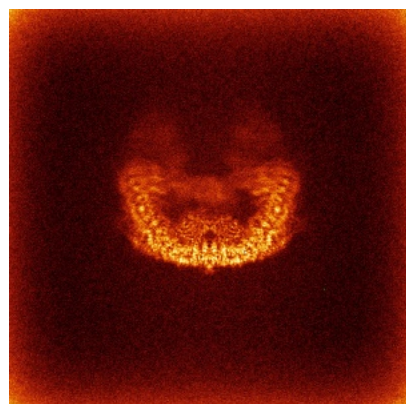


Y

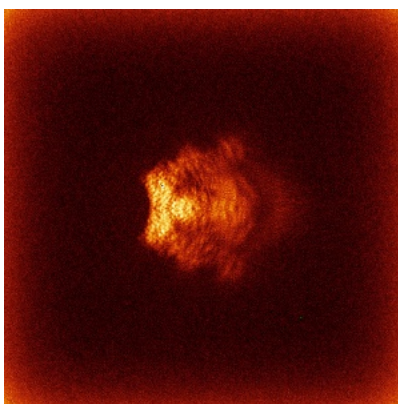


Z

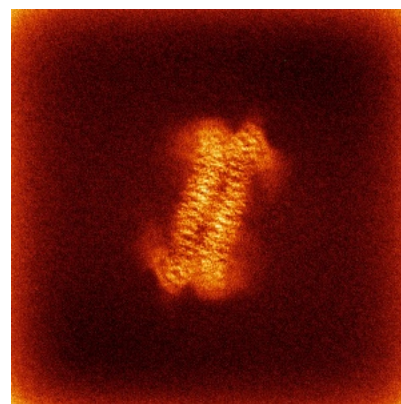
6.4.2 Raw map



X



Y

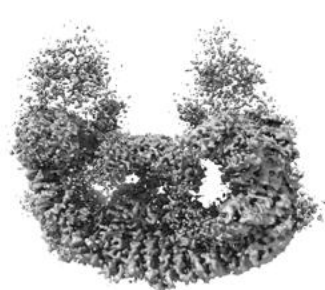


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



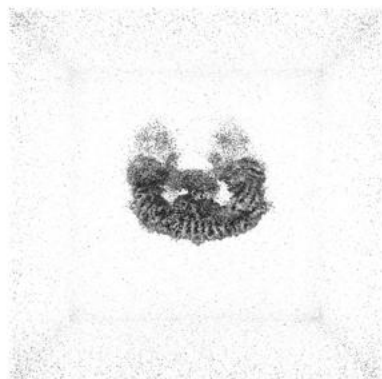
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

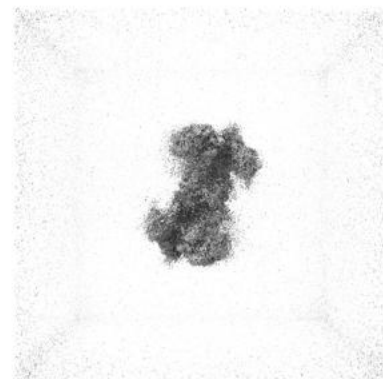
6.5.2 Raw map



X



Y



Z

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

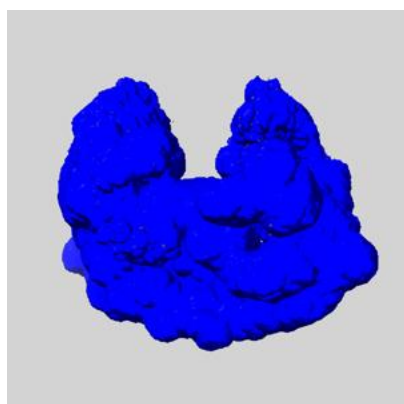
6.6 Mask visualisation [i](#)

