



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 03:50 AM UTC

PDB ID : 7WJI / pdb_00007wji
EMDB ID : EMD-32544
Title : Architecture of the human NALCN channelosome
Authors : Wu, J.P.; Yan, Z.; Zhou, L.; Liu, H.; Zhao, Q.
Deposited on : 2022-01-06
Resolution : 4.50 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

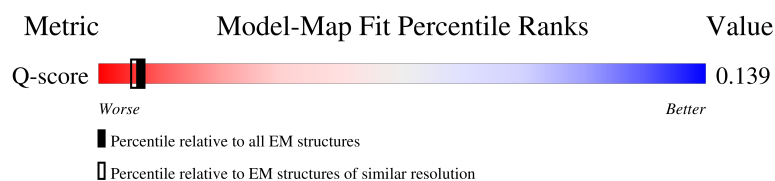
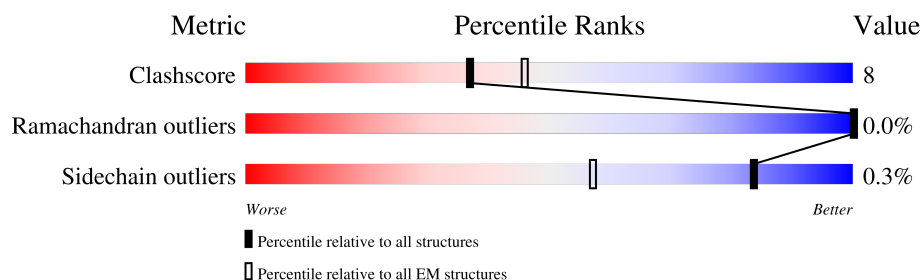
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	3258	28% 44%10%46%
2	B	2658	35% 50%12%37%
3	E	149	83% 71%13%15%
4	C	1992	44% 58%12%30%

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Mol	Chain	Length	Quality of chain
5	D	458	28%29%11%60%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41173 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 Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1763	Total	C	N	O	S	0	0
			14143	9070	2451	2525	97		

- Molecule 2 is a protein called Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1663	Total	C	N	O	S	0	0
			13146	8488	2188	2355	115		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2636	ASP	-	expression tag	UNP Q9P2D8
B	2637	GLU	-	expression tag	UNP Q9P2D8
B	2638	VAL	-	expression tag	UNP Q9P2D8
B	2639	ASP	-	expression tag	UNP Q9P2D8
B	2640	ALA	-	expression tag	UNP Q9P2D8
B	2641	GLY	-	expression tag	UNP Q9P2D8
B	2642	SER	-	expression tag	UNP Q9P2D8
B	2643	ASP	-	expression tag	UNP Q9P2D8
B	2644	TYR	-	expression tag	UNP Q9P2D8
B	2645	LYS	-	expression tag	UNP Q9P2D8
B	2646	ASP	-	expression tag	UNP Q9P2D8
B	2647	ASP	-	expression tag	UNP Q9P2D8
B	2648	ASP	-	expression tag	UNP Q9P2D8
B	2649	LYS	-	expression tag	UNP Q9P2D8
B	2650	GLY	-	expression tag	UNP Q9P2D8
B	2651	SER	-	expression tag	UNP Q9P2D8
B	2652	ASP	-	expression tag	UNP Q9P2D8
B	2653	TYR	-	expression tag	UNP Q9P2D8
B	2654	LYS	-	expression tag	UNP Q9P2D8
B	2655	ASP	-	expression tag	UNP Q9P2D8
B	2656	ASP	-	expression tag	UNP Q9P2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2657	ASP	-	expression tag	UNP Q9P2D8
B	2658	LYS	-	expression tag	UNP Q9P2D8

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	126	Total	C	N	O	S	0	0
			988	615	160	204	9		

- Molecule 4 is a protein called Sodium leak channel non-selective protein,Extended tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1394	Total	C	N	O	S	0	0
			11413	7523	1877	1926	87		

There are 15 discrepancies between the modelled and reference sequences:

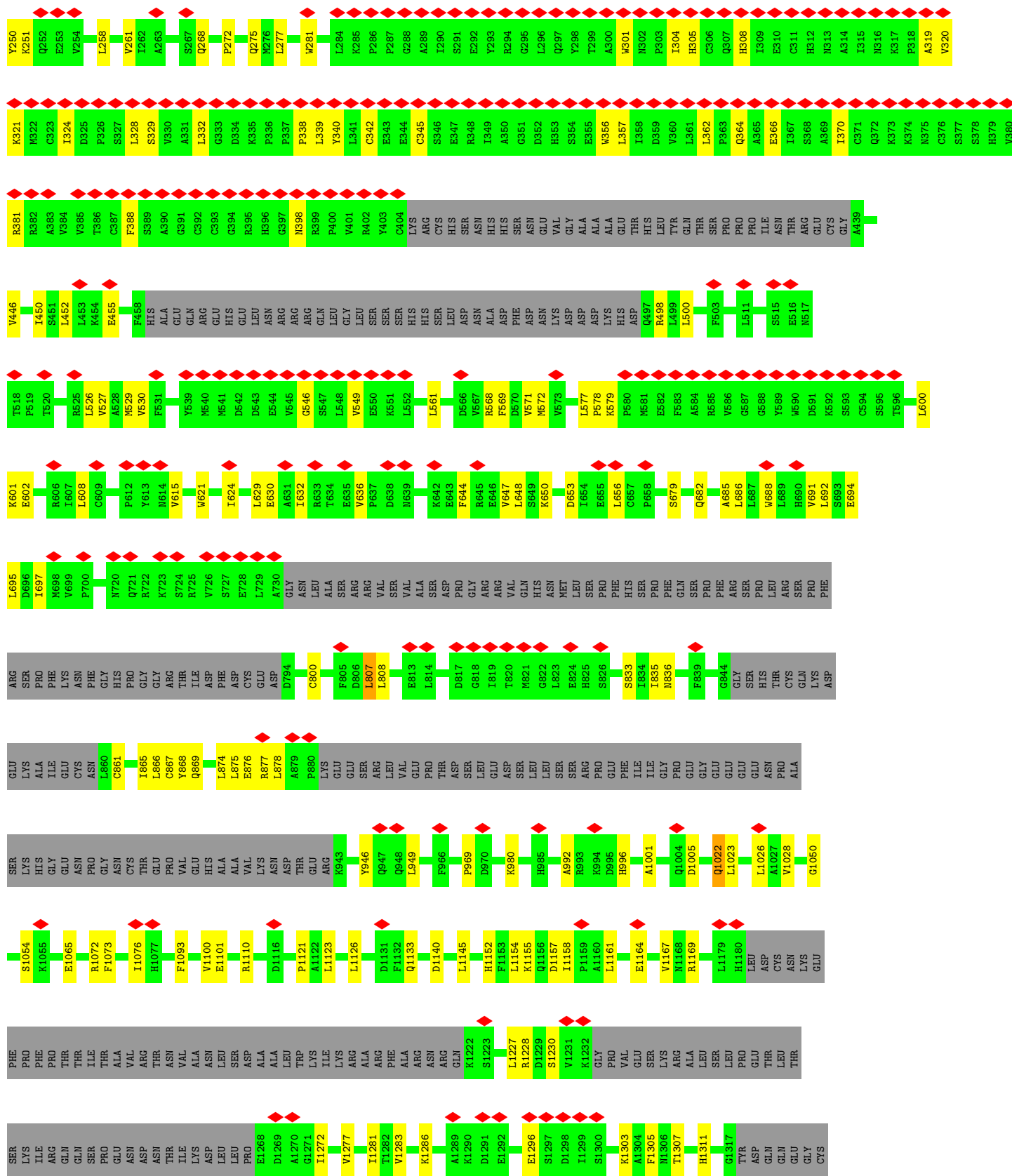
Chain	Residue	Modelled	Actual	Comment	Reference
C	1739	LEU	-	linker	UNP Q8IZF0
C	1740	GLU	-	linker	UNP Q8IZF0
C	1741	GLY	-	linker	UNP Q8IZF0
C	1742	SER	-	linker	UNP Q8IZF0
C	1743	GLU	-	linker	UNP Q8IZF0
C	1744	ASN	-	linker	UNP Q8IZF0
C	1745	LEU	-	linker	UNP Q8IZF0
C	1746	TYR	-	linker	UNP Q8IZF0
C	1747	PHE	-	linker	UNP Q8IZF0
C	1748	GLN	-	linker	UNP Q8IZF0
C	1749	GLY	-	linker	UNP Q8IZF0
C	1750	GLY	-	linker	UNP Q8IZF0
C	1751	GLY	-	linker	UNP Q8IZF0
C	1752	GLY	-	linker	UNP Q8IZF0
C	1753	SER	-	linker	UNP Q8IZF0

- Molecule 5 is a protein called Transmembrane protein FAM155A.

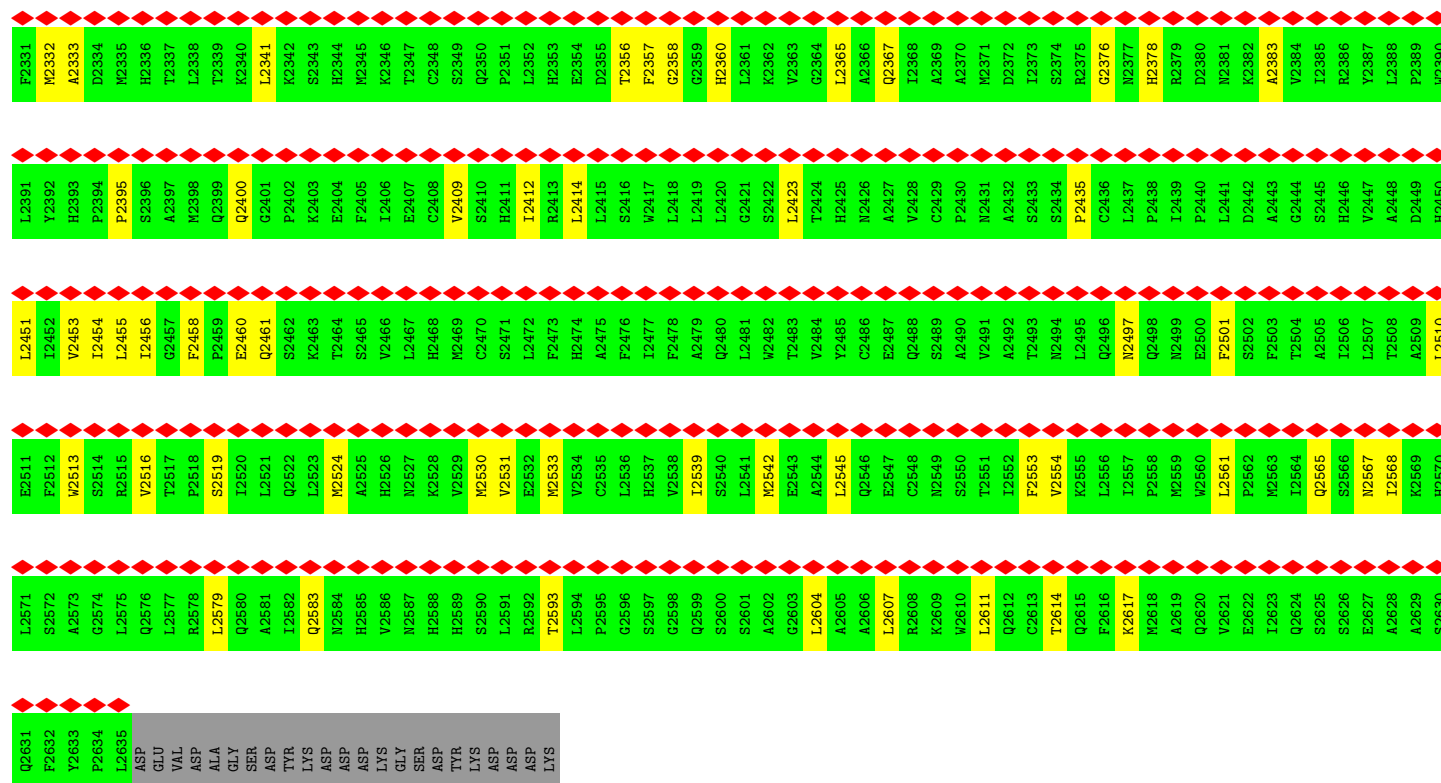
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	182	Total	C	N	O	S	0	0
			1483	934	243	292	14		



