Full wwPDB EM Validation Report

May 19, 2025 – 07:39 AM EDT

PDB ID	:	8E20 / pdb_00008e20
EMDB ID	:	EMD-27826
Title	:	Cryo-EM structure of the full-length human NF1 dimer
Authors	:	Darling, J.E.; Merk, A.; Grisshammer, R.; Ognjenovic, J.
Deposited on	:	2022-08-12
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

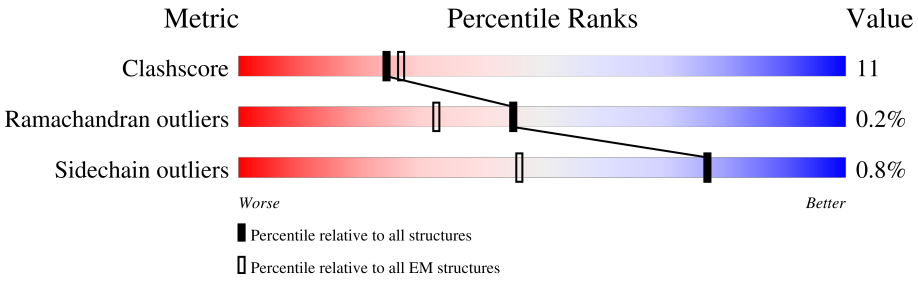
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2818	13% 67% 13% 20%
1	B	2818	13% 66% 13% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 29341 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 Isoform I of Neurofibromin.

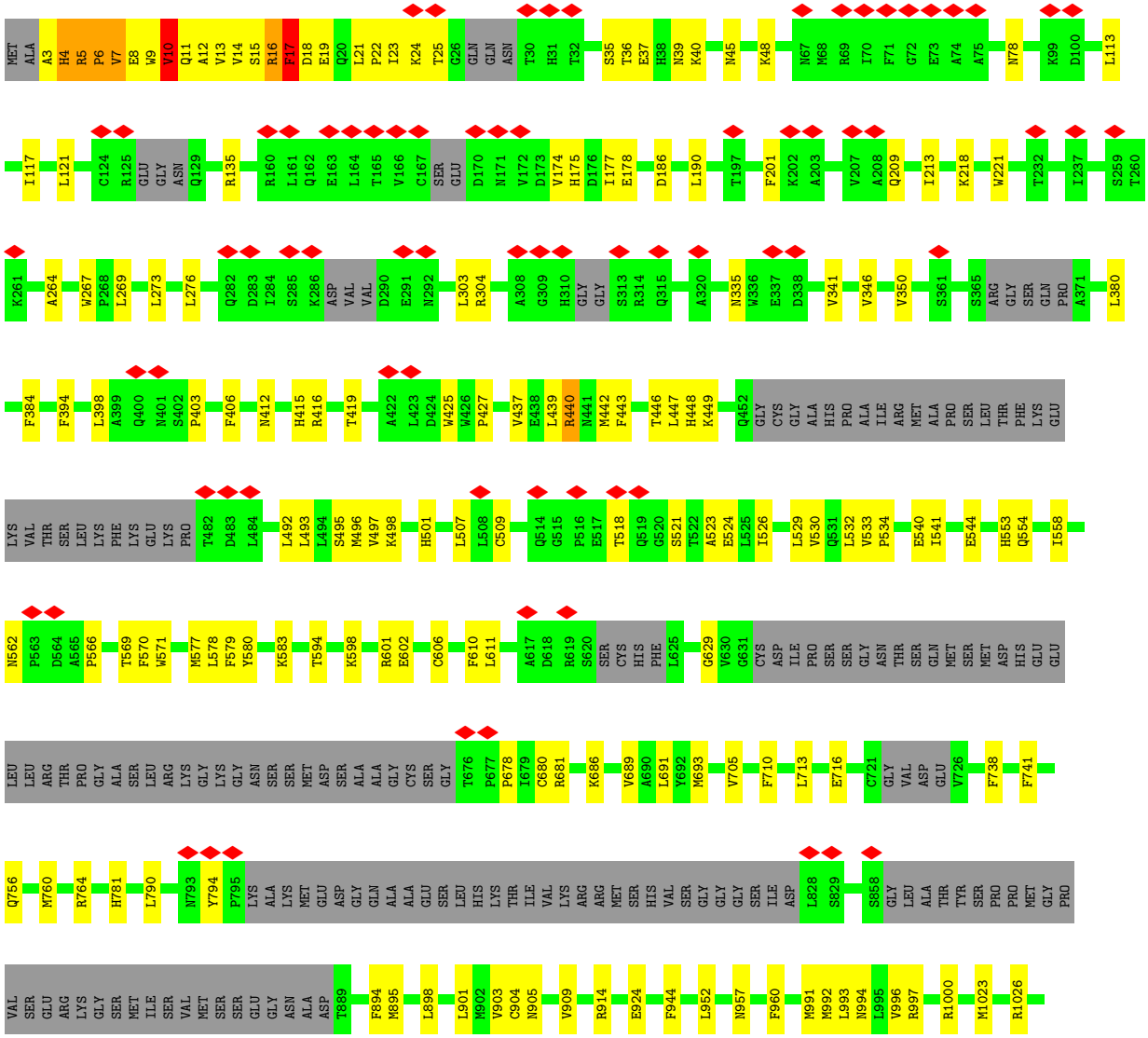
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2260	Total	C	N	O	S	0	0
			14633	9327	2661	2593	52		
1	B	2255	Total	C	N	O	S	0	0
			14708	9372	2661	2621	54		