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

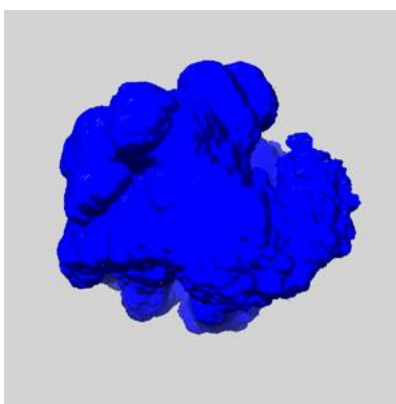
A mask typically either:

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

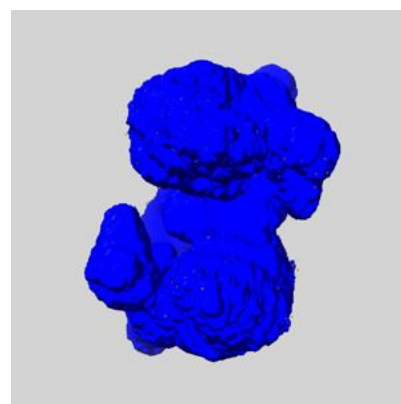
6.6.1 emd_27841_msk_1.map [i](#)



X

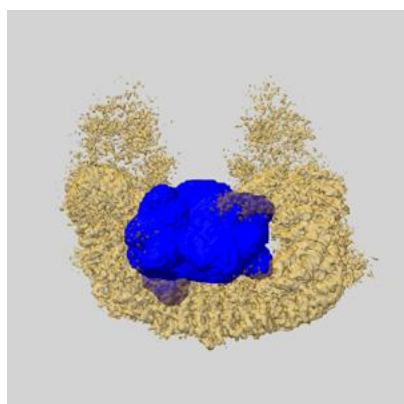


Y

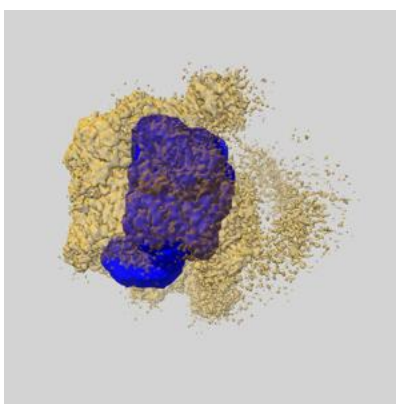


Z

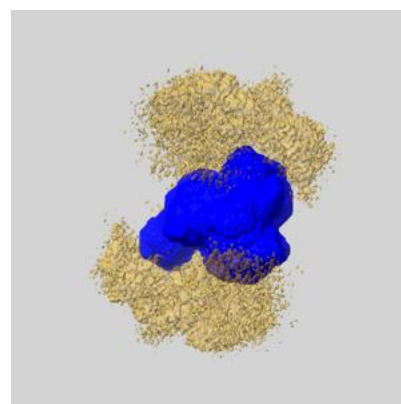
6.6.2 emd_27841_msk_2.map [i](#)