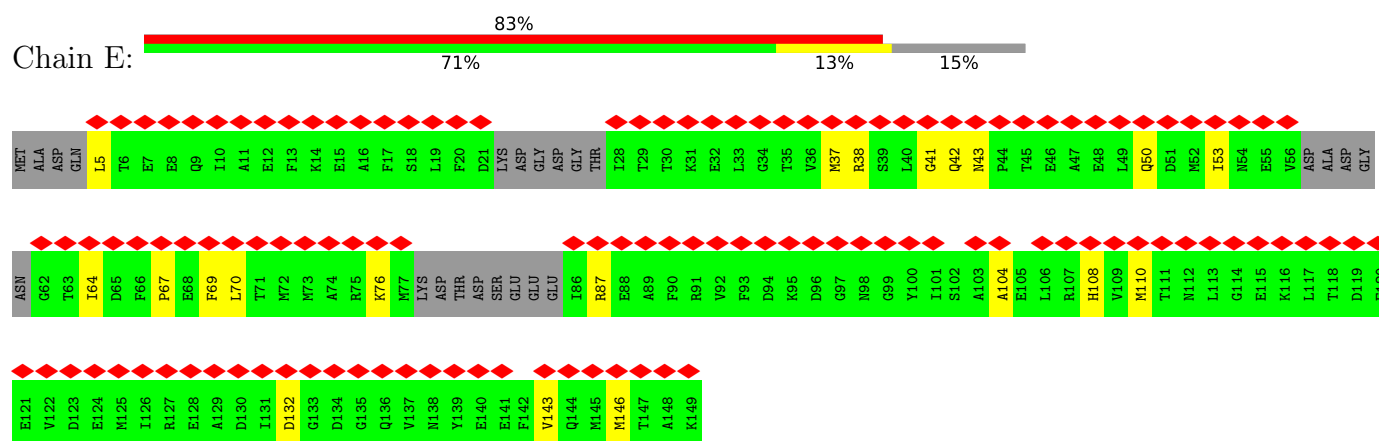




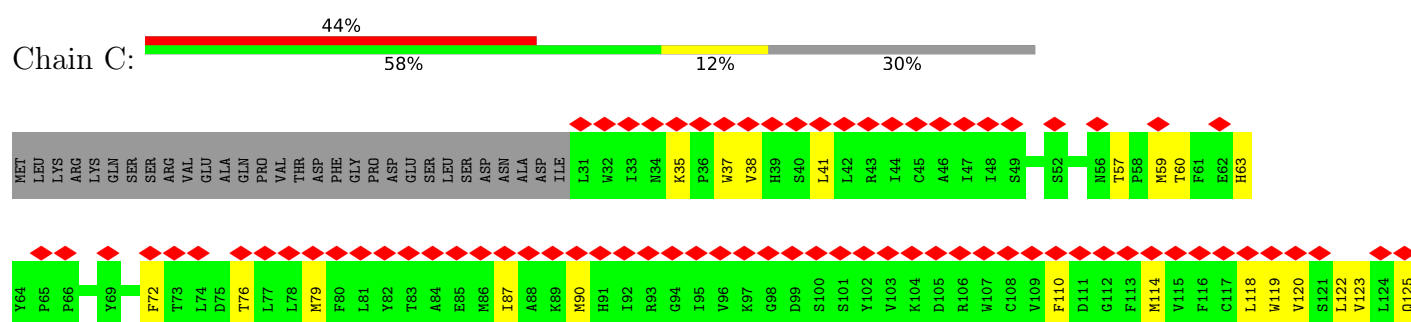


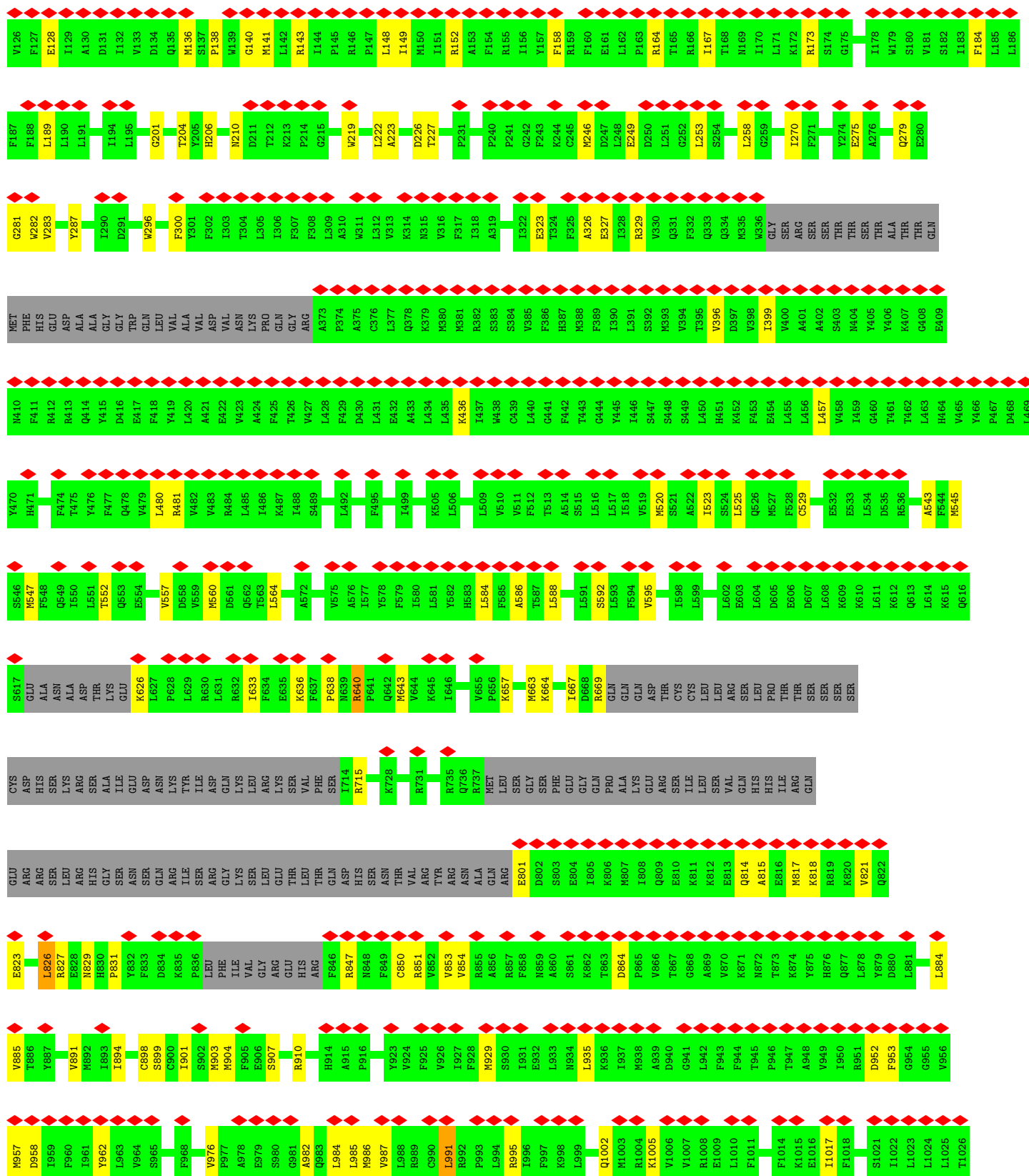


• Molecule 3: Calmodulin-1



• Molecule 4: Sodium leak channel non-selective protein, Extended tegument protein pp150







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174294	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.947	Depositor
Minimum map value	-1.055	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	556.544, 556.544, 556.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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	0.30	0/14450	0.67	2/19574 (0.0%)
2	B	0.30	0/13441	0.67	1/18238 (0.0%)
3	E	0.32	0/997	0.71	0/1335
4	C	0.31	0/11701	0.74	4/15843 (0.0%)
5	D	0.38	0/1522	0.88	0/2065
All	All	0.31	0/42111	0.70	7/57055 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1317	LYS	N-CA-C	6.44	121.27	113.41
4	C	991	LEU	N-CA-C	-6.32	105.52	112.72
4	C	1355	VAL	CA-C-N	-6.30	111.11	122.46
4	C	1355	VAL	C-N-CA	-6.30	111.11	122.46
1	A	2096	GLU	N-CA-CB	5.73	119.16	110.28
1	A	2734	GLN	N-CA-C	5.60	122.19	109.81
2	B	876	GLU	N-CA-CB	5.34	117.71	109.91