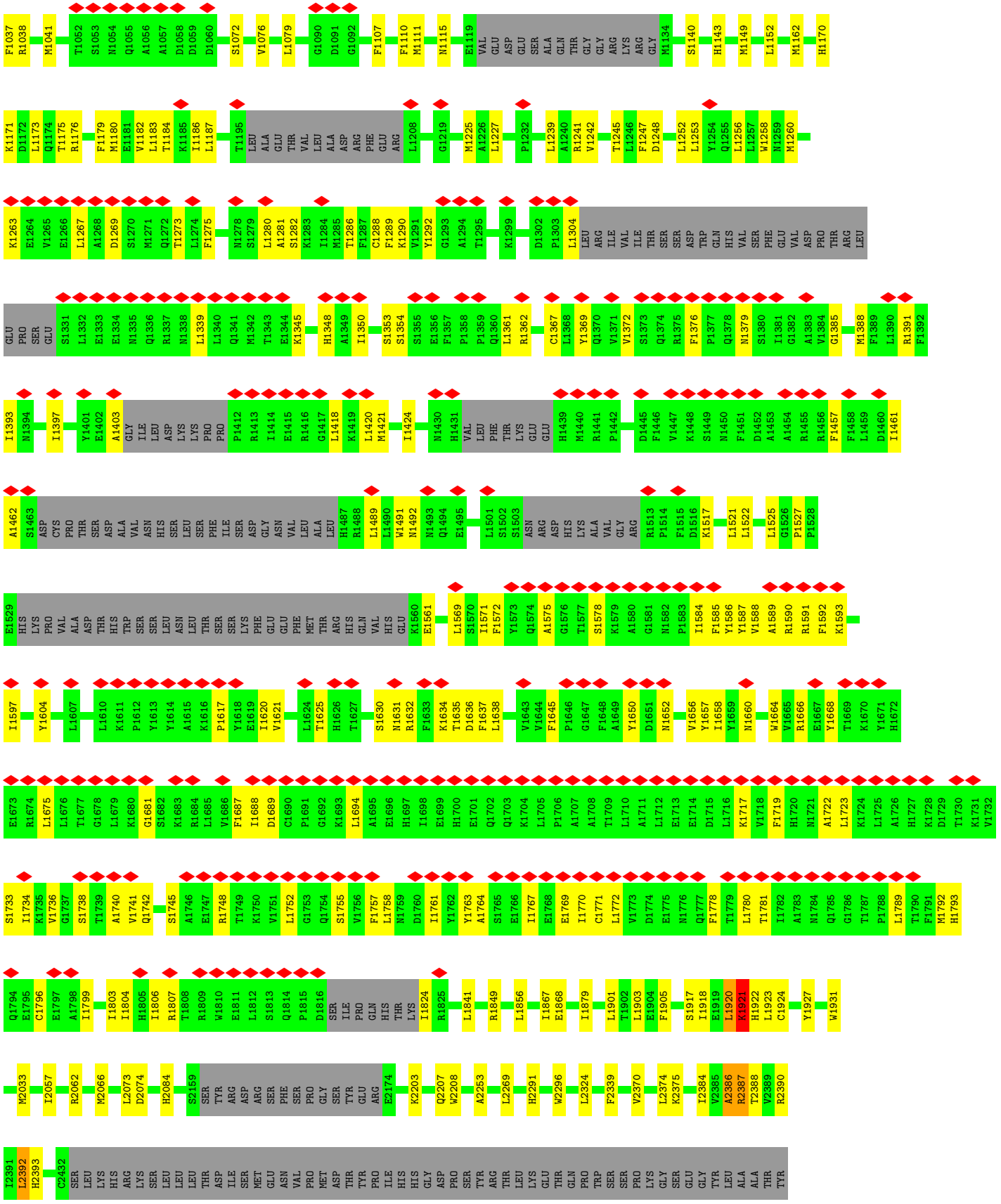
3 Residue-property plots (i)

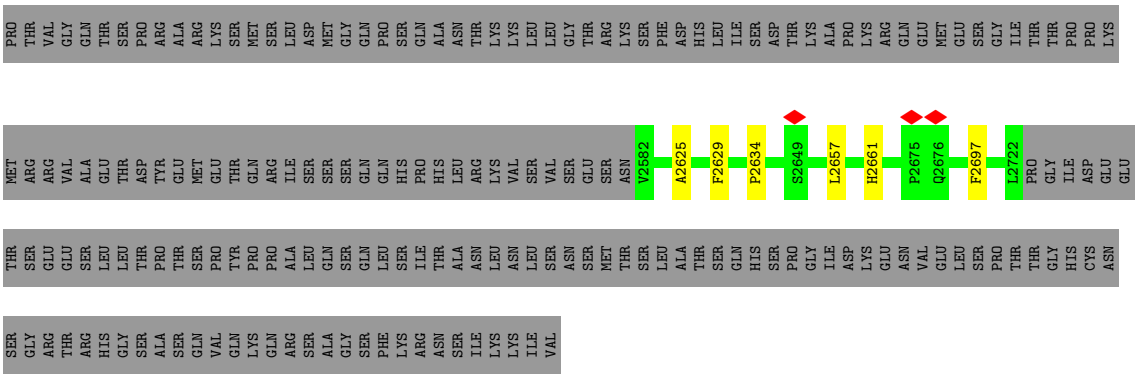
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Isoform I of Neurofibromin

Chain A:

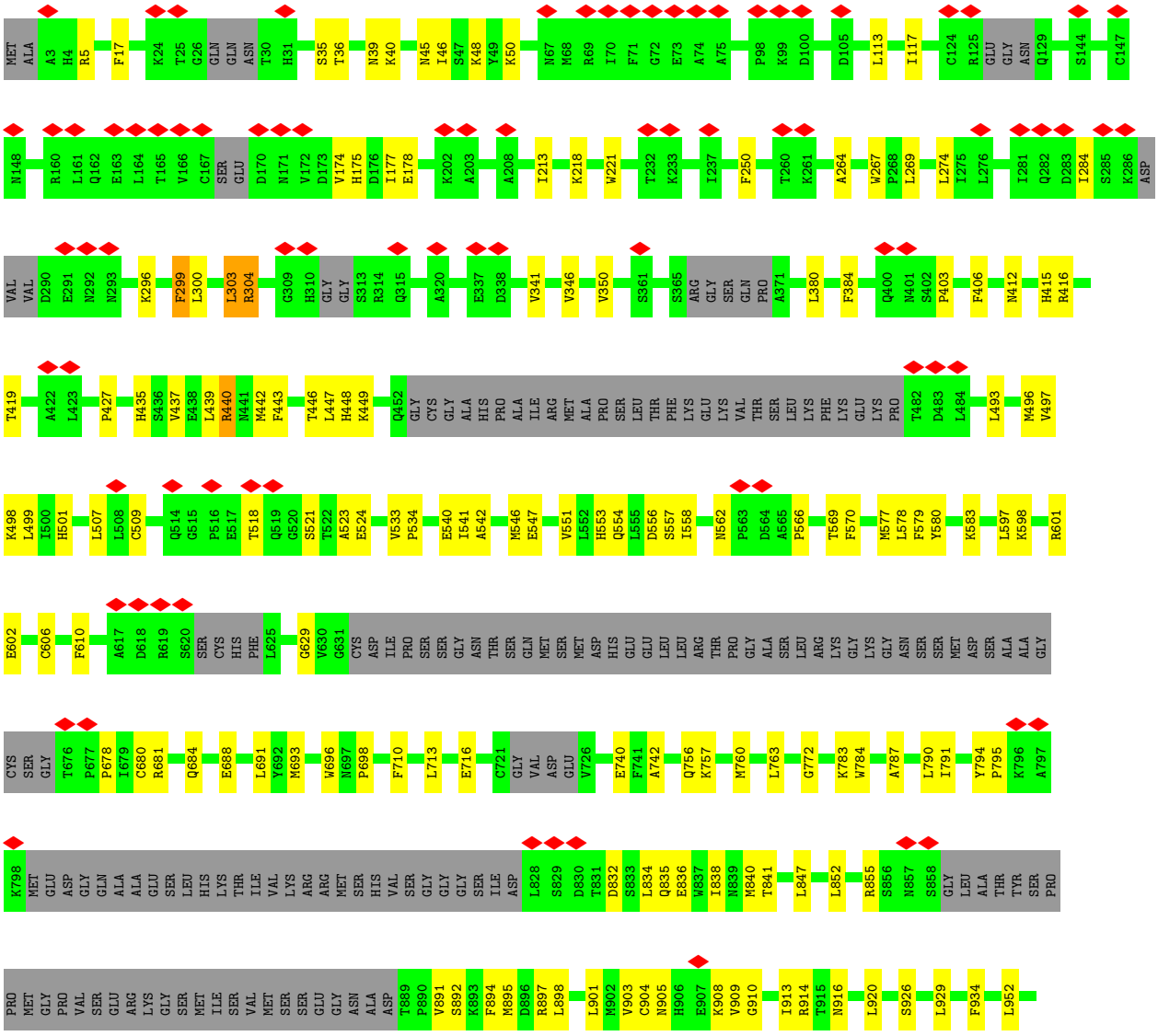


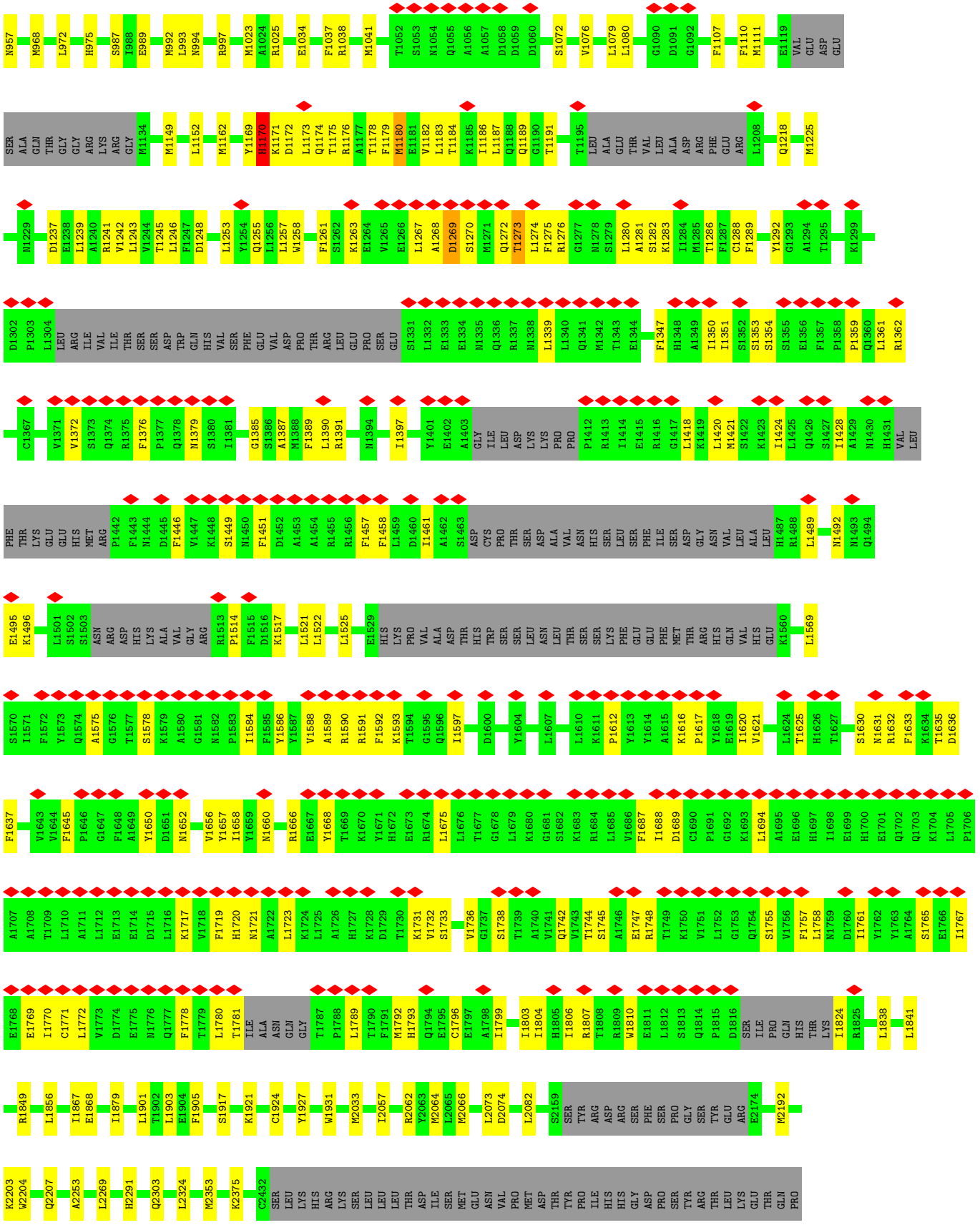


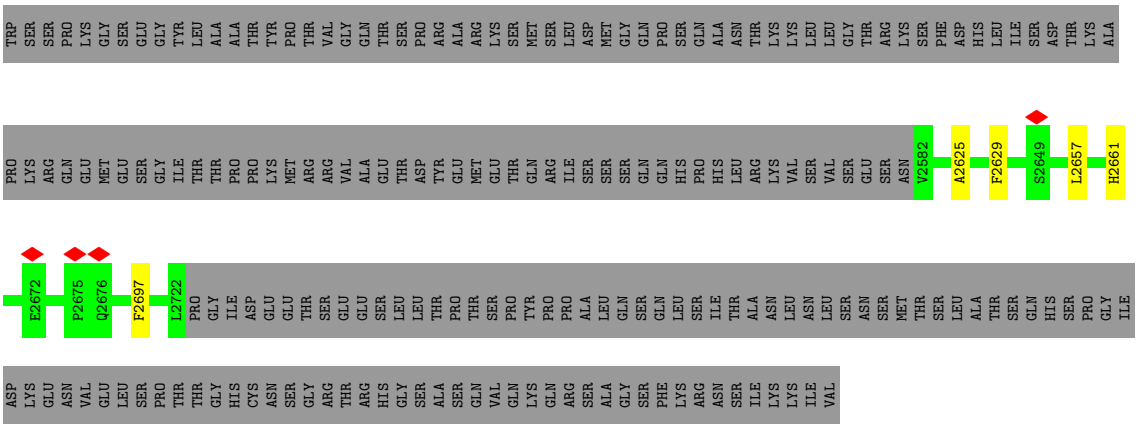


• Molecule 1: Isoform I of Neurofibromin

Chain B:






TRP SER SER PRO LYS GLY SER GLU GLY TYR LEU ALA ALA THR TYR PRO THR VAL GLY GLN THR SER PRO ARG ALA ARG LYS SER MET SER LEU ASP MET GLY GLN PRO SER GLN ALA ASN THR LYS LYS LEU LEU GLY THR ARG LYS SER PHE ASP HIS LEU ILE SER ASP THR LYS ALA
PRO LYS ARG GLN GLU MET GLU SER GLY ILE THR THR PRO PRO LYS MET ARG ARG VAL ALA GLU THR ASP TYR GLU MET GLU THR GLN ARG ILE SER SER SER GLN GLN HIS PRO HIS LEU ARG LYS VAL SER VAL SER GLU SER ASN V2582 A2625 F2629 S2649 L2657 H2661
E2672 P2675 Q2676 F2697 L2722 PRO GLY ILE ASP GLU GLU THR SER GLU GLU SER LEU LEU THR PRO THR SER PRO TYR PRO PRO ALA LEU GLN SER GLN LEU SER ILE THR ALA ASN LEU ASN LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER PRO GLY ILE
ASP LYS GLU ASN VAL GLU LEU SER PRO THR THR GLY HIS CYS ASN SER GLY ARG THR ARG HIS GLY SER ALA SER GLN VAL GLN LYS GLN ARG SER ALA GLY SER PHE LYS ARG ASN SER ILE LYS LYS ILE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	692875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	9.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0133	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/14889	0.54	8/20401 (0.0%)
1	B	0.24	0/14962	0.50	2/20488 (0.0%)
All	All	0.26	0/29851	0.52	10/40889 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1921	LYS	N-CA-C	-8.30	102.17	111.14
1	A	17	PHE	N-CA-C	-7.17	103.47	111.28
1	A	10	VAL	N-CA-C	-7.05	103.65	110.42
1	A	2392	LEU	N-CA-C	-6.11	104.54	111.14
1	A	6	PRO	N-CA-C	-5.95	100.21	112.47
1	A	16	ARG	N-CA-C	-5.43	105.91	112.54
1	A	2386	ALA	CA-C-N	-5.32	113.21	120.44
1	A	2386	ALA	C-N-CA	-5.32	113.21	120.44
1	B	1170	HIS	N-CA-C	5.31	116.85	109.31
1	B	1180	MET	N-CA-C	-5.07	106.35	112.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1170	HIS	Peptide
1	A	304	ARG	Sidechain
1	B	1169	TYR	Peptide
1	B	1170	HIS	Peptide
1	B	304	ARG	Sidechain
1	B	440	ARG	Sidechain
1	B	794	TYR	Peptide

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	14633	0	11225	284	0
1	B	14708	0	11423	259	0
All	All	29341	0	22648	542	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 11.