X



Y

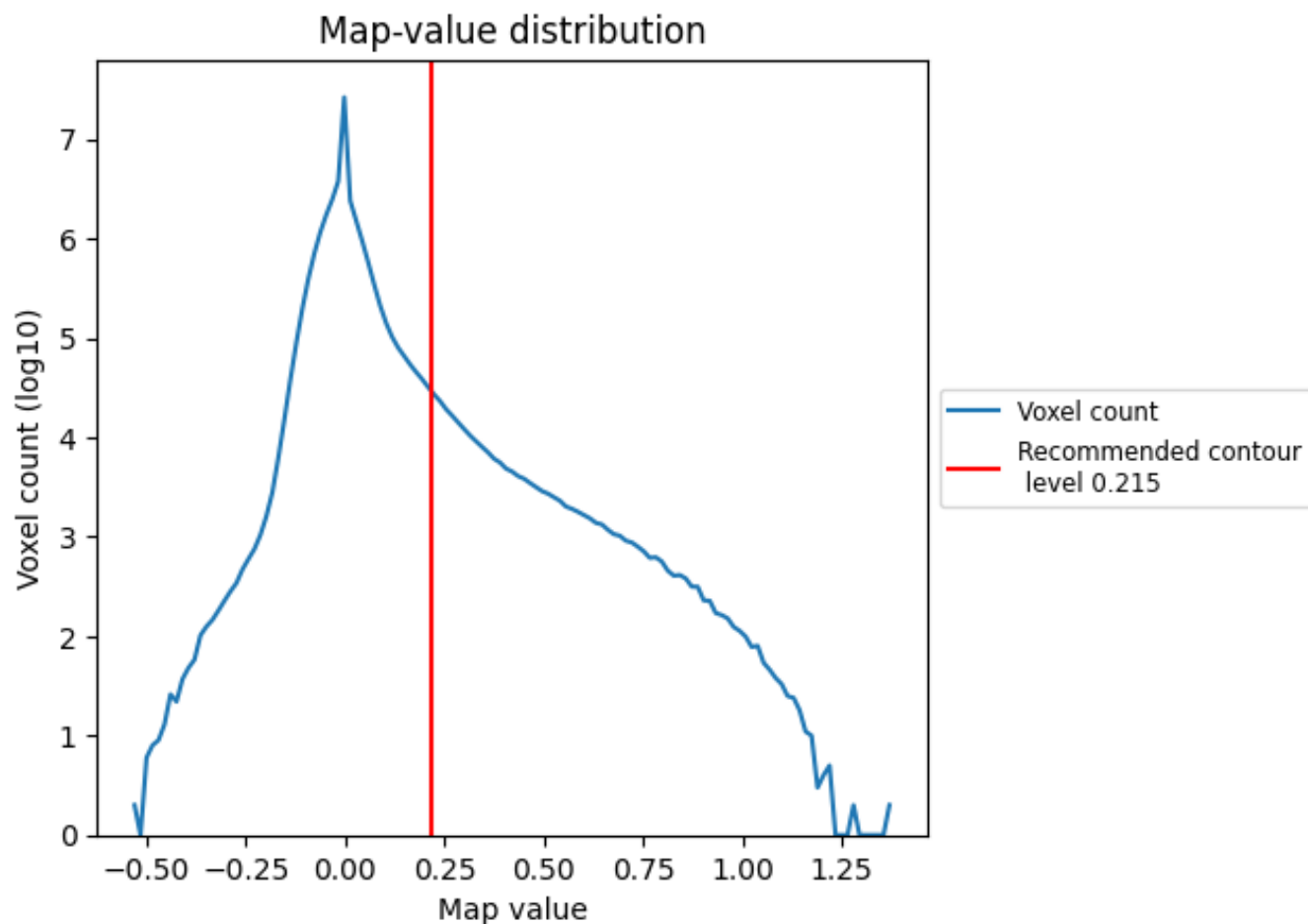


Z

7 Map analysis [i](#)

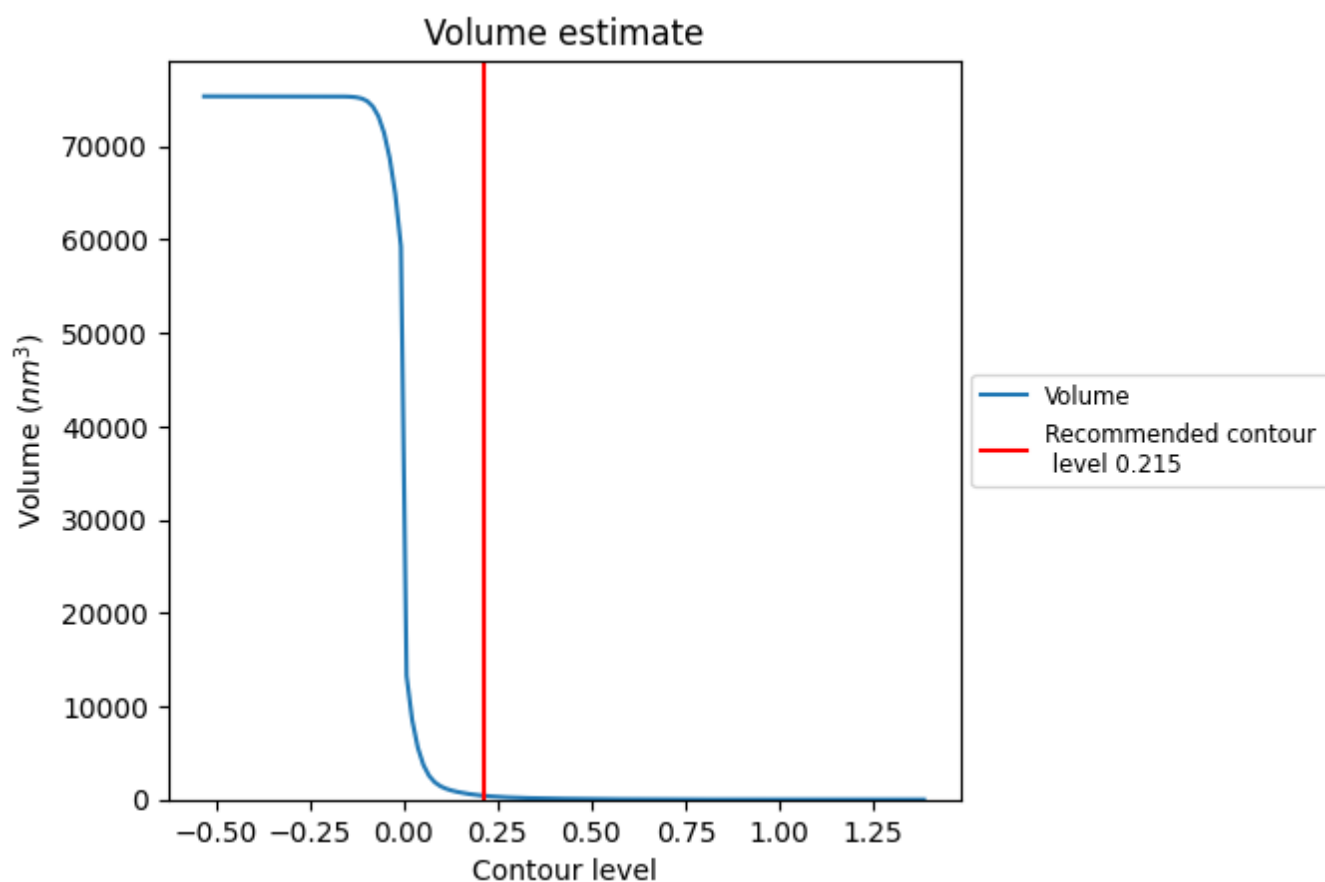
This section contains the results of statistical analysis of the map.

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.