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	14143	0	14323	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13146	0	13362	213	0
3	E	988	0	920	13	0
4	C	11413	0	11682	172	0
5	D	1483	0	1374	31	0
All	All	41173	0	41661	628	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 8.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:MET:SD	2:B:197:LEU:HD22	1.47	1.53
1:A:1460:LEU:HD22	1:A:1463:MET:CE	1.47	1.40
1:A:1460:LEU:CD2	1:A:1463:MET:HE2	1.74	1.17
2:B:178:MET:SD	2:B:197:LEU:CD2	2.34	1.15
3:E:110:MET:HG3	4:C:1576:LEU:HD11	1.30	1.11
2:B:874:LEU:HG	2:B:877:ARG:HH21	1.16	1.09
1:A:2169:LEU:HD11	1:A:2192:VAL:HG21	1.34	1.05
4:C:1318:HIS:CD2	4:C:1321:LEU:H	1.76	1.01
1:A:2169:LEU:CD1	1:A:2192:VAL:HG21	1.91	1.00
2:B:2054:ARG:HD3	2:B:2108:PHE:HB2	1.42	0.98
4:C:1347:LEU:CD2	4:C:1351:PHE:HE2	1.78	0.96
1:A:1463:MET:SD	1:A:1575:LEU:HD13	2.07	0.94
1:A:1460:LEU:HD22	1:A:1463:MET:HE1	1.48	0.93
1:A:1460:LEU:HD22	1:A:1463:MET:HE2	0.93	0.91
4:C:1318:HIS:HD2	4:C:1321:LEU:H	1.14	0.91
4:C:957:MET:HE1	4:C:991:LEU:HD23	1.50	0.90
1:A:1913:LEU:HD12	1:A:1914:LEU:N	1.89	0.88
2:B:197:LEU:HD23	2:B:201:PHE:HD2	1.39	0.88
5:D:261:CYS:O	5:D:265:VAL:HG23	1.72	0.88
4:C:1347:LEU:CD2	4:C:1351:PHE:CE2	2.58	0.87
2:B:304:ILE:CG2	2:B:340:TYR:CZ	2.58	0.86
2:B:1305:PHE:HZ	2:B:1359:LEU:HD21	1.38	0.86
4:C:457:LEU:HD11	4:C:481:ARG:HE	1.41	0.84
4:C:982:ALA:O	4:C:985:LEU:HB2	1.76	0.83
2:B:2053:GLY:HA3	2:B:2108:PHE:HE1	1.44	0.82
4:C:1347:LEU:HD21	4:C:1351:PHE:HE2	1.43	0.82
4:C:1347:LEU:HD23	4:C:1351:PHE:CE2	2.16	0.81
4:C:457:LEU:CD1	4:C:481:ARG:HE	1.92	0.81
2:B:874:LEU:HG	2:B:877:ARG:NH2	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ILE:CG2	2:B:340:TYR:CE2	2.64	0.80
1:A:2363:SER:O	1:A:2367:LEU:HG	1.81	0.80
2:B:992:ALA:HA	2:B:996:HIS:HB2	1.64	0.80
4:C:136:MET:HG2	4:C:136:MET:O	1.81	0.80
1:A:1460:LEU:CD2	1:A:1463:MET:CE	2.43	0.79
2:B:304:ILE:HG21	2:B:340:TYR:CZ	2.16	0.79
4:C:1347:LEU:HD21	4:C:1351:PHE:CE2	2.18	0.78
4:C:957:MET:HE1	4:C:991:LEU:CD2	2.12	0.78
1:A:2000:VAL:O	1:A:2009:PRO:HA	1.83	0.78
2:B:450:ILE:HD11	2:B:526:LEU:HD23	1.66	0.78
2:B:197:LEU:HD23	2:B:201:PHE:CD2	2.20	0.77
2:B:304:ILE:HG22	2:B:340:TYR:CE2	2.20	0.77
4:C:1318:HIS:NE2	4:C:1320:THR:HB	2.00	0.77
1:A:2169:LEU:CD1	1:A:2192:VAL:CG2	2.63	0.77
1:A:2748:LEU:HD22	1:A:2823:MET:CE	2.16	0.76
4:C:1114:LEU:HG	4:C:1114:LEU:O	1.84	0.76
4:C:1433:ILE:HG13	4:C:1434:ILE:HD12	1.69	0.75
1:A:922:PRO:O	1:A:925:LEU:HB2	1.86	0.74
2:B:450:ILE:HD11	2:B:526:LEU:CD2	2.17	0.74
2:B:193:ILE:O	2:B:197:LEU:HG	1.87	0.74
4:C:1031:PHE:HD2	4:C:1108:LEU:HD21	1.52	0.73
1:A:2367:LEU:CD1	1:A:2492:PRO:HB3	2.19	0.72
1:A:2748:LEU:HD22	1:A:2823:MET:HE2	1.72	0.72
2:B:835:ILE:HD11	2:B:874:LEU:HD22	1.71	0.72
1:A:1854:ILE:O	1:A:1858:MET:HG2	1.89	0.71
1:A:1350:LEU:HG	1:A:1575:LEU:HG	1.72	0.71
2:B:304:ILE:HG21	2:B:340:TYR:CE2	2.26	0.70
1:A:1910:LEU:HD13	1:A:1913:LEU:HD21	1.72	0.70
4:C:222:LEU:HD23	4:C:223:ALA:O	1.91	0.70
5:D:304:CYS:SG	5:D:341:CYS:HB2	2.31	0.69
1:A:1206:ALA:HB1	1:A:1287:ARG:HG3	1.74	0.69
4:C:552:THR:HG22	4:C:1114:LEU:HD11	1.75	0.68
2:B:304:ILE:HG22	2:B:340:TYR:CZ	2.28	0.68
2:B:304:ILE:CG2	2:B:340:TYR:OH	2.42	0.68
1:A:2378:LEU:HD21	1:A:2404:LEU:CD2	2.23	0.68
4:C:1352:ALA:HA	4:C:1355:VAL:HG12	1.75	0.68
2:B:2079:LYS:HE2	2:B:2112:LEU:HB3	1.75	0.67
2:B:833:SER:HA	2:B:836:ASN:HD22	1.60	0.67
2:B:2454:ILE:O	2:B:2458:PHE:HB2	1.94	0.67
2:B:324:ILE:HG22	2:B:338:PRO:HB3	1.77	0.67
1:A:1238:PRO:HD2	1:A:1241:MET:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1085:TRP:CD1	5:D:278:LYS:HG3	2.31	0.66
1:A:1852:LEU:HB3	1:A:1853:PRO:HD3	1.78	0.65
2:B:328:LEU:O	2:B:332:LEU:HB2	1.96	0.65
4:C:1213:LYS:HG2	4:C:1317:LYS:HE2	1.77	0.65
4:C:79:MET:HG3	4:C:122:LEU:HD11	1.76	0.65
1:A:1562:ARG:HA	1:A:1566:MET:HE3	1.77	0.65
4:C:1318:HIS:HB3	4:C:1322:LYS:HZ3	1.61	0.65
1:A:2367:LEU:HD12	1:A:2492:PRO:HB3	1.79	0.64
1:A:2125:GLU:OE1	1:A:2129:ARG:NH1	2.30	0.64
2:B:2524:MET:HG2	2:B:2531:VAL:HG22	1.78	0.64
2:B:561:LEU:HD13	2:B:615:VAL:HG13	1.81	0.63
1:A:1463:MET:SD	1:A:1575:LEU:CD1	2.86	0.63
2:B:694:GLU:HG3	2:B:695:LEU:HD12	1.80	0.63
4:C:850:CYS:HB2	4:C:935:LEU:HG	1.81	0.61
5:D:239:SER:HB3	5:D:243:THR:HB	1.81	0.61
5:D:341:CYS:SG	5:D:342:PRO:HD2	2.41	0.61
2:B:232:GLN:OE1	2:B:268:GLN:NE2	2.34	0.60
1:A:2367:LEU:CD1	1:A:2492:PRO:CB	2.79	0.60
1:A:819:ARG:HA	1:A:823:PHE:HB3	1.82	0.60
1:A:2379:GLN:OE1	1:A:2382:LYS:CE	2.50	0.60
4:C:884:LEU:HD12	4:C:885:VAL:HG13	1.82	0.60
1:A:123:ALA:O	1:A:127:CYS:HB3	2.02	0.60
3:E:64:ILE:HD11	3:E:69:PHE:HB2	1.83	0.60
2:B:630:GLU:HB3	2:B:688:TRP:HZ2	1.66	0.60
2:B:2046:LEU:HB3	2:B:2098:LEU:HD21	1.82	0.60
1:A:2580:PRO:HA	1:A:2583:ILE:HG12	1.83	0.59
4:C:1537:LEU:HD12	4:C:1538:SER:N	2.17	0.59
4:C:1002:GLN:HB3	4:C:1337:PHE:HE1	1.66	0.59
4:C:1400:VAL:H	4:C:1418:GLY:HA3	1.68	0.59
2:B:370:ILE:HG13	2:B:381:ARG:HB2	1.83	0.59
2:B:2205:LEU:HD11	2:B:2241:LEU:HD23	1.84	0.59
4:C:1343:PHE:O	4:C:1346:LEU:HG	2.02	0.59
4:C:1150:LEU:O	4:C:1154:VAL:HG12	2.02	0.59
1:A:2060:ASP:OD2	1:A:2135:ARG:NH1	2.35	0.59
2:B:2329:LEU:O	2:B:2333:ALA:HB2	2.02	0.59
2:B:304:ILE:HG22	2:B:340:TYR:OH	2.02	0.58
1:A:2558:ARG:HD2	1:A:2562:ARG:HH21	1.68	0.58
1:A:929:CYS:O	1:A:932:ARG:HB3	2.03	0.58
1:A:1973:LEU:O	1:A:1977:MET:HB2	2.03	0.58
1:A:2696:HIS:HA	1:A:2700:PRO:HD3	1.85	0.58
2:B:2192:CYS:SG	2:B:2193:SER:N	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:143:ARG:NH2	4:C:529:CYS:SG	2.76	0.58
2:B:202:LEU:HD11	2:B:247:LEU:HD13	1.85	0.58
1:A:2205:ALA:HB2	2:B:1072:ARG:HH12	1.69	0.58
4:C:227:THR:OG1	4:C:1368:ARG:NH2	2.37	0.58
2:B:577:LEU:HG	2:B:578:PRO:HD2	1.85	0.58
2:B:2234:THR:HA	2:B:2283:LEU:HD11	1.85	0.58
4:C:1393:LYS:HA	4:C:1396:HIS:HB2	1.86	0.58
1:A:1955:LEU:HA	1:A:1958:LEU:HB2	1.85	0.58
2:B:2524:MET:SD	2:B:2567:ASN:ND2	2.75	0.58
3:E:67:PRO:HA	3:E:70:LEU:HD12	1.86	0.58
2:B:450:ILE:HG23	2:B:529:MET:HG3	1.85	0.57
2:B:236:ASN:O	2:B:240:HIS:ND1	2.36	0.57
4:C:457:LEU:HD11	4:C:481:ARG:NE	2.14	0.57
2:B:2110:ARG:O	2:B:2110:ARG:HG2	2.04	0.57
2:B:1028:VAL:HG21	2:B:1073:PHE:HB3	1.84	0.57
4:C:520:MET:HA	4:C:523:ILE:HG12	1.85	0.57
2:B:608:LEU:HD22	2:B:647:VAL:HG13	1.85	0.57
2:B:621:TRP:HA	2:B:624:ILE:HG12	1.86	0.57
2:B:2079:LYS:CE	2:B:2112:LEU:HB3	2.34	0.57
1:A:933:GLN:O	1:A:936:GLN:HB3	2.04	0.57
1:A:2748:LEU:HD22	1:A:2823:MET:HE1	1.85	0.57
5:D:330:CYS:HB2	5:D:374:PRO:HG2	1.85	0.57
4:C:326:ALA:HA	4:C:329:ARG:HD2	1.87	0.57
1:A:2127:LEU:HA	1:A:2130:LEU:HD12	1.86	0.57
2:B:2400:GLN:HE22	2:B:2456:ILE:HB	1.69	0.57
4:C:1318:HIS:HD2	4:C:1321:LEU:N	1.95	0.57
4:C:1033:SER:O	4:C:1037:GLN:HB2	2.05	0.57
5:D:233:GLU:OE2	5:D:323:ASN:ND2	2.38	0.56
2:B:320:VAL:HG13	2:B:321:LYS:HG2	1.86	0.56
1:A:1600:LEU:HD11	1:A:1643:ASN:HD21	1.69	0.56
1:A:2354:VAL:HG12	1:A:2363:SER:HA	1.85	0.56
1:A:2711:LEU:HD11	1:A:2747:VAL:HG11	1.87	0.56
2:B:2089:LEU:HG	2:B:2094:ILE:HG21	1.88	0.56
1:A:1464:ILE:HG21	1:A:1587:MET:SD	2.46	0.56
4:C:520:MET:HE1	4:C:586:ALA:HB2	1.87	0.56
1:A:2589:LEU:HA	1:A:2592:MET:HG2	1.88	0.56
2:B:1395:ARG:NH2	2:B:1430:THR:O	2.38	0.56
1:A:2028:LEU:HD23	1:A:2033:ILE:HB	1.87	0.56
2:B:2332:MET:HG3	2:B:2414:LEU:HD23	1.88	0.56
1:A:1616:LEU:HD21	1:A:1662:MET:HE3	1.88	0.56
2:B:160:THR:HA	2:B:163:LEU:HG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2530:MET:HA	2:B:2533:MET:HG2	1.88	0.55
4:C:87:ILE:HG22	4:C:87:ILE:O	2.06	0.55
4:C:643:MET:HE1	4:C:657:LYS:HA	1.87	0.55
1:A:932:ARG:O	1:A:932:ARG:NH1	2.39	0.55
1:A:54:VAL:HG12	1:A:55:GLU:HG2	1.88	0.55
2:B:2149:ARG:O	2:B:2153:ASN:HB2	2.06	0.55
2:B:2542:MET:HE1	2:B:2579:LEU:HD12	1.86	0.55
4:C:976:VAL:HG21	4:C:986:MET:HE1	1.89	0.55
4:C:664:LYS:HA	4:C:667:ILE:HG22	1.88	0.55
5:D:269:GLN:HG2	5:D:273:HIS:CE1	2.40	0.55
2:B:866:LEU:HD23	2:B:869:GLN:HE21	1.72	0.55
2:B:2218:GLU:HG2	2:B:2219:PRO:HD3	1.89	0.55
1:A:2855:ILE:HD13	1:A:2859:LEU:HD12	1.88	0.55
2:B:2561:LEU:HD22	2:B:2583:GLN:HE21	1.72	0.55
4:C:136:MET:O	4:C:136:MET:CG	2.51	0.55
2:B:1145:LEU:HD21	2:B:1169:ARG:HH22	1.71	0.54
1:A:1572:PRO:HA	1:A:1575:LEU:HB2	1.89	0.54
1:A:2044:MET:HG3	1:A:2050:LEU:O	2.08	0.54
2:B:2278:ASP:HA	2:B:2281:LEU:HB2	1.89	0.54
2:B:2395:PRO:HB2	2:B:2453:VAL:HG21	1.89	0.54
1:A:82:LEU:HD22	1:A:184:THR:HB	1.89	0.54
2:B:601:LYS:NZ	2:B:602:GLU:OE2	2.40	0.54
4:C:57:THR:HB	4:C:60:THR:HG22	1.89	0.54
1:A:2379:GLN:OE1	1:A:2382:LYS:HE3	2.07	0.54
1:A:2169:LEU:HD13	1:A:2192:VAL:CG2	2.34	0.54
1:A:2277:VAL:HG21	1:A:2300:LEU:HD13	1.90	0.54
4:C:480:LEU:HD23	4:C:1030:VAL:HG21	1.89	0.54
1:A:2344:SER:HA	1:A:2347:ILE:HD12	1.90	0.54
1:A:1638:THR:HG21	1:A:1870:VAL:HG22	1.89	0.54
2:B:455:GLU:O	2:B:498:ARG:NH2	2.41	0.54
2:B:579:LYS:HE3	2:B:600:LEU:HD21	1.89	0.54
2:B:1227:LEU:O	2:B:1230:SER:HB3	2.07	0.54
5:D:333:TYR:O	5:D:336:GLU:HB2	2.07	0.54
1:A:2094:LYS:NZ	1:A:2141:GLU:OE1	2.37	0.54
2:B:319:ALA:HA	2:B:342:CYS:HA	1.89	0.53
4:C:891:VAL:HA	4:C:894:ILE:HG22	1.88	0.53
2:B:1360:LEU:HD11	2:B:1405:ILE:HG23	1.88	0.53
2:B:2254:ASP:HA	2:B:2257:TYR:HB2	1.91	0.53
1:A:1471:SER:HB2	1:A:1481:HIS:HE1	1.71	0.53
1:A:2169:LEU:HD13	1:A:2192:VAL:HG21	1.85	0.53
2:B:632:ILE:HD12	2:B:636:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2027:CYS:HB2	1:A:2074:LEU:HD22	1.91	0.53
1:A:1653:ARG:NH2	2:B:2021:GLU:OE1	2.41	0.53
1:A:2087:GLN:HG3	1:A:2150:ALA:HB2	1.91	0.53
2:B:2124:SER:HA	2:B:2127:ALA:HB3	1.91	0.53
1:A:2321:VAL:O	1:A:2325:LYS:NZ	2.38	0.53
4:C:1118:VAL:HB	4:C:1121:ARG:HH21	1.72	0.53
5:D:234:LEU:HG	5:D:319:VAL:HG11	1.90	0.53
1:A:1358:GLU:OE2	1:A:1578:LYS:NZ	2.41	0.53
4:C:210:ASN:HA	4:C:246:MET:HE2	1.89	0.53
1:A:82:LEU:O	1:A:86:LEU:HB2	2.09	0.52
1:A:2353:VAL:HG23	4:C:663:MET:HE1	1.91	0.52
2:B:1022:GLN:H	2:B:1022:GLN:NE2	2.07	0.52
2:B:1076:ILE:HD11	2:B:1121:PRO:HB3	1.91	0.52
4:C:1318:HIS:HB3	4:C:1322:LYS:NZ	2.24	0.52
1:A:815:GLY:O	1:A:819:ARG:NH1	2.42	0.52
1:A:1570:PRO:HA	1:A:1573:LEU:HD13	1.91	0.52
1:A:2390:THR:HG22	1:A:2392:PRO:HD2	1.90	0.52
3:E:76:LYS:HG2	4:C:1495:ARG:HH11	1.73	0.52
4:C:1343:PHE:HA	4:C:1346:LEU:HD21	1.92	0.52
2:B:2341:LEU:HD12	2:B:2358:GLY:HA2	1.91	0.52
4:C:991:LEU:O	4:C:991:LEU:HG	2.09	0.52
1:A:2043:LEU:HD12	1:A:2072:LEU:HD11	1.92	0.52
1:A:2200:HIS:HB2	1:A:2206:LEU:HD13	1.91	0.52
2:B:2565:GLN:HG2	2:B:2568:ILE:HD12	1.92	0.52
2:B:321:LYS:HB3	2:B:357:LEU:HB3	1.92	0.52
3:E:38:ARG:NH1	3:E:43:ASN:OD1	2.43	0.51
2:B:569:PHE:HB2	2:B:572:MET:HE2	1.92	0.51
1:A:1324:PHE:HB2	1:A:1498:ALA:HB1	1.93	0.51
1:A:924:ASN:O	1:A:928:TYR:N	2.43	0.51
1:A:2490:ARG:NH1	1:A:2553:GLN:OE1	2.43	0.51
1:A:2586:LEU:HD23	1:A:2589:LEU:HD21	1.92	0.51
2:B:2118:ASP:OD1	2:B:2118:ASP:N	2.44	0.51
4:C:114:MET:O	4:C:118:LEU:HB2	2.11	0.51
4:C:173:ARG:NH1	4:C:327:GLU:OE2	2.42	0.51
4:C:640:ARG:HE	4:C:831:PRO:HD3	1.75	0.51
2:B:1426:ILE:HD13	2:B:1429:ASN:HB3	1.92	0.51
4:C:1161:GLU:HA	4:C:1166:ALA:HB2	1.92	0.51
2:B:946:TYR:HD1	2:B:949:LEU:HD12	1.76	0.51
1:A:1347:GLN:HA	1:A:1350:LEU:HB2	1.93	0.51
1:A:2134:PRO:HD3	1:A:2188:LEU:HD12	1.92	0.51
2:B:653:ASP:HB3	2:B:656:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:396:VAL:HA	4:C:399:ILE:HG22	1.93	0.51
1:A:34:LEU:HD22	2:B:2510:LEU:HD13	1.92	0.51
1:A:847:ARG:O	1:A:851:ASN:ND2	2.44	0.51
1:A:2859:LEU:O	1:A:2873:ARG:NH1	2.42	0.51
2:B:452:LEU:HD11	2:B:500:LEU:HB2	1.93	0.51
2:B:644:PHE:HB3	2:B:648:LEU:HD12	1.93	0.51
2:B:1426:ILE:HA	2:B:1429:ASN:HB3	1.93	0.51
2:B:2328:VAL:HG13	2:B:2365:LEU:HB3	1.93	0.51
4:C:823:GLU:O	4:C:827:ARG:NH2	2.43	0.51
1:A:86:LEU:HG	1:A:191:LEU:HD12	1.93	0.50
1:A:2193:PHE:HB3	1:A:2210:TYR:HE1	1.76	0.50
2:B:272:PRO:HA	2:B:275:GLN:HB3	1.93	0.50
2:B:1065:GLU:HB3	2:B:1110:ARG:HH12	1.76	0.50
4:C:1346:LEU:C	4:C:1346:LEU:HD12	2.35	0.50
5:D:275:ALA:HA	5:D:278:LYS:HE2	1.91	0.50
5:D:330:CYS:SG	5:D:376:CYS:SG	3.09	0.50
1:A:2848:PHE:HA	1:A:2851:LEU:HB2	1.93	0.50
2:B:2539:ILE:HG12	2:B:2542:MET:HE2	1.93	0.50
2:B:2455:LEU:HD13	2:B:2519:SER:HB3	1.93	0.50
1:A:2558:ARG:O	1:A:2562:ARG:HB2	2.11	0.50
4:C:801:GLU:HG3	4:C:1558:GLN:HG3	1.94	0.50
4:C:1076:ARG:HD2	4:C:1078:GLY:H	1.77	0.50
4:C:149:ILE:O	4:C:152:ARG:HB3	2.11	0.50
4:C:59:MET:O	4:C:63:HIS:ND1	2.44	0.50
4:C:592:SER:HA	4:C:595:VAL:HG22	1.93	0.50
4:C:1321:LEU:HB3	4:C:1322:LYS:NZ	2.27	0.49
1:A:101:HIS:ND1	1:A:104:LYS:O	2.45	0.49
3:E:37:MET:HG2	3:E:42:GLN:HB2	1.95	0.49
4:C:158:PHE:O	4:C:164:ARG:NH2	2.45	0.49
4:C:958:ASP:OD2	4:C:995:ARG:NH1	2.46	0.49
2:B:2147:MET:HE1	2:B:2188:LEU:HD23	1.94	0.49
1:A:96:ARG:NH2	1:A:198:ARG:O	2.45	0.49
1:A:901:VAL:HA	1:A:904:MET:HG3	1.94	0.49
1:A:1183:GLY:O	1:A:1186:ARG:HB3	2.12	0.49
1:A:1920:PHE:HE1	1:A:1925:SER:HB3	1.77	0.49
2:B:324:ILE:HG12	2:B:356:TRP:HB3	1.94	0.49
1:A:1226:ALA:HB1	1:A:1351:GLU:HG3	1.95	0.49
1:A:2044:MET:HG2	1:A:2045:ASP:N	2.27	0.49
4:C:1517:TYR:HD2	4:C:1563:ILE:HG23	1.78	0.49
1:A:1958:LEU:HA	1:A:1961:VAL:HB	1.94	0.49
2:B:1155:LYS:HG3	2:B:1158:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:GLN:HA	3:E:53:ILE:HG22	1.93	0.49
4:C:1346:LEU:HD12	4:C:1347:LEU:N	2.28	0.49
4:C:1463:SER:OG	4:C:1464:TYR:N	2.44	0.49
2:B:2082:LEU:HA	2:B:2085:ILE:HG12	1.94	0.49
1:A:931:ILE:HA	1:A:934:LEU:HB3	1.95	0.49
1:A:2691:ASP:CG	1:A:2692:PHE:H	2.21	0.49
1:A:2742:GLN:HA	1:A:2745:ILE:HG12	1.95	0.49
1:A:817:ARG:HG3	1:A:818:LEU:HD12	1.95	0.49
4:C:1178:LEU:HD13	4:C:1461:LEU:HD21	1.95	0.49
1:A:2531:VAL:HG12	1:A:2535:MET:HE2	1.95	0.48
1:A:2810:GLY:HA2	1:A:2813:TRP:CH2	2.48	0.48
2:B:206:ILE:HG21	2:B:250:TYR:HB3	1.95	0.48
2:B:2451:LEU:HD23	2:B:2454:ILE:HD12	1.95	0.48
1:A:1627:ASP:HA	1:A:1630:MET:HG2	1.95	0.48
1:A:1298:SER:O	1:A:1302:LEU:N	2.44	0.48
2:B:679:SER:HA	2:B:682:GLN:HB2	1.96	0.48
2:B:875:LEU:HD23	2:B:878:LEU:HD12	1.94	0.48
4:C:814:GLN:HA	4:C:817:MET:HE2	1.94	0.48
4:C:1315:CYS:HA	4:C:1322:LYS:HE3	1.94	0.48
1:A:2286:ALA:HB3	1:A:2558:ARG:HB2	1.96	0.48
3:E:104:ALA:O	3:E:108:HIS:ND1	2.40	0.48
1:A:1913:LEU:HD12	1:A:1913:LEU:C	2.38	0.48
2:B:1140:ASP:OD1	2:B:1228:ARG:NH1	2.46	0.48
4:C:1537:LEU:HD12	4:C:1537:LEU:C	2.39	0.48
2:B:2357:PHE:HA	2:B:2360:HIS:HB2	1.95	0.48
4:C:901:ILE:HA	4:C:904:MET:HE3	1.94	0.48
4:C:1017:ILE:HD11	4:C:1154:VAL:HG13	1.96	0.48
4:C:1343:PHE:HA	4:C:1346:LEU:CD2	2.44	0.48
1:A:2357:ALA:HB3	4:C:667:ILE:HD11	1.94	0.48
4:C:1048:ASP:OD2	4:C:1088:ARG:NE	2.47	0.48
1:A:22:ILE:HG12	1:A:65:LEU:HD12	1.95	0.48
1:A:2860:LEU:O	1:A:2873:ARG:NH2	2.46	0.47
2:B:364:GLN:NE2	2:B:366:GLU:O	2.47	0.47
2:B:569:PHE:HA	2:B:572:MET:HG2	1.95	0.47
1:A:2014:VAL:HG12	1:A:2059:ARG:HH21	1.78	0.47
4:C:907:SER:HB3	4:C:910:ARG:HB3	1.94	0.47
2:B:39:LEU:HA	2:B:42:PHE:HB2	1.96	0.47
2:B:132:VAL:HA	2:B:135:VAL:HG22	1.95	0.47
2:B:969:PRO:HB3	2:B:1023:LEU:HD11	1.97	0.47