All (542) 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:B:1273:THR:HB	1:B:1276:ARG:HE	1.19	1.01
1:A:5:ARG:HA	1:A:8:GLU:HB2	1.53	0.87
1:B:1248:ASP:HA	1:B:1253:LEU:HB2	1.56	0.87
1:A:1248:ASP:HA	1:A:1253:LEU:HB2	1.61	0.81
1:B:698:PRO:HB3	1:B:836:GLU:HG2	1.61	0.80
1:A:1183:LEU:HA	1:A:1187:LEU:H	1.50	0.75
1:B:1621:VAL:HG22	1:B:1657:TYR:HB2	1.68	0.73
1:B:975:HIS:CE1	1:B:1025:ARG:NH2	2.57	0.73
1:A:398:LEU:HD23	1:A:442:MET:HE1	1.71	0.73
1:B:1273:THR:HB	1:B:1276:ARG:NE	2.02	0.73
1:B:756:GLN:HG3	1:B:760:MET:HE2	1.71	0.72
1:B:2625:ALA:O	1:B:2629:PHE:N	2.23	0.71
1:A:1258:TRP:CD1	1:A:1367:CYS:HG	2.07	0.71
1:A:1171:LYS:HD3	1:A:1176:ARG:H	1.55	0.71
1:B:784:TRP:HE1	1:B:841:THR:HG22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2625:ALA:O	1:A:2629:PHE:N	2.24	0.71
1:A:1621:VAL:HG22	1:A:1657:TYR:HB2	1.72	0.70
1:B:1171:LYS:HE3	1:B:1173:LEU:HA	1.72	0.70
1:B:1171:LYS:HG3	1:B:1173:LEU:N	2.06	0.70
1:A:1171:LYS:HG3	1:A:1173:LEU:N	2.07	0.70
1:A:5:ARG:HA	1:A:8:GLU:CB	2.21	0.70
1:A:1778:PHE:HD2	1:A:1796:CYS:HB3	1.57	0.69
1:B:972:LEU:O	1:B:1025:ARG:NH2	2.26	0.69
1:A:4:HIS:O	1:A:7:VAL:N	2.25	0.69
1:B:1780:LEU:HB2	1:B:1789:LEU:HB2	1.75	0.68
1:A:1247:PHE:HD2	1:A:1256:LEU:HD13	1.58	0.68
1:B:440:ARG:HA	1:B:443:PHE:CE2	2.28	0.68
1:B:1742:GLN:HG2	1:B:1761:ILE:HG12	1.75	0.68
1:A:1239:LEU:HD22	1:A:1280:LEU:HD21	1.76	0.67
1:B:1592:PHE:HE1	1:B:1597:ILE:HB	1.59	0.67
1:A:1180:MET:HA	1:A:1183:LEU:HB2	1.75	0.67
1:A:1769:GLU:HB2	1:A:1781:THR:HB	1.76	0.67
1:A:1385:GLY:HA2	1:A:1388:MET:HE2	1.74	0.67
1:B:412:ASN:HB3	1:B:416:ARG:HH12	1.58	0.67
1:A:952:LEU:O	1:A:957:ASN:ND2	2.28	0.67
1:B:975:HIS:HE1	1:B:1025:ARG:NH2	1.92	0.66
1:A:12:ALA:O	1:A:16:ARG:N	2.27	0.66
1:A:23:ILE:HA	1:A:78:ASN:CB	2.26	0.66
1:B:579:PHE:O	1:B:583:LYS:HG2	1.96	0.66
1:B:1635:THR:HG23	1:B:1675:LEU:HD11	1.76	0.66
1:B:1778:PHE:HD2	1:B:1796:CYS:HB3	1.61	0.66
1:A:579:PHE:O	1:A:583:LYS:HG2	1.96	0.66
1:A:1569:LEU:O	1:A:1591:ARG:NH1	2.29	0.65
1:B:439:LEU:HA	1:B:442:MET:HE2	1.78	0.65
1:B:443:PHE:HB3	1:B:496:MET:HE1	1.78	0.65
1:B:1359:PRO:HA	1:B:1362:ARG:HB2	1.78	0.65
1:A:5:ARG:HB2	1:A:9:TRP:CZ2	2.32	0.65
1:B:992:MET:HE3	1:B:992:MET:O	1.96	0.65
1:B:2303:GLN:NE2	1:B:2353:MET:SD	2.67	0.64
1:B:1180:MET:HA	1:B:1183:LEU:HG	1.78	0.64
1:B:1339:LEU:HD21	1:B:1420:LEU:HD22	1.78	0.64
1:A:1592:PHE:HE1	1:A:1597:ILE:HB	1.62	0.64
1:B:835:GLN:HA	1:B:838:ILE:HD12	1.79	0.64
1:A:1917:SER:O	1:A:1918:ILE:C	2.40	0.64
1:B:542:ALA:O	1:B:546:MET:HG2	1.97	0.63
1:A:4:HIS:CE1	1:A:6:PRO:HB2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:GLY:HA2	1:B:913:ILE:HD12	1.79	0.63
1:A:1241:ARG:HH11	1:A:1242:VAL:HG12	1.64	0.63
1:B:1242:VAL:HA	1:B:1245:THR:HG22	1.81	0.62
1:B:213:ILE:HG12	1:B:269:LEU:HD22	1.80	0.62
1:B:1362:ARG:HG2	1:B:1461:ILE:HG23	1.81	0.62
1:B:852:LEU:HD12	1:B:929:LEU:HD23	1.82	0.61
1:B:1489:LEU:HA	1:B:1492:ASN:HB2	1.81	0.61
1:B:1569:LEU:O	1:B:1591:ARG:NH1	2.34	0.61
1:A:448:HIS:CE1	1:A:493:LEU:HD11	2.35	0.61
1:A:738:PHE:HA	1:A:741:PHE:HD2	1.64	0.61
1:A:2392:LEU:O	1:A:2393:HIS:C	2.42	0.61
1:B:562:ASN:HB3	1:B:566:PRO:HA	1.83	0.61
1:A:5:ARG:O	1:A:6:PRO:C	2.44	0.61
1:A:534:PRO:HG2	1:A:580:TYR:HE1	1.66	0.61
1:A:1489:LEU:HA	1:A:1492:ASN:HB2	1.83	0.60
1:B:905:ASN:OD1	1:B:914:ARG:NH2	2.34	0.60
1:A:1171:LYS:HE3	1:A:1173:LEU:HA	1.83	0.60
1:A:1227:LEU:HB3	1:A:1239:LEU:HD11	1.83	0.60
1:A:14:VAL:O	1:A:17:PHE:HB2	2.01	0.60
1:A:213:ILE:HG12	1:A:269:LEU:HD22	1.82	0.60
1:A:1183:LEU:HD22	1:A:1187:LEU:HB2	1.82	0.60
1:A:201:PHE:O	1:A:209:GLN:NE2	2.31	0.60
1:B:1748:ARG:HB3	1:B:1755:SER:HB3	1.84	0.59
1:B:993:LEU:HG	1:B:997:ARG:HE	1.66	0.59
1:B:1589:ALA:O	1:B:1631:ASN:ND2	2.35	0.59
1:A:905:ASN:OD1	1:A:914:ARG:NH2	2.35	0.59
1:B:284:ILE:HG21	1:B:300:LEU:HD12	1.85	0.59
1:B:412:ASN:HB3	1:B:416:ARG:NH1	2.18	0.59
1:A:1263:LYS:HE3	1:A:1281:ALA:HB2	1.84	0.59
1:B:113:LEU:O	1:B:117:ILE:N	2.36	0.59
1:A:439:LEU:HA	1:A:442:MET:HE2	1.85	0.59
1:B:17:PHE:CZ	1:B:40:LYS:HA	2.38	0.59
1:B:629:GLY:HA3	1:B:680:CYS:HB3	1.85	0.59
1:A:446:THR:O	1:A:449:LYS:HG2	2.03	0.58
1:B:934:PHE:HE1	1:B:968:MET:HE1	1.69	0.58
1:B:1625:THR:HG22	1:B:1660:ASN:HD22	1.68	0.58