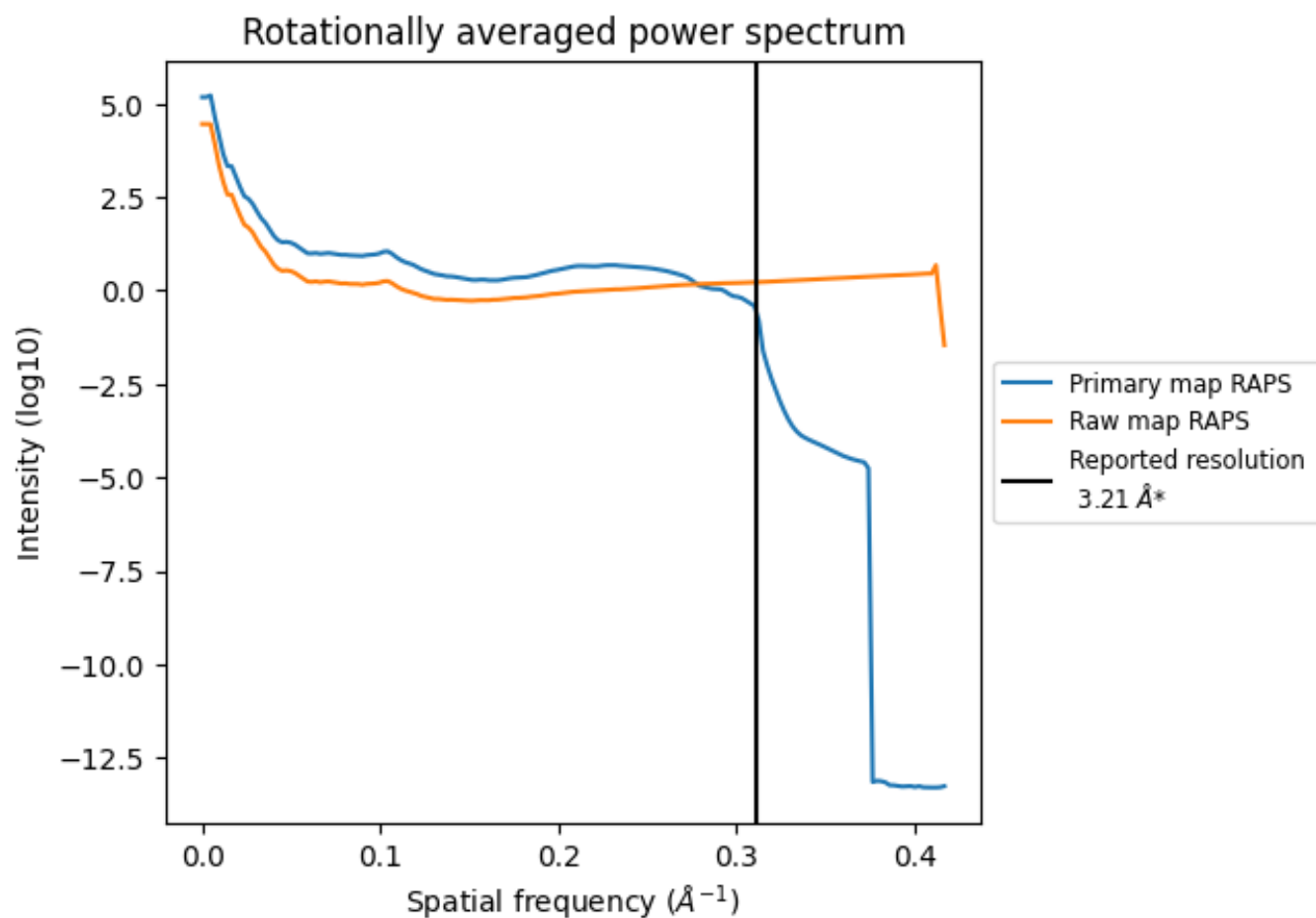
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm³; this corresponds to an approximate mass of 366 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 ⓘ