4:C:1375:ALA:HA	4:C:1378:ALA:HB3	1.96	0.47
5:D:345:LEU:HA	5:D:357:SER:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1862:GLU:HB2	1:A:1870:VAL:HG21	1.96	0.47
2:B:2423:LEU:HD23	2:B:2611:LEU:HD13	1.97	0.47
4:C:1368:ARG:HH22	5:D:290:LEU:HD22	1.80	0.47
2:B:141:VAL:HG22	2:B:151:LEU:HD21	1.97	0.47
2:B:1100:VAL:HG11	2:B:1154:LEU:HD11	1.96	0.47
2:B:2545:LEU:HD22	2:B:2553:PHE:HB2	1.96	0.47
4:C:1031:PHE:HD2	4:C:1108:LEU:CD2	2.23	0.47
1:A:935:VAL:O	1:A:939:LYS:N	2.47	0.47
1:A:1184:MET:HE2	1:A:1220:ALA:HB1	1.97	0.47
1:A:2745:ILE:HD12	1:A:2819:GLN:HG2	1.97	0.47
2:B:980:LYS:HE3	2:B:1026:LEU:HD22	1.97	0.47
4:C:864:ASP:OD1	4:C:864:ASP:N	2.47	0.47
4:C:899:SER:O	4:C:903:MET:HB3	2.15	0.47
4:C:929:MET:HE2	4:C:962:TYR:HB2	1.96	0.47
1:A:2189:PHE:O	1:A:2192:VAL:HG22	2.15	0.47
1:A:2826:ARG:HB3	1:A:2828:VAL:HG23	1.97	0.47
2:B:807:LEU:HD23	2:B:808:LEU:HD23	1.97	0.47
1:A:871:GLU:OE2	1:A:933:GLN:NE2	2.47	0.47
2:B:686:LEU:HD21	2:B:800:CYS:HB3	1.97	0.47
2:B:2554:VAL:HG21	2:B:2593:THR:HG21	1.97	0.47
4:C:638:PRO:HG2	4:C:640:ARG:HH12	1.80	0.46
1:A:1869:ALA:HB3	1:A:1873:VAL:HG13	1.95	0.46
2:B:248:MET:HE3	2:B:388:PHE:HD1	1.79	0.46
2:B:1335:SER:OG	2:B:1337:CYS:SG	2.63	0.46
2:B:2460:GLU:HG3	2:B:2461:GLN:HG2	1.96	0.46
1:A:2241:TYR:O	1:A:2251:ARG:NH1	2.47	0.46
2:B:1403:LEU:CD1	2:B:2029:VAL:HB	2.46	0.46
4:C:899:SER:O	4:C:903:MET:CB	2.64	0.46
1:A:953:ALA:H	1:A:1187:PHE:HZ	1.62	0.46
2:B:329:SER:HB3	2:B:339:LEU:HG	1.96	0.46
2:B:1403:LEU:HD12	2:B:2029:VAL:HG21	1.97	0.46
4:C:898:CYS:HA	4:C:901:ILE:HG12	1.96	0.46
4:C:1114:LEU:O	4:C:1114:LEU:CG	2.57	0.46
4:C:1536:MET:HE1	4:C:1556:ARG:HH12	1.79	0.46
5:D:214:PRO:HD2	5:D:215:LEU:H	1.80	0.46
1:A:1908:TYR:OH	2:B:1101:GLU:O	2.29	0.46
2:B:527:VAL:HA	2:B:530:VAL:HG12	1.97	0.46
2:B:1354:ASN:OD1	2:B:1355:LEU:N	2.45	0.46
4:C:110:PHE:O	4:C:114:MET:HG3	2.15	0.46
1:A:121:LEU:HD21	1:A:214:ILE:HB	1.97	0.46
1:A:126:ASP:HA	1:A:129:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:CYS:SG	1:A:1475:THR:N	2.88	0.46
1:A:2186:ILE:O	1:A:2190:LEU:HG	2.15	0.46
2:B:2034:ILE:HG12	2:B:2041:ALA:HB3	1.97	0.46
4:C:184:PHE:HD1	4:C:1321:LEU:HG	1.81	0.46
4:C:201:GLY:HA2	4:C:1230:LYS:HD2	1.98	0.46
1:A:113:LEU:HD23	1:A:116:LEU:HD12	1.97	0.46
1:A:2126:ASP:O	1:A:2130:LEU:HG	2.16	0.46
4:C:189:LEU:HD21	4:C:270:ILE:HG23	1.97	0.46
2:B:172:SER:O	2:B:218:HIS:ND1	2.48	0.46
2:B:1296:GLU:OE2	2:B:1358:HIS:NE2	2.49	0.46
3:E:41:GLY:HA2	4:C:1489:ARG:HH21	1.81	0.46
4:C:815:ALA:HA	4:C:818:LYS:HE2	1.97	0.46
4:C:847:ARG:NH1	4:C:850:CYS:SG	2.83	0.46
4:C:1534:LEU:HA	4:C:1537:LEU:HG	1.97	0.46
1:A:215:TRP:HA	1:A:218:MET:HG2	1.97	0.46
1:A:1185:LYS:O	1:A:1188:GLN:HB3	2.16	0.46
1:A:1853:PRO:HA	1:A:1856:HIS:HB2	1.98	0.46
2:B:1001:ALA:O	2:B:1005:ASP:HB2	2.15	0.46
2:B:1157:ASP:OD1	2:B:1157:ASP:N	2.48	0.46
4:C:525:LEU:HD13	4:C:543:ALA:HB2	1.98	0.46
4:C:1149:THR:HA	4:C:1152:VAL:HG22	1.97	0.46
5:D:375:GLU:O	5:D:376:CYS:SG	2.74	0.46
1:A:1874:ALA:HA	1:A:1877:VAL:HG12	1.97	0.45
1:A:2025:LYS:HA	1:A:2025:LYS:HD3	1.83	0.45
1:A:2214:VAL:HA	1:A:2217:THR:HG22	1.97	0.45
1:A:2586:LEU:HA	1:A:2589:LEU:HG	1.98	0.45
2:B:2195:ASP:OD1	2:B:2195:ASP:N	2.49	0.45
1:A:2712:LEU:HD13	1:A:2905:LEU:HD13	1.97	0.45
5:D:335:LEU:HD11	5:D:368:PHE:HB2	1.98	0.45
2:B:301:TRP:H	2:B:301:TRP:CD1	2.34	0.45
4:C:282:TRP:HZ2	4:C:1387:THR:HG21	1.82	0.45
1:A:78:VAL:HG13	1:A:119:MET:HB2	1.97	0.45
1:A:1574:SER:HA	1:A:1577:ILE:HD12	1.99	0.45
2:B:2329:LEU:O	2:B:2333:ALA:CB	2.64	0.45
4:C:164:ARG:HH11	4:C:167:ILE:HG13	1.81	0.45
4:C:826:LEU:HD12	4:C:826:LEU:HA	1.79	0.45
1:A:2422:MET:HG2	1:A:2547:LEU:HD13	1.98	0.45
2:B:2082:LEU:HD23	2:B:2085:ILE:HD11	1.98	0.45
1:A:2046:LYS:HA	1:A:2046:LYS:HD3	1.83	0.45
4:C:1392:ASN:OD1	4:C:1393:LYS:N	2.49	0.45
1:A:1959:TRP:HB2	1:A:2102:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2342:SER:OG	1:A:2343:ILE:N	2.49	0.45
4:C:640:ARG:HG3	4:C:829:ASN:HA	1.98	0.45
4:C:1286:VAL:HA	4:C:1289:VAL:HG22	1.99	0.45
1:A:953:ALA:HB1	1:A:1180:ILE:HG13	1.99	0.45
2:B:238:VAL:HG22	2:B:301:TRP:HA	1.98	0.45
2:B:446:VAL:O	2:B:450:ILE:HG12	2.16	0.45
2:B:692:LEU:CD1	2:B:697:ILE:HG13	2.47	0.45
4:C:984:LEU:HA	4:C:987:VAL:HG22	1.97	0.45
1:A:2405:ALA:HA	1:A:2408:LEU:HD12	1.99	0.45
2:B:2295:LYS:O	2:B:2367:GLN:NE2	2.48	0.45
5:D:274:HIS:O	5:D:278:LYS:HD3	2.17	0.45
2:B:629:LEU:HB3	2:B:688:TRP:CD1	2.52	0.45
2:B:650:LYS:HG3	2:B:656:LEU:HD23	1.98	0.45
3:E:146:MET:HE1	4:C:1579:CYS:HA	1.99	0.45
4:C:545:MET:SD	4:C:1121:ARG:NH1	2.90	0.45
2:B:1305:PHE:CZ	2:B:1359:LEU:HD21	2.31	0.44
2:B:2604:LEU:HA	2:B:2607:LEU:HB2	1.99	0.44
4:C:275:GLU:HG2	4:C:557:VAL:HG21	1.99	0.44
4:C:715:ARG:NH1	4:C:715:ARG:O	2.50	0.44
5:D:284:SER:HA	5:D:287:HIS:HD2	1.82	0.44
1:A:1588:TYR:HA	1:A:1591:ILE:HG22	1.99	0.44
1:A:1945:GLU:HG3	1:A:2048:TRP:HA	1.99	0.44
1:A:2187:MET:HE3	1:A:2187:MET:HB3	1.72	0.44
1:A:2701:PHE:O	1:A:2707:ARG:NE	2.42	0.44
2:B:2054:ARG:HA	2:B:2054:ARG:HD2	1.77	0.44
1:A:1994:GLY:HA2	1:A:2063:PRO:HA	1.99	0.44
2:B:251:LYS:HA	2:B:251:LYS:HD2	1.81	0.44
2:B:2356:THR:HG1	2:B:2360:HIS:CD2	2.35	0.44
1:A:2853:PRO:O	1:A:2857:CYS:HB2	2.17	0.44
2:B:342:CYS:H	2:B:345:CYS:HB3	1.81	0.44
4:C:72:PHE:O	4:C:76:THR:OG1	2.30	0.44
4:C:1051:ILE:HD12	4:C:1051:ILE:HA	1.85	0.44
1:A:1315:LEU:HD23	1:A:1315:LEU:HA	1.88	0.44
1:A:2033:ILE:HD12	1:A:2041:TYR:HE2	1.82	0.44
2:B:179:ILE:HG21	2:B:226:MET:HG2	2.00	0.44
2:B:1422:HIS:O	2:B:1425:HIS:HB3	2.18	0.44
2:B:2093:GLY:O	2:B:2097:GLN:NE2	2.50	0.44
1:A:852:LYS:NZ	1:A:853:ASP:OD2	2.45	0.44
1:A:865:LEU:HD21	1:A:897:GLU:HA	2.00	0.44
1:A:2094:LYS:HG3	1:A:2157:LEU:HD13	2.00	0.44
2:B:1286:LYS:HE3	2:B:1286:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:283:VAL:O	4:C:287:TYR:HB3	2.17	0.44
4:C:952:ASP:HB3	4:C:953:PHE:H	1.54	0.44
2:B:1164:GLU:HA	2:B:1167:VAL:HG12	2.00	0.44
4:C:1142:LEU:O	4:C:1146:ILE:HG22	2.17	0.44
2:B:2214:ARG:HA	2:B:2217:LEU:HD13	2.00	0.43
4:C:138:PRO:O	4:C:141:MET:HG2	2.18	0.43
4:C:1321:LEU:HB3	4:C:1322:LYS:HZ2	1.83	0.43
1:A:887:VAL:HB	1:A:948:ARG:HH22	1.82	0.43
2:B:1429:ASN:O	2:B:1433:ALA:N	2.51	0.43
2:B:2196:SER:N	2:B:2199:ARG:HH21	2.16	0.43
2:B:2270:LEU:HD13	2:B:2365:LEU:HD11	1.98	0.43
2:B:2614:THR:HA	2:B:2617:LYS:HB2	2.00	0.43
3:E:132:ASP:N	3:E:132:ASP:OD1	2.50	0.43
4:C:114:MET:HE2	4:C:148:LEU:HD12	2.00	0.43
4:C:204:THR:HG21	4:C:249:GLU:HB2	1.99	0.43
4:C:633:ILE:HA	4:C:636:LYS:HE2	1.99	0.43
1:A:904:MET:HE1	1:A:908:LEU:HD22	1.99	0.43
1:A:2564:ILE:HG21	1:A:2614:LEU:HA	2.01	0.43
2:B:2617:LYS:HD3	2:B:2617:LYS:HA	1.79	0.43
3:E:87:ARG:HG2	3:E:143:VAL:HG21	1.99	0.43
4:C:957:MET:CE	4:C:991:LEU:CD2	2.91	0.43
5:D:303:ASP:HA	5:D:306:ILE:HG12	2.01	0.43
1:A:2108:THR:HG22	1:A:2119:HIS:HE2	1.84	0.43
2:B:1152:HIS:HB2	2:B:1161:LEU:HD13	2.00	0.43
4:C:1060:ILE:HA	4:C:1087:PRO:HA	2.01	0.43
1:A:1600:LEU:HG	1:A:1647:LYS:HE3	2.00	0.43
2:B:1145:LEU:HD22	2:B:1283:VAL:HG21	2.00	0.43
4:C:38:VAL:HA	4:C:41:LEU:HG	2.00	0.43
5:D:332:GLN:HA	5:D:335:LEU:HD13	2.01	0.43
1:A:1972:ASP:OD1	1:A:1972:ASP:N	2.49	0.43
2:B:2100:GLN:NE2	2:B:2146:ALA:O	2.46	0.43
2:B:2170:TRP:HA	2:B:2173:ILE:HD13	2.01	0.43
4:C:1348:CYS:HA	4:C:1351:PHE:HD2	1.84	0.43
1:A:868:PHE:HE2	1:A:930:ASP:HB3	1.82	0.43
2:B:2328:VAL:HA	2:B:2365:LEU:HD13	2.00	0.43
4:C:669:ARG:HD2	4:C:669:ARG:HA	1.82	0.43
5:D:348:ASN:HB3	5:D:352:ILE:HA	2.00	0.43
1:A:1879:TRP:O	1:A:1883:ILE:N	2.52	0.43
1:A:2345:GLU:HA	1:A:2348:LYS:HB3	2.01	0.43
4:C:584:LEU:HD12	4:C:588:LEU:HB2	2.00	0.43
4:C:1094:ARG:NH2	4:C:1396:HIS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:207:VAL:HG23	5:D:212:PRO:HG3	1.99	0.43
1:A:2843:THR:HG23	1:A:2845:ILE:HG23	2.01	0.43
4:C:520:MET:HE2	4:C:547:MET:HE2	2.00	0.43
5:D:283:GLU:OE1	5:D:287:HIS:NE2	2.52	0.43
1:A:2735:PRO:O	1:A:2739:LEU:HG	2.18	0.43
2:B:861:CYS:O	2:B:865:ILE:HD12	2.19	0.43
2:B:1050:GLY:O	2:B:1054:SER:OG	2.37	0.43
4:C:120:VAL:HA	4:C:123:VAL:HG12	2.00	0.43
1:A:90:ALA:HB2	1:A:191:LEU:HB3	2.00	0.42
1:A:677:LEU:HA	1:A:680:VAL:HG22	2.01	0.42
1:A:1317:LYS:NZ	1:A:1321:GLU:OE1	2.47	0.42
1:A:2489:PHE:O	1:A:2493:ARG:NH1	2.41	0.42
1:A:2683:LEU:HA	1:A:2686:GLN:HE21	1.83	0.42
2:B:362:LEU:HB2	2:B:398:ASN:HB2	2.01	0.42
4:C:850:CYS:HA	4:C:853:VAL:HG12	2.00	0.42
5:D:241:PRO:HB2	5:D:264:CYS:HB2	2.01	0.42
5:D:349:ASP:N	5:D:349:ASP:OD1	2.49	0.42
1:A:1357:ARG:HD2	1:A:1454:HIS:HB2	2.00	0.42
1:A:2140:ALA:HB3	1:A:2142:PHE:CE1	2.54	0.42
4:C:1462:LEU:HD13	4:C:1470:PHE:HE1	1.84	0.42
2:B:39:LEU:HD23	2:B:154:SER:HB2	2.01	0.42
2:B:1093:PHE:HB2	2:B:1126:LEU:HD22	2.01	0.42
4:C:281:GLY:N	4:C:1389:GLU:OE1	2.52	0.42
1:A:787:ARG:NH1	1:A:845:THR:O	2.53	0.42
1:A:1984:VAL:HG13	1:A:1992:MET:HB3	2.02	0.42
1:A:2395:ARG:HA	1:A:2395:ARG:HD3	1.82	0.42
2:B:319:ALA:HB2	2:B:340:TYR:HD2	1.84	0.42
4:C:206:HIS:CD2	4:C:226:ASP:OD2	2.72	0.42
4:C:818:LYS:HA	4:C:821:VAL:HG12	2.00	0.42
4:C:1138:VAL:O	4:C:1142:LEU:HG	2.19	0.42
1:A:824:ARG:HD2	1:A:824:ARG:HA	1.88	0.42
1:A:1601:SER:HB2	1:A:1607:ALA:HB2	2.01	0.42
1:A:1903:GLN:HA	1:A:1906:LEU:HB2	2.00	0.42
2:B:308:HIS:HE2	2:B:332:LEU:HB3	1.85	0.42
4:C:1102:GLY:HA2	4:C:1105:MET:HE3	2.01	0.42
4:C:1283:LEU:HA	4:C:1286:VAL:HG12	2.02	0.42
1:A:214:ILE:HD13	1:A:226:VAL:HG21	2.01	0.42
1:A:2088:LYS:HD2	1:A:2088:LYS:HA	1.81	0.42
2:B:1133:GLN:HE22	2:B:1227:LEU:HD22	1.85	0.42
2:B:1360:LEU:HD11	2:B:1405:ILE:HD12	2.01	0.42
2:B:2217:LEU:O	2:B:2257:TYR:OH	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:125:GLN:HA	4:C:128:GLU:HB2	2.01	0.42
4:C:1121:ARG:NH1	4:C:1122:ASP:OD1	2.52	0.42
1:A:1500:LYS:HZ3	1:A:1566:MET:HE1	1.85	0.42
1:A:2160:LEU:HD11	2:B:1110:ARG:HG3	2.01	0.42
2:B:258:LEU:HA	2:B:261:VAL:HG12	2.01	0.42
4:C:436:LYS:HA	4:C:436:LYS:HD3	1.90	0.42
4:C:1005:LYS:HB2	4:C:1005:LYS:HE2	1.81	0.42
4:C:1327:THR:O	4:C:1331:SER:OG	2.38	0.42
4:C:1421:ALA:HA	4:C:1424:LEU:HG	2.02	0.42
5:D:213:THR:HG23	5:D:216:TRP:HB2	2.02	0.42
1:A:51:ARG:O	1:A:57:LYS:N	2.52	0.42
3:E:5:LEU:HD22	3:E:70:LEU:HD22	2.01	0.42
1:A:73:SER:HB3	1:A:76:GLU:HG3	2.00	0.42
2:B:156:PHE:HB3	2:B:196:TYR:CE2	2.55	0.42
2:B:175:PRO:O	2:B:178:MET:HB3	2.20	0.42
2:B:526:LEU:HD23	2:B:526:LEU:HA	1.92	0.42
2:B:685:ALA:HA	2:B:688:TRP:HE3	1.85	0.42
4:C:296:TRP:O	4:C:300:PHE:HB2	2.20	0.42
4:C:1123:VAL:HG22	4:C:1127:ARG:HH21	1.85	0.42
4:C:1204:TYR:HE1	4:C:1263:MET:HB3	1.85	0.42
1:A:125:GLN:O	1:A:129:ASN:ND2	2.46	0.42
2:B:230:ALA:O	2:B:234:THR:OG1	2.38	0.42
2:B:1303:LYS:O	2:B:1307:THR:OG1	2.28	0.42
2:B:2376:GLY:HA3	2:B:2383:ALA:HB2	2.02	0.42
2:B:11:LYS:HD2	2:B:11:LYS:HA	1.92	0.41
2:B:1413:ASP:HB2	2:B:1416:ILE:HD11	2.02	0.41
4:C:560:MET:HB2	4:C:564:LEU:HD23	2.02	0.41
1:A:1309:GLU:HA	1:A:1312:LYS:HD3	2.02	0.41
1:A:1347:GLN:HG2	1:A:1568:LEU:HD22	2.01	0.41
1:A:2731:TRP:HE1	1:A:2808:GLN:HG3	1.84	0.41
2:B:305:HIS:O	2:B:340:TYR:OH	2.33	0.41
2:B:2163:MET:SD	2:B:2163:MET:N	2.93	0.41
4:C:626:LYS:HB3	4:C:626:LYS:HE2	1.86	0.41
4:C:657:LYS:HE3	4:C:657:LYS:HB3	1.84	0.41
4:C:1322:LYS:H	4:C:1322:LYS:HG2	1.56	0.41
2:B:867:CYS:SG	2:B:868:TYR:N	2.94	0.41
4:C:119:TRP:HA	4:C:122:LEU:HD12	2.02	0.41
1:A:217:PRO:HG2	1:A:224:PRO:HB3	2.03	0.41
1:A:870:MET:SD	1:A:870:MET:N	2.88	0.41
1:A:1613:MET:HB3	1:A:1613:MET:HE3	1.63	0.41
1:A:2496:LEU:HD12	1:A:2540:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1401:ALA:O	2:B:1405:ILE:HG12	2.19	0.41
2:B:163:LEU:HD13	2:B:204:MET:HG2	2.03	0.41
4:C:457:LEU:CD1	4:C:481:ARG:NE	2.72	0.41
1:A:85:VAL:HB	1:A:112:LEU:HD11	2.01	0.41
1:A:1920:PHE:O	2:B:1351:TYR:OH	2.36	0.41
1:A:2536:ARG:O	1:A:2540:ILE:HG13	2.20	0.41
1:A:2601:THR:HG22	1:A:2604:ARG:HH21	1.86	0.41
2:B:49:ILE:HG22	2:B:50:LEU:HD12	2.02	0.41
2:B:2513:TRP:HA	2:B:2516:VAL:HG12	2.01	0.41
4:C:323:GLU:OE2	4:C:1451:SER:OG	2.28	0.41
4:C:1318:HIS:CD2	4:C:1321:LEU:N	2.61	0.41
2:B:1123:LEU:HB3	2:B:1158:ILE:HD13	2.02	0.41
2:B:2117:MET:HE2	2:B:2117:MET:HB3	1.97	0.41
4:C:219:TRP:HB2	4:C:1067:VAL:HG21	2.03	0.41
4:C:1327:THR:HG23	4:C:1449:ASN:HB2	2.01	0.41
1:A:1977:MET:HG2	1:A:1983:GLU:HA	2.02	0.41
1:A:2789:SER:HA	1:A:2792:GLN:HG3	2.03	0.41
2:B:568:ARG:HB3	2:B:571:VAL:HG22	2.03	0.41
2:B:2154:ILE:HD12	2:B:2154:ILE:HA	1.94	0.41
2:B:2295:LYS:HE3	2:B:2310:VAL:HG23	2.02	0.41
2:B:2497:ASN:OD1	2:B:2501:PHE:N	2.52	0.41
4:C:279:GLN:O	4:C:1115:LYS:NZ	2.49	0.41
1:A:2086:ILE:HG22	1:A:2144:LEU:HD11	2.01	0.41
1:A:2133:PHE:HA	1:A:2134:PRO:HA	1.75	0.41
2:B:140:LEU:HG	2:B:143:LEU:HD12	2.02	0.41
2:B:688:TRP:HA	2:B:691:VAL:HG22	2.03	0.41
2:B:2047:ASP:OD1	2:B:2047:ASP:N	2.53	0.41
2:B:2204:LEU:HD21	2:B:2216:LEU:HD12	2.02	0.41
2:B:2328:VAL:HG22	2:B:2365:LEU:HD22	2.03	0.41
4:C:35:LYS:HG3	4:C:37:TRP:H	1.86	0.41
4:C:223:ALA:HA	5:D:288:LYS:HB3	2.03	0.41
4:C:851:ARG:HA	4:C:854:VAL:HG12	2.02	0.41
5:D:295:TYR:OH	5:D:340:ARG:O	2.38	0.41
1:A:116:LEU:HA	1:A:119:MET:HE2	2.03	0.41
1:A:2487:GLU:HG2	1:A:2490:ARG:HH21	1.85	0.41
2:B:277:LEU:O	2:B:281:TRP:N	2.53	0.41
2:B:546:GLY:HA2	2:B:549:VAL:HG12	2.03	0.41
4:C:1374:SER:O	4:C:1378:ALA:N	2.54	0.41
1:A:214:ILE:HG23	1:A:215:TRP:HD1	1.86	0.40
1:A:793:LEU:HD13	1:A:831:LEU:HD21	2.04	0.40
1:A:831:LEU:HA	1:A:831:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:GLN:O	1:A:940:GLU:N	2.52	0.40
2:B:577:LEU:HD23	2:B:579:LYS:H	1.85	0.40
1:A:2555:MET:HB3	1:A:2610:PRO:HB2	2.03	0.40
2:B:190:HIS:HD2	2:B:193:ILE:HD12	1.86	0.40
2:B:1367:LEU:HD21	2:B:1402:LEU:HD21	2.02	0.40
2:B:2249:PHE:O	2:B:2255:LYS:NZ	2.54	0.40
5:D:311:TRP:HA	5:D:314:SER:HB3	2.03	0.40
1:A:849:TYR:HA	1:A:852:LYS:HE3	2.04	0.40
1:A:2103:PHE:O	1:A:2107:LEU:HB2	2.22	0.40
1:A:2849:VAL:O	2:B:225:SER:OG	2.29	0.40
4:C:90:MET:HE3	4:C:90:MET:HB2	1.89	0.40
4:C:253:LEU:HD13	4:C:258:LEU:HD21	2.04	0.40
1:A:795:LYS:O	1:A:799:SER:OG	2.31	0.40
1:A:1863:VAL:HG11	2:B:1272:ILE:HG23	2.04	0.40
1:A:2710:MET:HB2	1:A:2710:MET:HE3	1.92	0.40
2:B:1277:VAL:O	2:B:1281:ILE:HG12	2.22	0.40
2:B:2378:HIS:CE1	2:B:2435:PRO:HD2	2.57	0.40
2:B:2409:VAL:HA	2:B:2412:ILE:HG22	2.04	0.40
4:C:1124:ILE:HG21	4:C:1136:ILE:HD13	2.04	0.40
4:C:1172:GLN:NE2	4:C:1549:GLN:HB3	2.37	0.40
5:D:239:SER:OG	5:D:268:TYR:OH	2.36	0.40
1:A:1924:THR:HA	1:A:1927:ILE:HG22	2.03	0.40
1:A:2162:LYS:HE2	1:A:2199:LEU:HD22	2.03	0.40
1:A:2367:LEU:HD13	1:A:2492:PRO:HA	2.04	0.40
4:C:140:GLY:O	4:C:143:ARG:HB2	2.20	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	1739/3258 (53%)	1635 (94%)	104 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1639/2658 (62%)	1527 (93%)	112 (7%)	0	100	100
3	E	118/149 (79%)	111 (94%)	7 (6%)	0	100	100
4	C	1382/1992 (69%)	1311 (95%)	71 (5%)	0	100	100
5	D	178/458 (39%)	162 (91%)	15 (8%)	1 (1%)	21	58
All	All	5056/8515 (59%)	4746 (94%)	309 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	214	PRO