1:A:756:GLN:O	1:A:760:MET:HG3	2.04	0.58
1:A:1635:THR:HG23	1:A:1675:LEU:HD11	1.83	0.58
1:B:952:LEU:O	1:B:957:ASN:ND2	2.36	0.58
1:A:4:HIS:C	1:A:6:PRO:HD2	2.29	0.58
1:A:1748:ARG:HB3	1:A:1755:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:117:ILE:N	2.36	0.58
1:A:9:TRP:O	1:A:12:ALA:HB3	2.03	0.57
1:A:1171:LYS:HB3	1:A:1175:THR:OG1	2.03	0.57
1:B:446:THR:O	1:B:449:LYS:HG2	2.04	0.57
1:A:1905:PHE:HE2	1:A:1931:TRP:CD1	2.23	0.57
1:A:273:LEU:HA	1:A:276:LEU:HD12	1.86	0.57
1:A:1038:ARG:NH2	1:A:1079:LEU:O	2.37	0.57
1:B:1182:VAL:O	1:B:1186:ILE:N	2.38	0.57
1:A:562:ASN:HB3	1:A:566:PRO:HA	1.85	0.57
1:B:855:ARG:HH22	1:B:892:SER:H	1.52	0.57
1:B:1179:PHE:CE2	1:B:1183:LEU:HD21	2.40	0.57
1:A:1571:ILE:HG12	1:A:1591:ARG:HB2	1.86	0.56
1:A:895:MET:HA	1:A:898:LEU:HB2	1.86	0.56
1:A:1180:MET:HG2	1:A:1183:LEU:HD12	1.88	0.56
1:A:1522:LEU:HA	1:A:1525:LEU:HB2	1.86	0.56
1:B:1171:LYS:HB3	1:B:1175:THR:OG1	2.04	0.56
1:B:2291:HIS:HB3	1:B:2324:LEU:HD21	1.87	0.56
1:B:1905:PHE:HE2	1:B:1931:TRP:CD1	2.23	0.56
1:A:1666:ARG:HD3	1:A:1758:LEU:HD21	1.87	0.56
1:A:2384:ILE:O	1:A:2387:ARG:HG2	2.06	0.56
1:A:1183:LEU:HD13	1:A:1187:LEU:HD23	1.86	0.56
1:A:2657:LEU:O	1:A:2661:HIS:ND1	2.25	0.56
1:B:1372:VAL:HG13	1:B:1376:PHE:HD2	1.70	0.56
1:B:1272:GLN:C	1:B:1274:LEU:H	2.12	0.56
1:A:3:ALA:O	1:A:4:HIS:C	2.47	0.56
1:A:2291:HIS:HB3	1:A:2324:LEU:HD21	1.88	0.56
1:A:415:HIS:O	1:A:419:THR:N	2.39	0.56
1:A:1354:SER:HB3	1:A:1457:PHE:CD1	2.41	0.55
1:A:1362:ARG:HG2	1:A:1461:ILE:HG23	1.88	0.55
1:B:1660:ASN:HD21	1:B:1761:ILE:HD11	1.71	0.55
1:B:1849:ARG:NH1	1:B:1879:ILE:O	2.39	0.55
1:B:174:VAL:O	1:B:178:GLU:N	2.40	0.55
1:A:629:GLY:HA3	1:A:680:CYS:HB3	1.88	0.55
1:A:781:HIS:HE1	1:A:894:PHE:CD1	2.24	0.55
1:B:916:ASN:O	1:B:920:LEU:HG	2.07	0.55
1:A:1242:VAL:HA	1:A:1245:THR:HG22	1.89	0.55
1:A:1632:ARG:HB3	1:A:1664:TRP:HZ2	1.72	0.55
1:A:1849:ARG:NH1	1:A:1879:ILE:O	2.39	0.55
1:B:757:LYS:HA	1:B:760:MET:HE3	1.89	0.55
1:A:1799:ILE:O	1:A:1803:ILE:HG13	2.07	0.54
1:B:895:MET:HA	1:B:898:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1183:LEU:HD22	1:B:1187:LEU:HB2	1.88	0.54
1:A:895:MET:HA	1:A:898:LEU:HD12	1.89	0.54
1:A:13:VAL:HA	1:A:16:ARG:CB	2.38	0.54
1:A:598:LYS:HA	1:A:601:ARG:HD3	1.87	0.54
1:B:1171:LYS:CB	1:B:1175:THR:H	2.20	0.54
1:B:1179:PHE:CZ	1:B:1183:LEU:HD21	2.42	0.54
1:B:1522:LEU:HA	1:B:1525:LEU:HB2	1.87	0.54
1:B:1283:LYS:HA	1:B:1286:THR:HG22	1.90	0.54
1:B:1269:ASP:C	1:B:1273:THR:HG1	2.15	0.54
1:B:2657:LEU:O	1:B:2661:HIS:ND1	2.26	0.54
1:B:1183:LEU:HA	1:B:1187:LEU:H	1.72	0.54
1:A:1171:LYS:CB	1:A:1175:THR:H	2.21	0.54
1:A:691:LEU:HB3	1:A:710:PHE:CE1	2.43	0.53
1:A:1572:PHE:HD1	1:A:1587:TYR:HD2	1.56	0.53
1:A:1742:GLN:HG2	1:A:1761:ILE:HG12	1.90	0.53
1:B:1218:GLN:NE2	1:B:1514:PRO:HB3	2.23	0.53
1:A:598:LYS:O	1:A:602:GLU:HG2	2.07	0.53
1:B:437:VAL:O	1:B:440:ARG:HG2	2.08	0.53
1:B:554:GLN:O	1:B:558:ILE:HG12	2.07	0.53
1:B:1255:GLN:O	1:B:1258:TRP:HD1	1.91	0.53
1:B:901:LEU:HA	1:B:904:CYS:SG	2.48	0.53
1:B:975:HIS:HE1	1:B:1025:ARG:HH21	1.56	0.53
1:B:1799:ILE:O	1:B:1803:ILE:HG13	2.09	0.53
1:A:764:ARG:NH2	1:A:924:GLU:HA	2.23	0.53
1:A:1354:SER:HB3	1:A:1457:PHE:HD1	1.74	0.53
1:B:598:LYS:O	1:B:602:GLU:HG2	2.09	0.53
1:A:21:LEU:O	1:A:22:PRO:C	2.50	0.53
1:B:1397:ILE:HG22	1:B:1418:LEU:HB3	1.90	0.53
1:B:1688:ILE:HG13	1:B:1694:LEU:HB2	1.91	0.53
1:B:787:ALA:HA	1:B:790:LEU:HB2	1.89	0.53
1:B:553:HIS:HD2	1:B:606:CYS:HB2	1.74	0.53
1:A:1767:ILE:HG22	1:A:1770:ILE:HD11	1.90	0.52
1:A:1585:PHE:HB2	1:A:1620:ILE:HD12	1.92	0.52
1:B:1239:LEU:HD22	1:B:1280:LEU:HD21	1.91	0.52
1:A:446:THR:HG21	1:A:496:MET:HE1	1.91	0.52
1:A:1372:VAL:HG13	1:A:1376:PHE:HD2	1.75	0.52
1:B:1171:LYS:HB2	1:B:1175:THR:H	1.72	0.52
1:B:1767:ILE:HG22	1:B:1770:ILE:HD11	1.92	0.52
1:A:764:ARG:HH21	1:A:924:GLU:HA	1.75	0.52
1:A:394:PHE:O	1:A:398:LEU:HD12	2.09	0.52
1:A:1286:THR:O	1:A:1391:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1617:PRO:HA	1:A:1652:ASN:HB3	1.92	0.52
1:A:1917:SER:O	1:A:1920:LEU:N	2.42	0.52
1:B:903:VAL:O	1:B:914:ARG:NH2	2.31	0.52
1:B:1149:MET:HA	1:B:1152:LEU:HD13	1.92	0.52
1:B:2192:MET:CE	1:B:2204:TRP:HB3	2.40	0.52