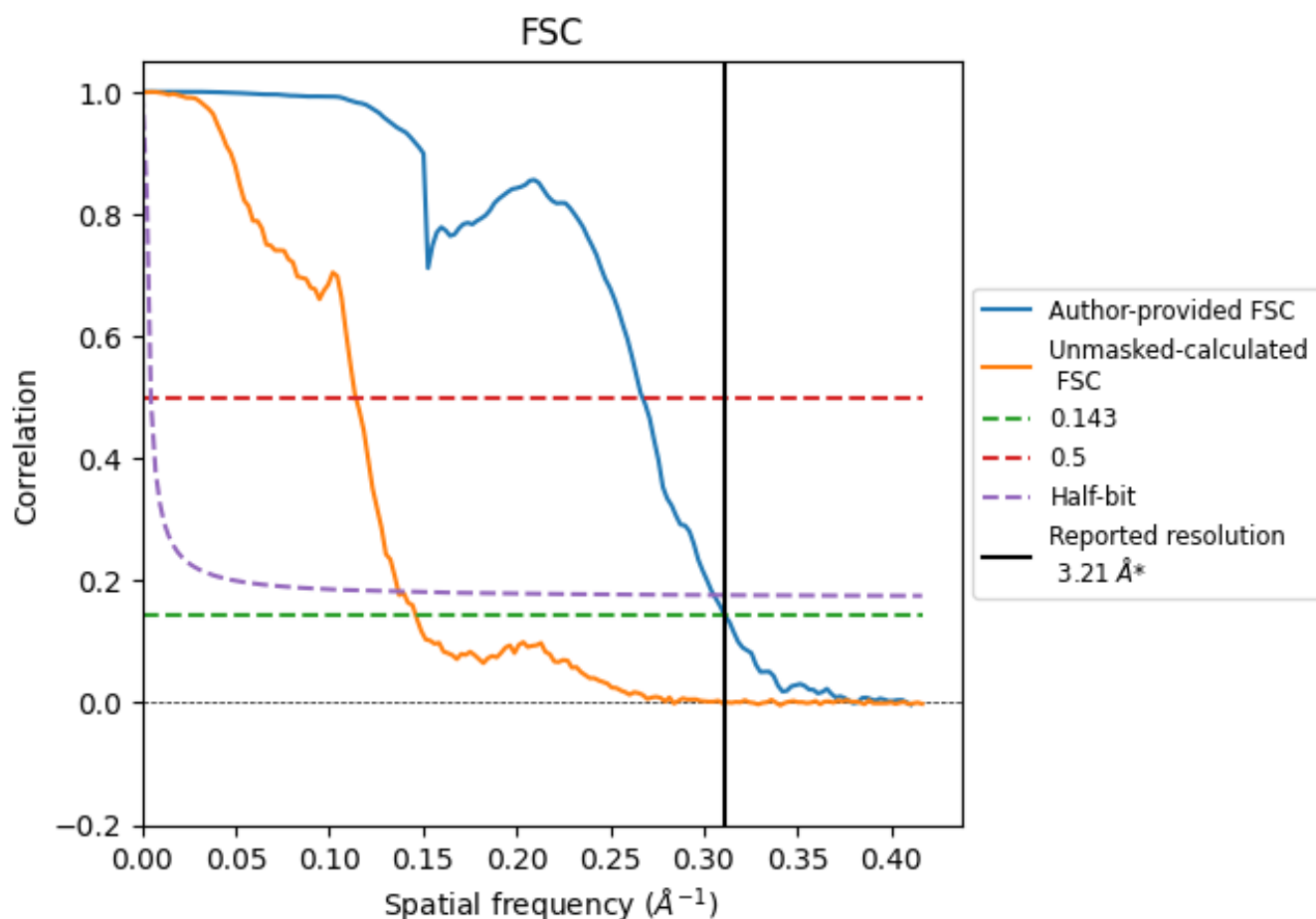


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

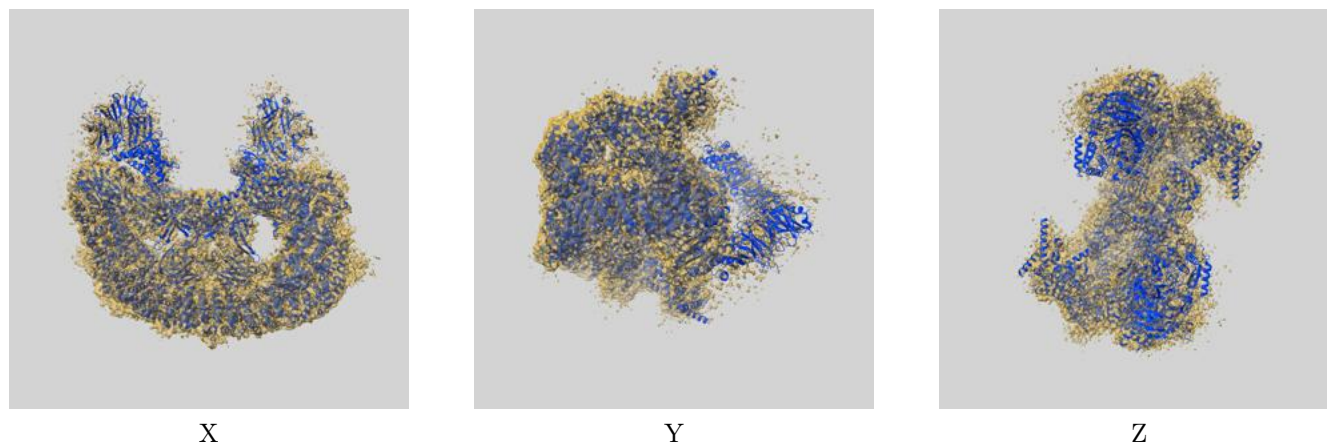
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.74	3.27
Unmasked-calculated*	6.84	8.76	7.30