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	1563/2853 (55%)	1558 (100%)	5 (0%)	86	84
2	B	1486/2380 (62%)	1481 (100%)	5 (0%)	86	84
3	E	103/127 (81%)	103 (100%)	0	100	100
4	C	1261/1787 (71%)	1258 (100%)	3 (0%)	87	85
5	D	168/397 (42%)	168 (100%)	0	100	100
All	All	4581/7544 (61%)	4568 (100%)	13 (0%)	84	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1613	MET
1	A	1852	LEU
1	A	2187	MET
1	A	2188	LEU
1	A	2596	ILE
2	B	807	LEU
2	B	1022	GLN

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Mol	Chain	Res	Type
2	B	1311	HIS
2	B	2110	ARG
2	B	2112	LEU
4	C	640	ARG
4	C	826	LEU
4	C	1371	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	223	GLN
1	A	357	GLN
1	A	361	HIS
1	A	695	ASN
1	A	820	HIS
1	A	826	ASN
1	A	829	ASN
1	A	851	ASN
1	A	1270	GLN
1	A	1289	ASN
1	A	1456	ASN
1	A	1481	HIS
1	A	1643	ASN
1	A	1880	ASN
1	A	1923	GLN
1	A	2076	HIS
1	A	2220	HIS
1	A	2808	GLN
2	B	312	HIS
2	B	313	ASN
2	B	398	ASN
2	B	555	GLN
2	B	684	GLN
2	B	713	ASN
2	B	799	ASN
2	B	836	ASN
2	B	869	GLN
2	B	996	HIS
2	B	1006	HIS
2	B	1022	GLN
2	B	1429	ASN