1:A:1339:LEU:HD21	1:A:1420:LEU:HD22	1.92	0.52
1:B:1867:ILE:O	1:B:1868:GLU:HB2	2.10	0.52
1:A:7:VAL:HG12	1:A:8:GLU:N	2.25	0.52
1:A:554:GLN:O	1:A:558:ILE:HG12	2.10	0.52
1:A:1149:MET:HA	1:A:1152:LEU:HD13	1.91	0.52
1:A:37:GLU:HA	1:A:40:LYS:HG2	1.91	0.51
1:A:1180:MET:HA	1:A:1183:LEU:CB	2.41	0.51
1:B:1658:ILE:HG13	1:B:1687:PHE:HA	1.90	0.51
1:B:993:LEU:HD13	1:B:1041:MET:HE2	1.91	0.51
1:A:5:ARG:HD3	1:A:9:TRP:CZ2	2.46	0.51
1:A:1225:MET:HE2	1:A:1225:MET:N	2.26	0.51
1:B:1241:ARG:HH11	1:B:1242:VAL:HG12	1.75	0.51
1:A:5:ARG:HB2	1:A:9:TRP:CE2	2.46	0.51
1:A:1660:ASN:HD21	1:A:1761:ILE:HD11	1.74	0.51
1:B:534:PRO:HG2	1:B:580:TYR:HE1	1.76	0.51
1:B:1288:CYS:SG	1:B:1289:PHE:N	2.84	0.51
1:B:2062:ARG:O	1:B:2066:MET:HG2	2.10	0.51
1:B:2657:LEU:C	1:B:2661:HIS:HD1	2.18	0.51
1:A:437:VAL:HA	1:A:440:ARG:NH1	2.25	0.51
1:A:1517:LYS:HE3	1:A:1521:LEU:HD21	1.93	0.51
1:B:1917:SER:O	1:B:1921:LYS:N	2.40	0.51
1:A:2386:ALA:O	1:A:2390:ARG:HG3	2.10	0.50
1:B:791:ILE:O	1:B:795:PRO:HD3	2.10	0.50
1:A:5:ARG:HA	1:A:8:GLU:CG	2.40	0.50
1:A:2062:ARG:O	1:A:2066:MET:HG2	2.10	0.50
1:B:35:SER:O	1:B:39:ASN:N	2.43	0.50
1:A:36:THR:O	1:A:40:LYS:N	2.45	0.50
1:A:1037:PHE:CE2	1:A:1041:MET:HE1	2.46	0.50
1:A:1393:ILE:O	1:A:1397:ILE:HG12	2.11	0.50
1:B:498:LYS:HA	1:B:501:HIS:HD2	1.76	0.50
1:A:1780:LEU:O	1:A:1789:LEU:N	2.29	0.50
1:B:264:ALA:HA	1:B:267:TRP:CE3	2.46	0.50
1:B:897:ARG:O	1:B:901:LEU:HG	2.12	0.50
1:A:11:GLN:O	1:A:15:SER:N	2.33	0.50
1:A:2084:HIS:CD2	1:A:2208:TRP:HZ3	2.28	0.50
1:B:1225:MET:N	1:B:1225:MET:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:LYS:HE3	1:B:1281:ALA:HB2	1.93	0.50
1:A:1658:ILE:HG13	1:A:1687:PHE:HA	1.94	0.50
1:A:13:VAL:O	1:A:17:PHE:N	2.45	0.49
1:A:521:SER:O	1:A:524:GLU:N	2.45	0.49
1:A:1256:LEU:HG	1:A:1260:MET:HE1	1.93	0.49
1:A:1288:CYS:SG	1:A:1289:PHE:N	2.85	0.49
1:B:1666:ARG:HD3	1:B:1758:LEU:HD21	1.94	0.49
1:B:1720:HIS:ND1	1:B:1721:ASN:OD1	2.41	0.49
1:A:1171:LYS:HB2	1:A:1175:THR:H	1.78	0.49
1:A:1922:HIS:O	1:A:1923:LEU:C	2.52	0.49
1:A:994:ASN:HA	1:A:997:ARG:HD2	1.95	0.49
1:B:521:SER:O	1:B:524:GLU:N	2.46	0.49
1:B:597:LEU:O	1:B:601:ARG:HG3	2.13	0.49
1:B:678:PRO:HD2	1:B:681:ARG:HD3	1.95	0.49
1:B:443:PHE:HE2	1:B:507:LEU:HD23	1.77	0.49
1:A:1620:ILE:HG23	1:A:1656:VAL:HG13	1.95	0.49
1:B:274:LEU:HD22	1:B:299:PHE:HE2	1.78	0.49
1:A:264:ALA:HA	1:A:267:TRP:CE3	2.48	0.49
1:A:1290:LYS:HB2	1:A:1391:ARG:HH22	1.77	0.49
1:B:1175:THR:O	1:B:1179:PHE:N	2.46	0.49
1:B:1270:SER:OG	1:B:1273:THR:HG23	2.13	0.49
1:A:4:HIS:O	1:A:7:VAL:HB	2.12	0.48
1:A:562:ASN:ND2	1:A:569:THR:OG1	2.46	0.48
1:A:1397:ILE:HG22	1:A:1418:LEU:HB3	1.95	0.48
1:A:1578:SER:HB3	1:A:1584:ILE:HD11	1.93	0.48
1:B:45:ASN:HA	1:B:48:LYS:HE2	1.93	0.48
1:B:443:PHE:CE2	1:B:507:LEU:HD23	2.47	0.48
1:B:1350:ILE:O	1:B:1353:SER:OG	2.27	0.48
1:A:447:LEU:HB3	1:A:449:LYS:HE3	1.93	0.48
1:A:1179:PHE:CE2	1:A:1183:LEU:HD11	2.48	0.48
1:B:448:HIS:CE1	1:B:493:LEU:HD11	2.48	0.48
1:B:540:GLU:HG2	1:B:541:ILE:N	2.28	0.48
1:A:35:SER:O	1:A:39:ASN:N	2.42	0.48
1:B:562:ASN:ND2	1:B:569:THR:OG1	2.37	0.48
1:B:1901:LEU:C	1:B:1903:LEU:H	2.21	0.48
1:A:2657:LEU:C	1:A:2661:HIS:HD1	2.17	0.48
1:B:300:LEU:HA	1:B:303:LEU:HD12	1.94	0.48
1:A:1182:VAL:O	1:A:1186:ILE:N	2.46	0.48
1:A:1918:ILE:HG22	1:A:1922:HIS:HE1	1.78	0.48
1:A:1740:ALA:HB1	1:A:1763:TYR:HA	1.96	0.48
1:B:1245:THR:HG23	1:B:1246:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1272:GLN:C	1:B:1274:LEU:N	2.72	0.48
1:B:1617:PRO:HA	1:B:1652:ASN:HB3	1.95	0.48
1:A:346:VAL:O	1:A:350:VAL:HG23	2.13	0.48
1:A:1183:LEU:O	1:A:1184:THR:C	2.56	0.48
1:B:693:MET:SD	1:B:783:LYS:NZ	2.86	0.48
1:A:1286:THR:C	1:A:1391:ARG:HH21	2.21	0.48
1:A:1764:ALA:HA	1:A:1767:ILE:HG13	1.96	0.48
1:A:1901:LEU:C	1:A:1903:LEU:H	2.21	0.48
1:A:501:HIS:NE2	1:A:544:GLU:O	2.47	0.48
1:A:1645:PHE:HB2	1:A:1650:TYR:OH	2.13	0.48
1:B:763:LEU:HD22	1:B:847:LEU:HD11	1.96	0.47
1:B:2033:MET:HE1	1:B:2057:ILE:O	2.13	0.47
1:A:4:HIS:O	1:A:5:ARG:C	2.55	0.47
1:A:12:ALA:O	1:A:15:SER:N	2.47	0.47
1:A:1867:ILE:O	1:A:1868:GLU:HB2	2.14	0.47
1:B:1736:VAL:HG21	1:B:1799:ILE:HG23	1.96	0.47
1:A:17:PHE:CZ	1:A:40:LYS:HA	2.49	0.47
1:A:1162:MET:HA	1:A:1824:ILE:HG13	1.96	0.47