*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 6.84 differs from the reported value 3.21 by more than 10 %

9 Map-model fit [i](#)

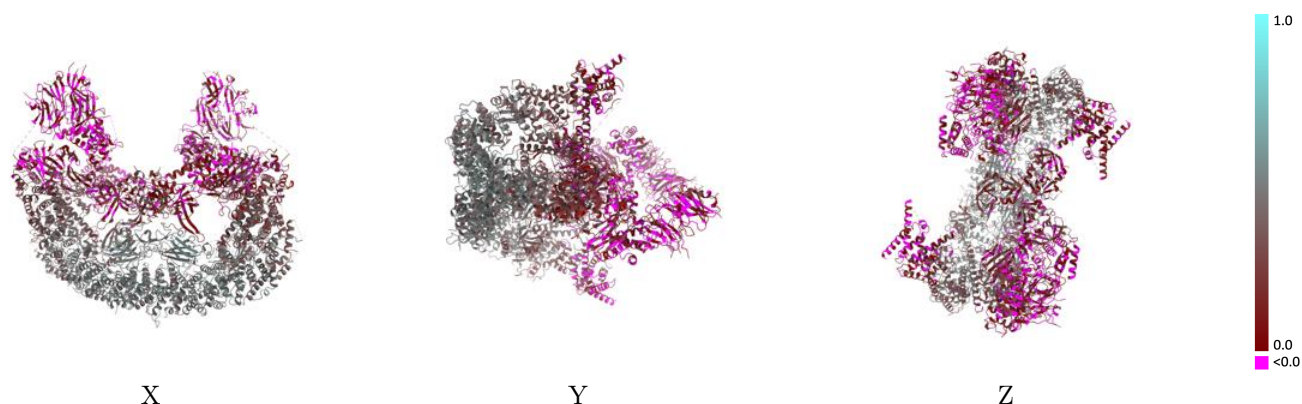
This section contains information regarding the fit between EMDB map EMD-27841 and PDB model 8E2K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



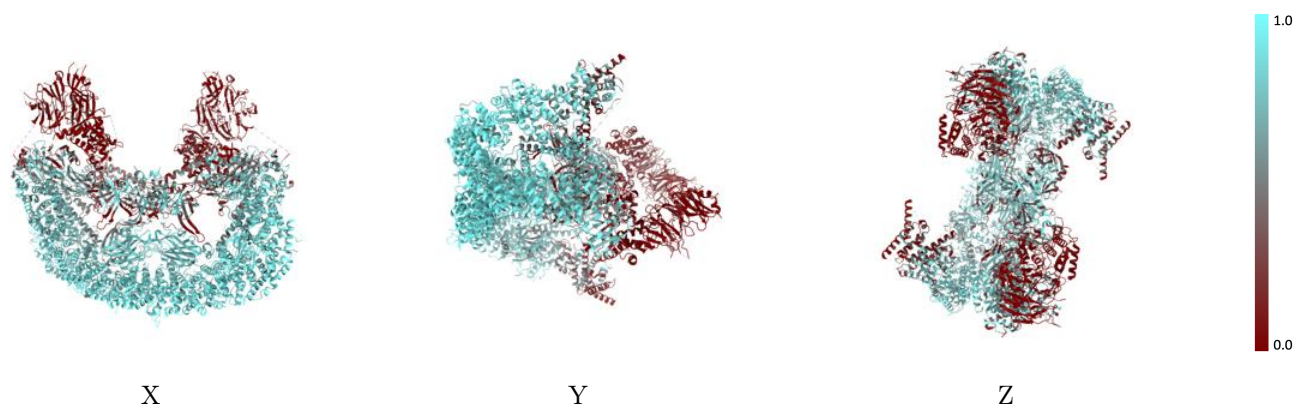
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