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Mol	Chain	Res	Type
2	B	2140	ASN
2	B	2326	ASN
2	B	2400	GLN
2	B	2425	HIS
2	B	2426	ASN
2	B	2488	GLN
3	E	112	ASN
3	E	138	ASN
4	C	68	GLN
4	C	220	ASN
4	C	256	GLN
4	C	333	GLN
4	C	414	GLN
4	C	934	ASN
4	C	1037	GLN
4	C	1092	ASN
4	C	1172	GLN
4	C	1274	ASN
4	C	1291	HIS
4	C	1318	HIS
4	C	1440	ASN
4	C	1449	ASN
5	D	242	ASN
5	D	269	GLN
5	D	273	HIS
5	D	315	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

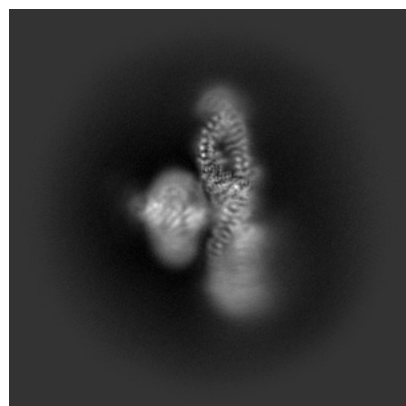
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32544. These allow visual inspection of the internal detail of the map and identification of artifacts.

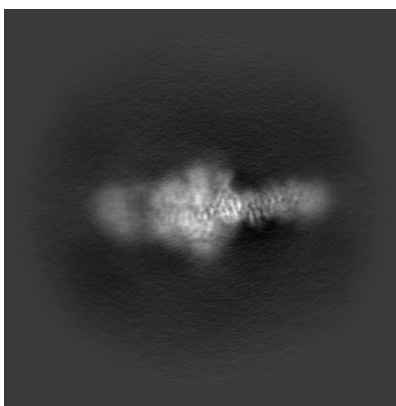
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

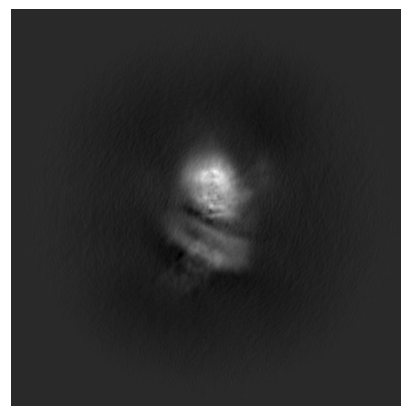
6.1.1 Primary map



X

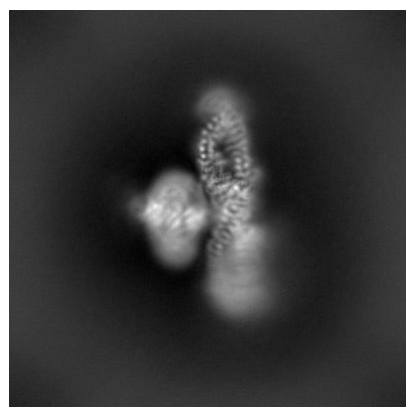


Y

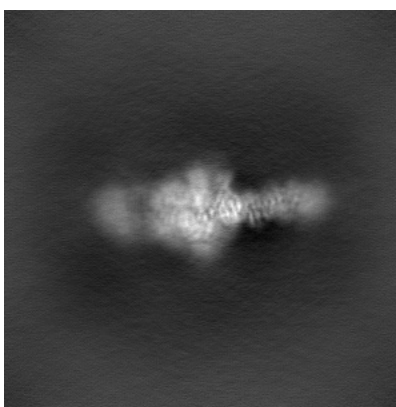


Z

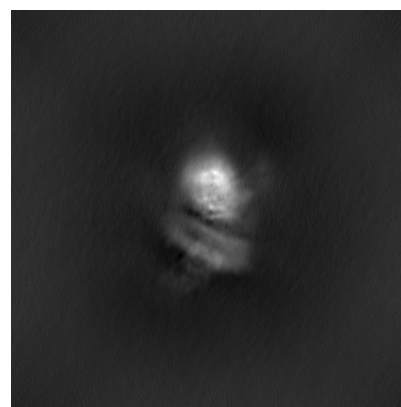
6.1.2 Raw map



X



Y

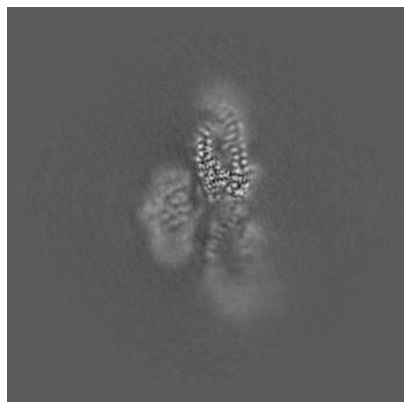


Z

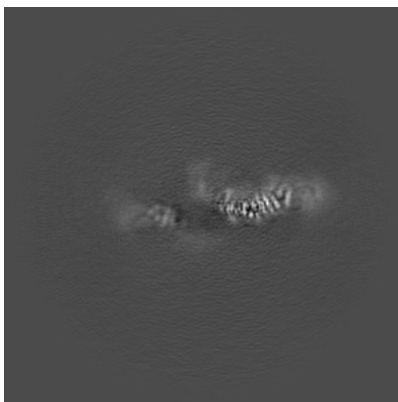
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

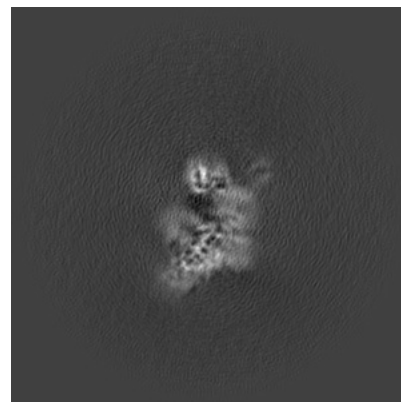
6.2.1 Primary map



X Index: 256

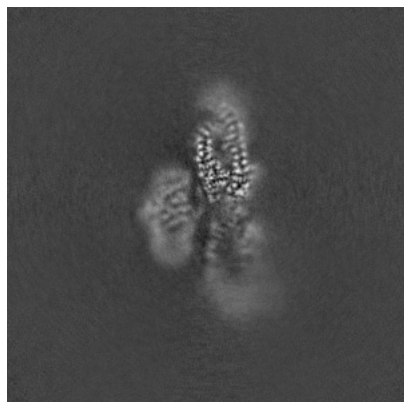


Y Index: 256

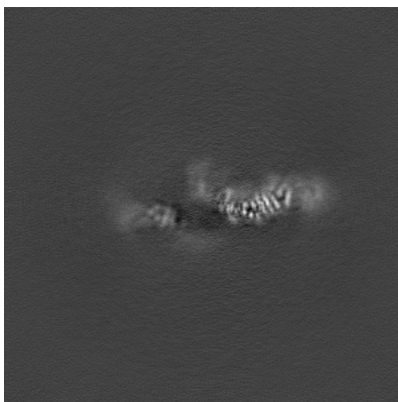


Z Index: 256

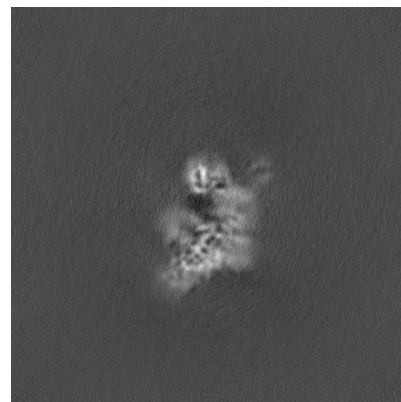
6.2.2 Raw map



X Index: 256



Y Index: 256

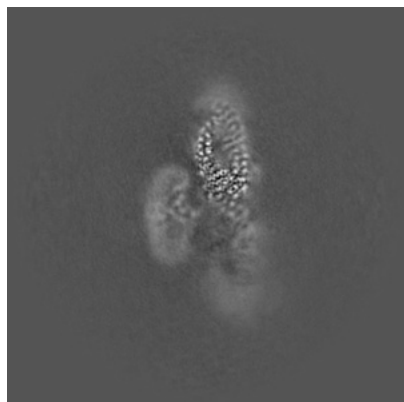


Z Index: 256

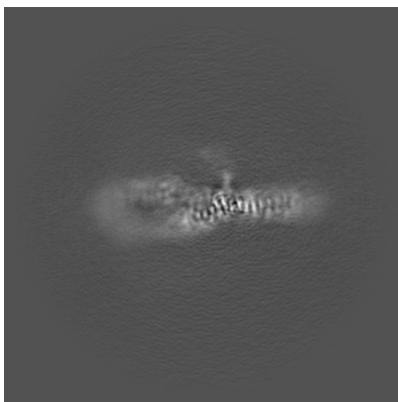
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

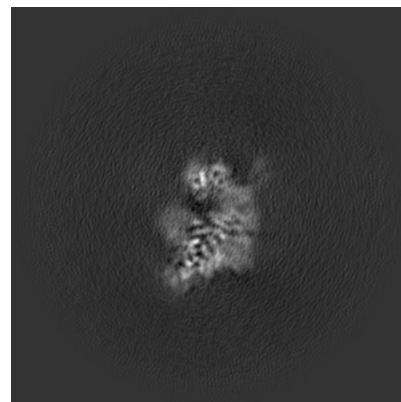
6.3.1 Primary map



X Index: 261

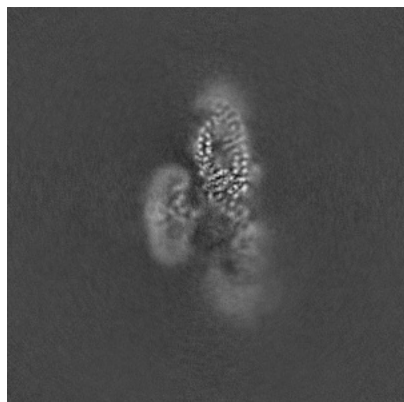


Y Index: 293

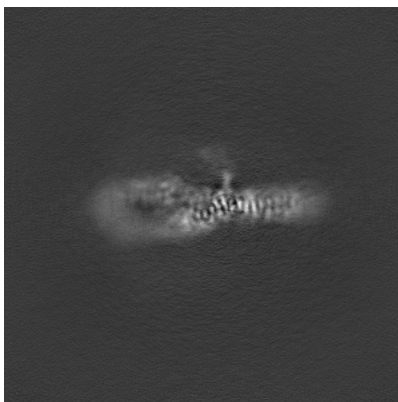


Z Index: 249

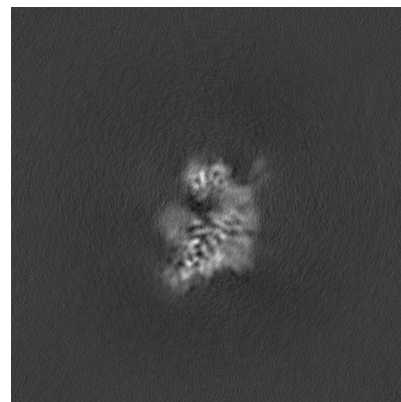
6.3.2 Raw map



X Index: 261



Y Index: 293

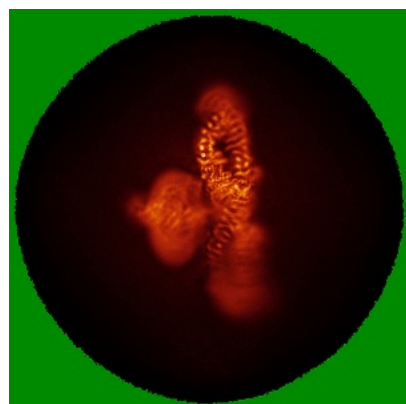


Z Index: 249

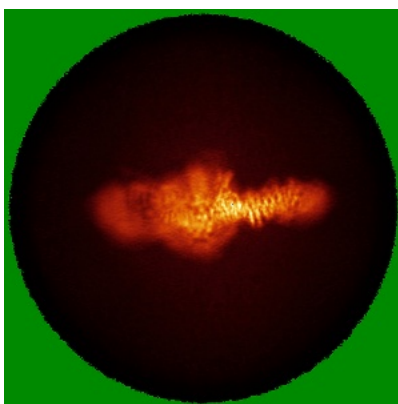
The images above show the largest variance slices of the map in three orthogonal directions.