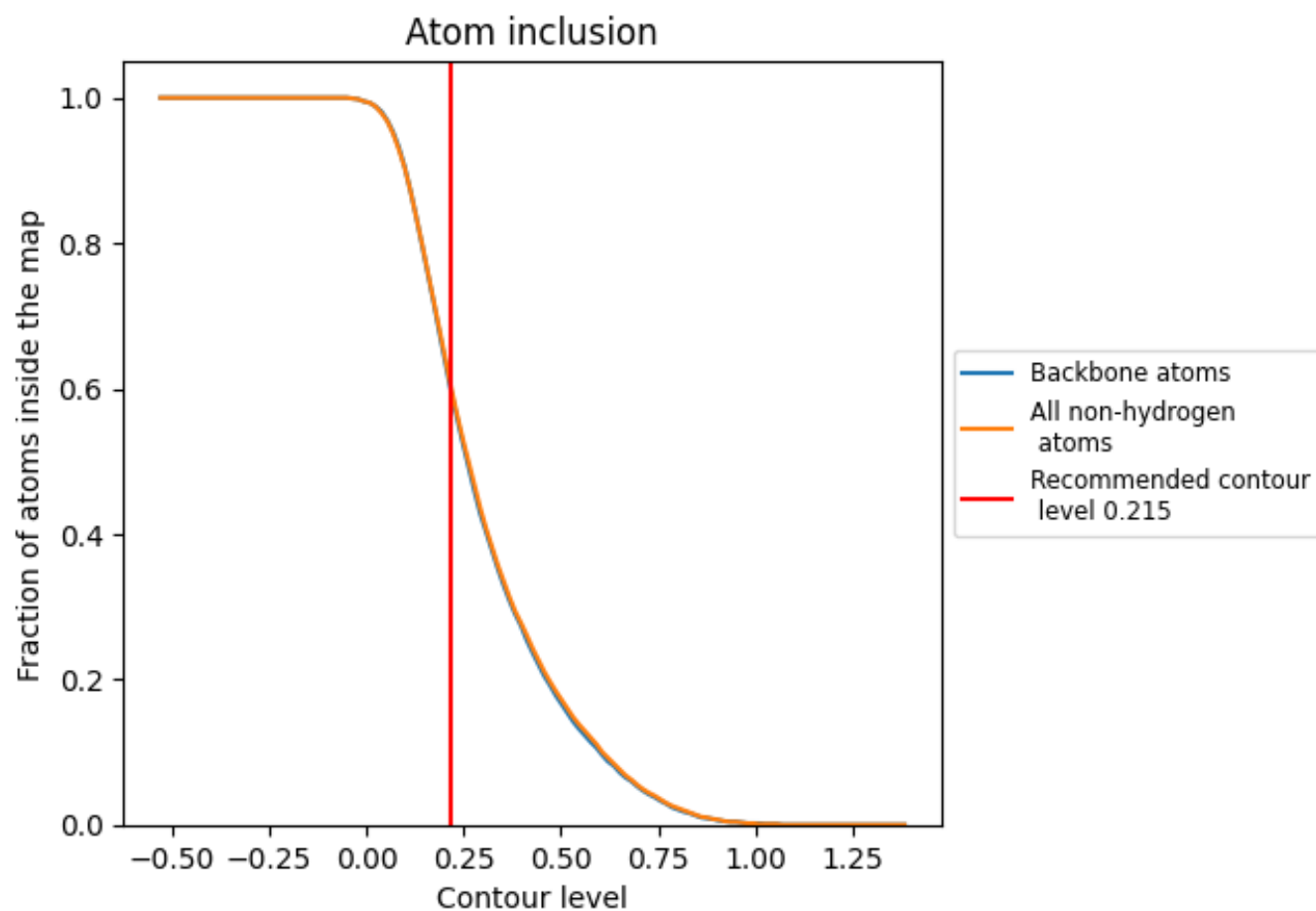
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.215).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 61% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6080	0.2770
A	0.6220	0.2830
B	0.6390	0.2890
X	0.5490	0.2640
Y	0.4590	0.1440
Z	0.4610	0.1690