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

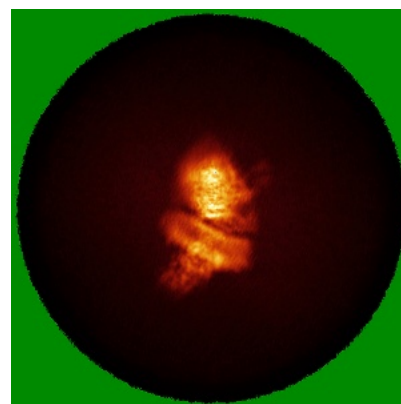
6.4.1 Primary map



X

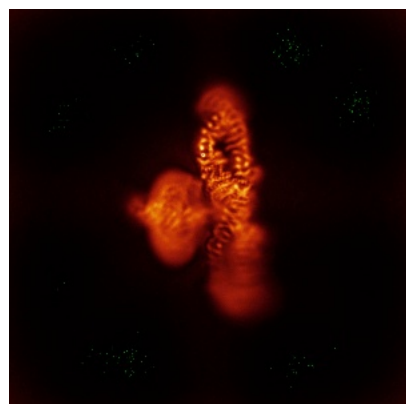


Y

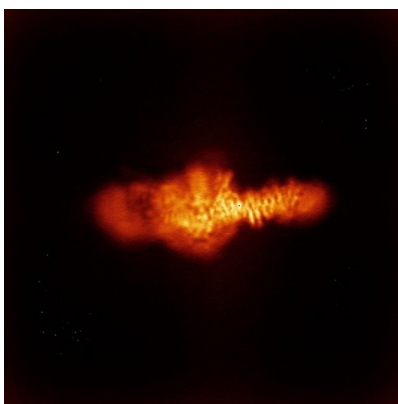


Z

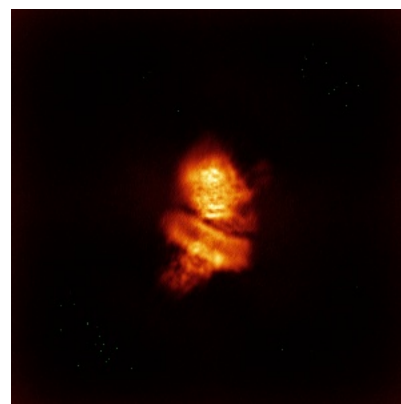
6.4.2 Raw map



X



Y

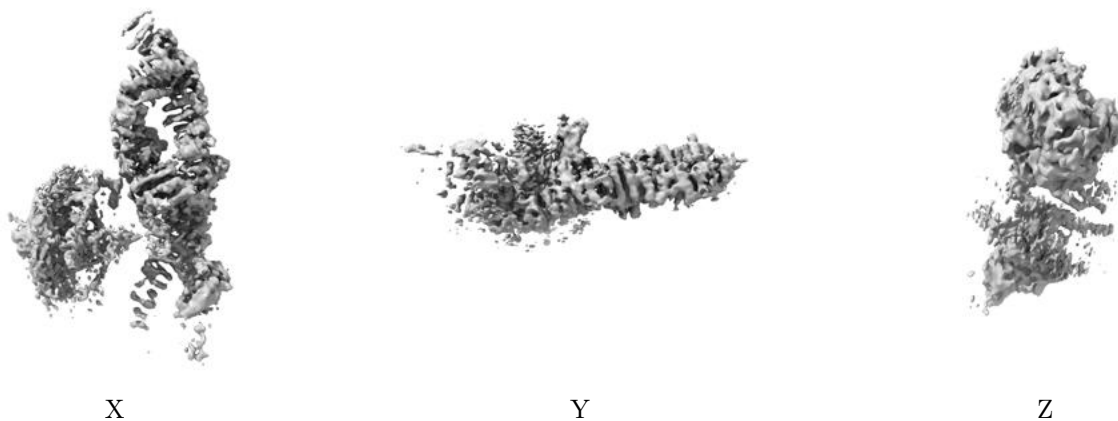


Z

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

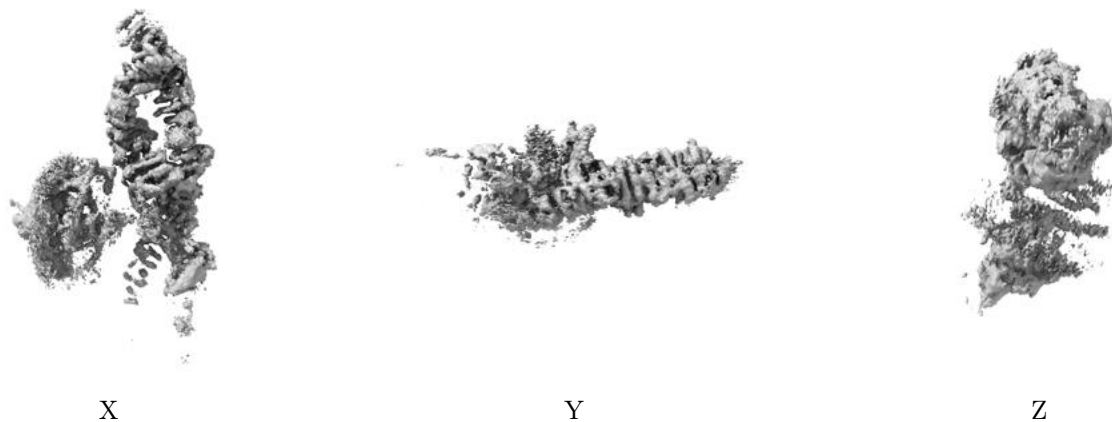
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

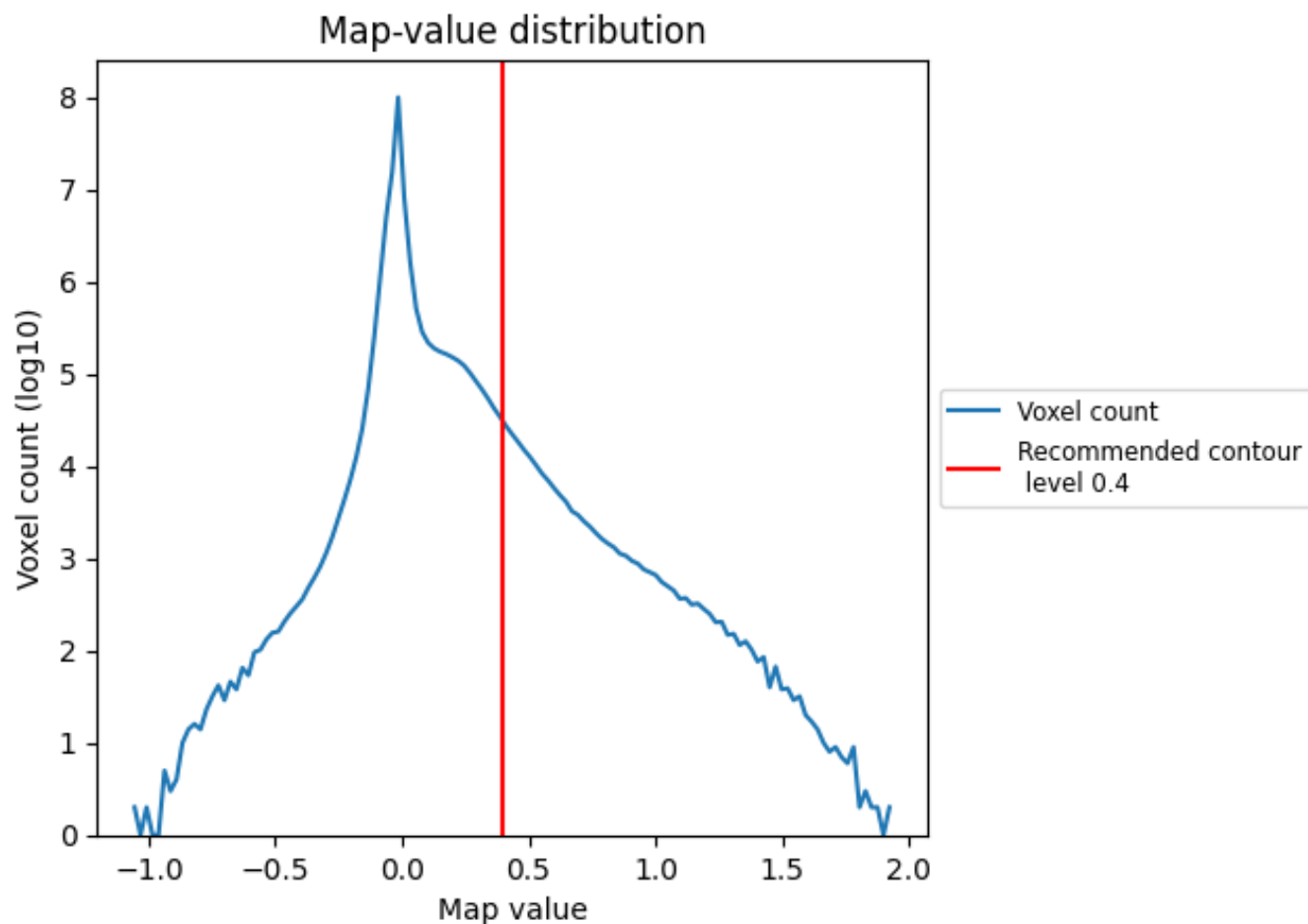
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

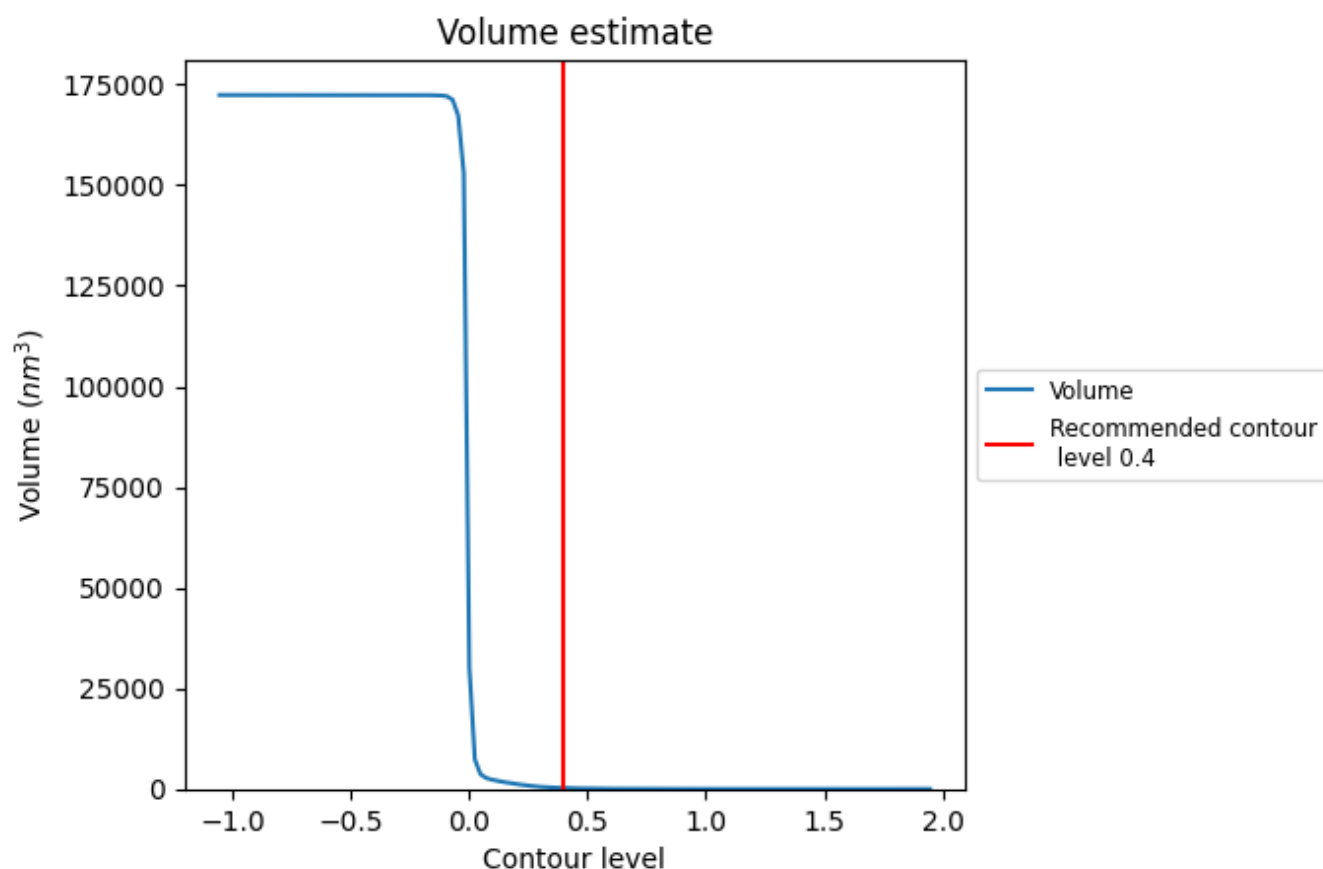
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

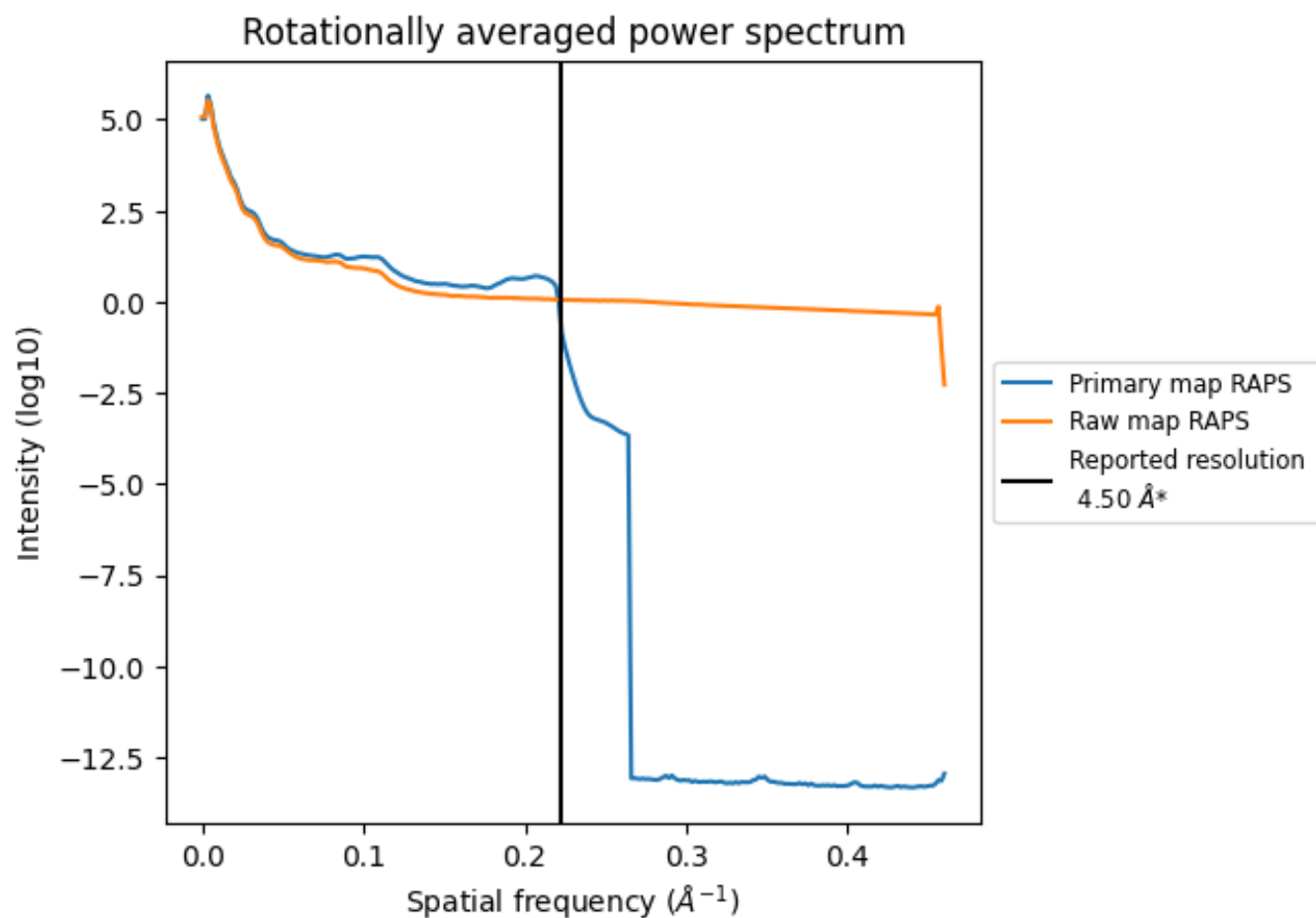
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm^3 ; this corresponds to an approximate mass of 207 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 ⓘ

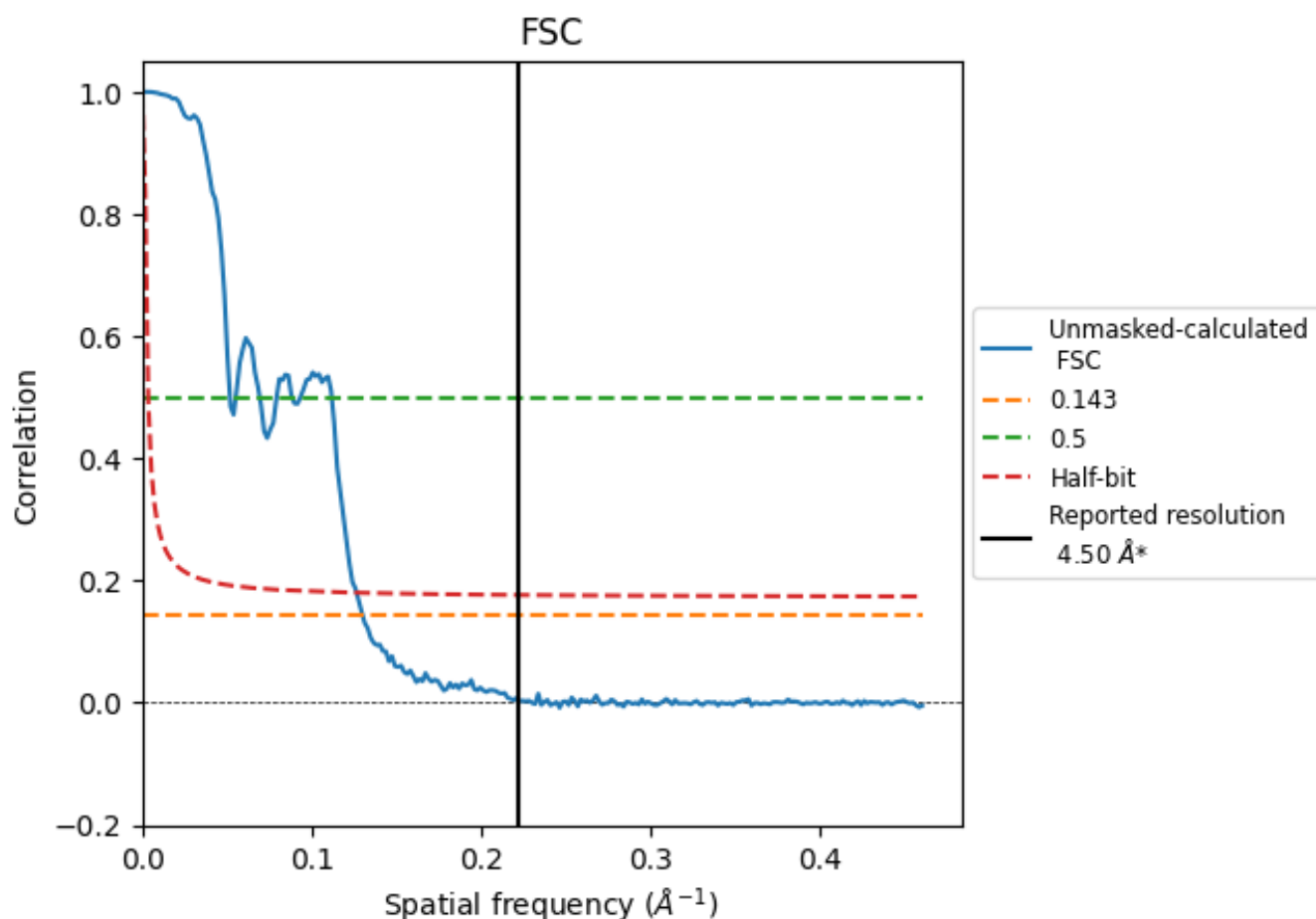


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

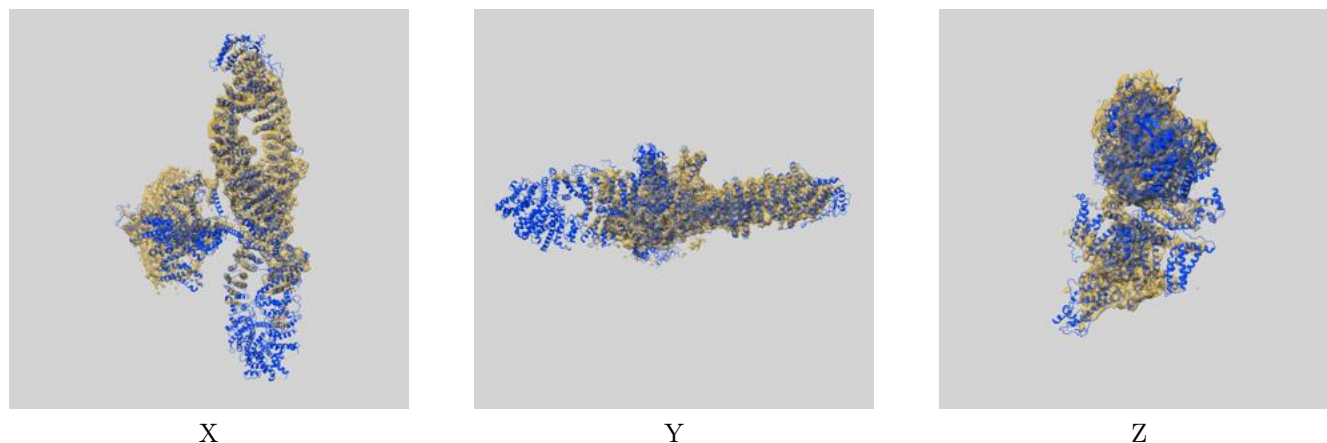
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.70	19.31	7.91

*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 7.70 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

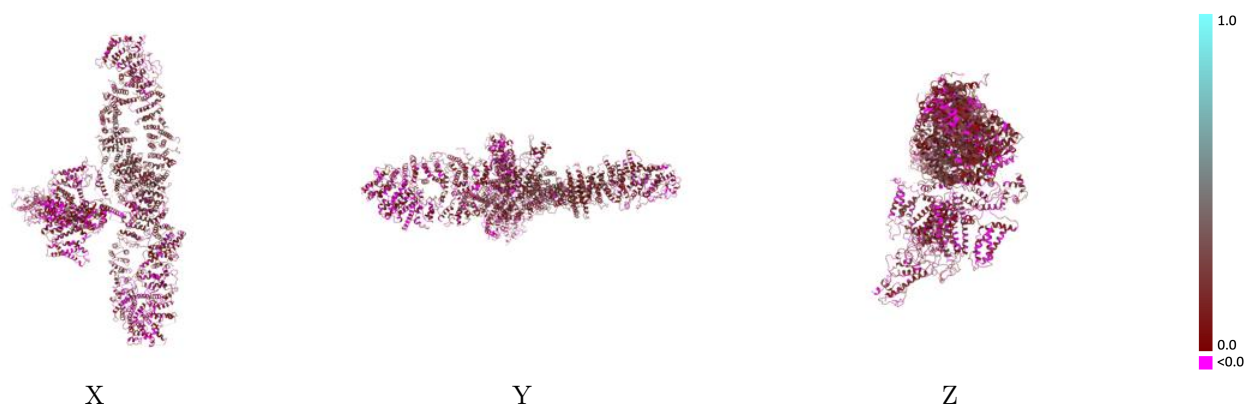
This section contains information regarding the fit between EMDB map EMD-32544 and PDB model 7WJI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



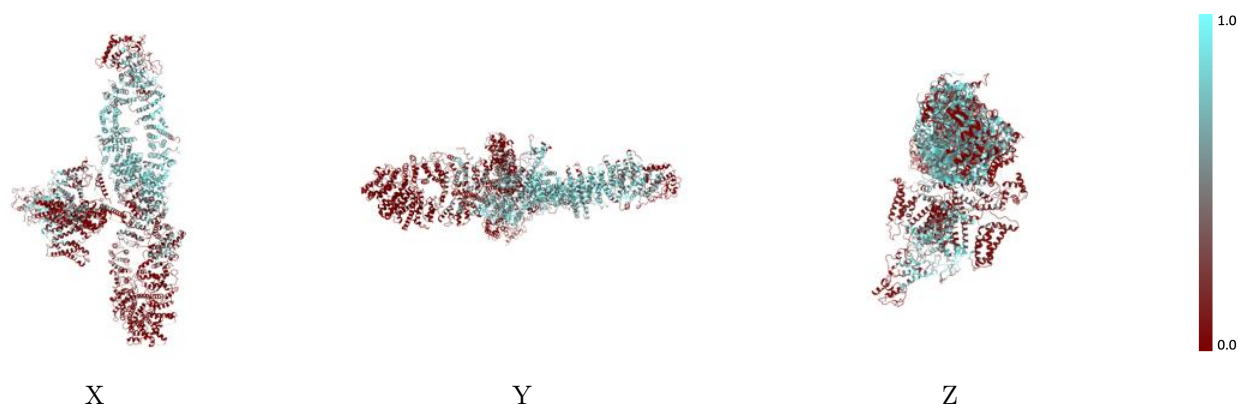
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



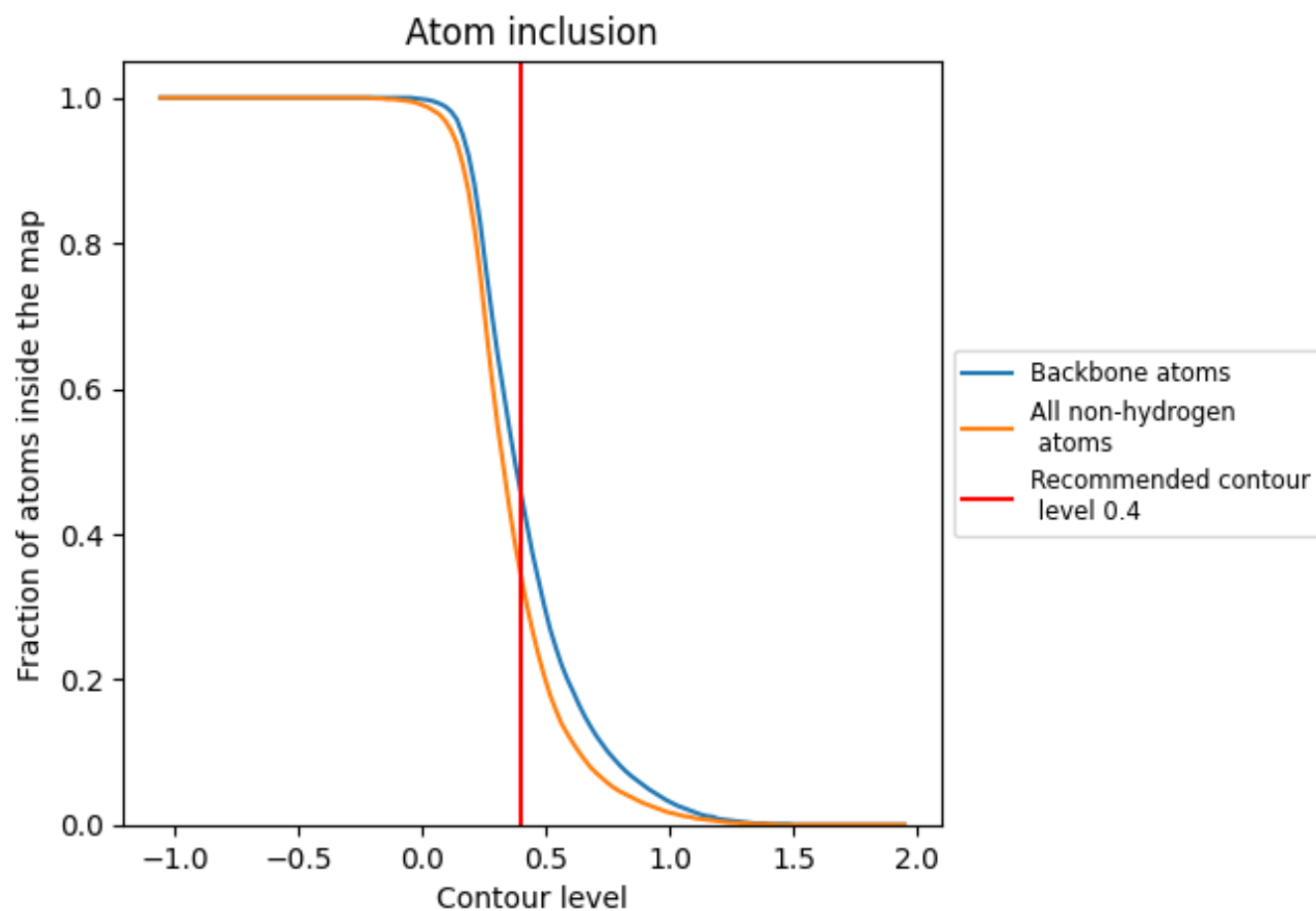
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 34% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3410	0.1390
A	0.3790	0.1700
B	0.3520	0.1440
C	0.3140	0.0990
D	0.2650	0.1070
E	0.0530	0.1160