1:B:1772:LEU:HA	1:B:1778:PHE:HE1	1.79	0.47
1:A:529:LEU:HD12	1:A:532:LEU:HD12	1.96	0.47
1:B:1162:MET:HA	1:B:1824:ILE:HG13	1.96	0.47
1:A:440:ARG:HH21	1:A:507:LEU:HA	1.80	0.47
1:B:498:LYS:O	1:B:501:HIS:HB2	2.15	0.47
1:B:1636:ASP:OD1	1:B:1637:PHE:N	2.47	0.47
1:A:24:LYS:O	1:A:25:THR:C	2.58	0.47
1:A:440:ARG:NH1	1:A:509:CYS:O	2.47	0.47
1:A:1688:ILE:HG13	1:A:1694:LEU:HB2	1.96	0.47
1:A:2296:TRP:NE1	1:A:2339:PHE:O	2.41	0.47
1:B:1038:ARG:NH2	1:B:1079:LEU:O	2.48	0.47
1:B:1354:SER:HB3	1:B:1457:PHE:CD1	2.49	0.47
1:B:1421:MET:HA	1:B:1424:ILE:HD13	1.97	0.47
1:A:6:PRO:O	1:A:10:VAL:N	2.47	0.47
1:A:1723:LEU:HB3	1:A:1792:MET:HB2	1.97	0.47
1:B:346:VAL:O	1:B:350:VAL:HG23	2.14	0.47
1:B:795:PRO:HB2	1:B:908:LYS:HD2	1.96	0.47
1:B:1183:LEU:HD22	1:B:1187:LEU:CB	2.44	0.47
1:B:1645:PHE:HB2	1:B:1650:TYR:OH	2.14	0.47
1:A:3:ALA:HB3	1:A:8:GLU:CD	2.40	0.47
1:B:440:ARG:NH1	1:B:509:CYS:O	2.47	0.47
1:A:993:LEU:HG	1:A:997:ARG:HE	1.80	0.47
1:A:1292:TYR:HB3	1:A:1361:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:MET:O	1:B:1184:THR:HG23	2.14	0.47
1:B:1738:SER:HA	1:B:1806:ILE:HG21	1.97	0.47
1:B:1778:PHE:CD2	1:B:1796:CYS:HB3	2.45	0.47
1:A:713:LEU:O	1:A:716:GLU:HG3	2.15	0.46
1:A:1636:ASP:OD1	1:A:1637:PHE:N	2.48	0.46
1:B:299:PHE:CE1	1:B:303:LEU:HD21	2.50	0.46
1:B:1765:SER:OG	1:B:1810:TRP:NE1	2.48	0.46
1:A:121:LEU:HD11	1:A:135:ARG:HA	1.98	0.46
1:A:174:VAL:O	1:A:178:GLU:N	2.47	0.46
1:A:1037:PHE:O	1:A:1041:MET:HE2	2.16	0.46
1:B:412:ASN:O	1:B:416:ARG:HG2	2.16	0.46
1:A:1588:VAL:HG12	1:A:1590:ARG:HG2	1.96	0.46
1:B:1171:LYS:HD3	1:B:1176:ARG:H	1.80	0.46
1:B:1385:GLY:HA3	1:B:1458:PHE:CE2	2.51	0.46
1:B:1723:LEU:HB3	1:B:1792:MET:HG2	1.97	0.46
1:B:2203:LYS:O	1:B:2207:GLN:HG3	2.15	0.46
1:A:540:GLU:HG2	1:A:541:ILE:N	2.30	0.46
1:A:1738:SER:HA	1:A:1806:ILE:HG21	1.97	0.46
1:A:2033:MET:HE1	1:A:2057:ILE:O	2.14	0.46
1:A:1772:LEU:HA	1:A:1778:PHE:HE1	1.81	0.46
1:B:1689:ASP:OD1	1:B:1689:ASP:N	2.41	0.46
1:B:2064:MET:HE3	1:B:2064:MET:HB2	1.71	0.46
1:A:1107:PHE:CD2	1:A:1111:MET:HE1	2.51	0.46
1:B:17:PHE:HZ	1:B:40:LYS:HA	1.81	0.46
1:A:17:PHE:O	1:A:18:ASP:C	2.59	0.46
1:A:992:MET:O	1:A:992:MET:HE3	2.16	0.46
1:B:1660:ASN:HD21	1:B:1761:ILE:CD1	2.28	0.46
1:B:1901:LEU:O	1:B:1903:LEU:N	2.49	0.46
1:A:440:ARG:HA	1:A:443:PHE:HD1	1.81	0.46
1:A:1111:MET:O	1:A:1115:ASN:N	2.42	0.46
1:B:713:LEU:O	1:B:716:GLU:HG3	2.15	0.46
1:B:2192:MET:HE3	1:B:2204:TRP:HB3	1.97	0.46
1:A:493:LEU:HA	1:A:496:MET:HE3	1.97	0.45
1:A:991:MET:SD	1:A:992:MET:N	2.90	0.45
1:B:447:LEU:HB3	1:B:449:LYS:HE3	1.96	0.45
1:A:5:ARG:O	1:A:8:GLU:N	2.49	0.45
1:A:1350:ILE:O	1:A:1353:SER:OG	2.30	0.45
1:B:1731:LYS:H	1:B:1747:GLU:CD	2.24	0.45
1:A:493:LEU:O	1:A:496:MET:HG2	2.15	0.45
1:B:415:HIS:O	1:B:419:THR:N	2.46	0.45
1:B:1575:ALA:HB3	1:B:1586:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:MET:HE3	1:A:1023:MET:O	2.16	0.45
1:A:1901:LEU:O	1:A:1903:LEU:N	2.50	0.45
1:B:299:PHE:CE1	1:B:303:LEU:HD11	2.52	0.45
1:A:493:LEU:O	1:A:497:VAL:HG23	2.16	0.45
1:A:1183:LEU:HD22	1:A:1187:LEU:CB	2.45	0.45
1:A:1369:TYR:CG	1:A:1462:ALA:HB1	2.51	0.45
1:B:1286:THR:C	1:B:1391:ARG:HH21	2.25	0.45
1:B:1593:LYS:HD3	1:B:1630:SER:HB3	1.98	0.45
1:A:448:HIS:CE1	1:A:532:LEU:HD21	2.52	0.45
1:B:1717:LYS:HA	1:B:1717:LYS:HD3	1.77	0.45
1:B:1803:ILE:HA	1:B:1806:ILE:HG12	1.97	0.45
1:A:5:ARG:O	1:A:9:TRP:N	2.36	0.45
1:A:1345:LYS:HA	1:A:1348:HIS:HE1	1.81	0.45
1:B:1037:PHE:HD2	1:B:1038:ARG:HG3	1.80	0.45
1:B:691:LEU:HB3	1:B:710:PHE:CE1	2.52	0.45
1:A:45:ASN:HA	1:A:48:LYS:HE2	1.99	0.45
1:A:1252:LEU:O	1:A:1256:LEU:N	2.48	0.45
1:A:1593:LYS:HD3	1:A:1630:SER:HB3	1.99	0.45
1:B:498:LYS:HA	1:B:501:HIS:CD2	2.51	0.45
1:B:1180:MET:HE3	1:B:1183:LEU:HD12	1.99	0.45
1:A:1803:ILE:HA	1:A:1806:ILE:HG12	1.99	0.44
1:A:5:ARG:CA	1:A:8:GLU:HB2	2.36	0.44
1:A:1918:ILE:HG22	1:A:1922:HIS:CE1	2.52	0.44
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.84	0.44
1:B:435:HIS:O	1:B:439:LEU:HG	2.17	0.44
1:B:577:MET:SD	1:B:578:LEU:HG	2.57	0.44
1:B:2253:ALA:HB2	1:B:2269:LEU:HD22	1.98	0.44
1:A:1687:PHE:CZ	1:A:1689:ASP:HB3	2.52	0.44
1:B:46:ILE:O	1:B:50:LYS:N	2.45	0.44
1:B:533:VAL:HB	1:B:534:PRO:HD3	2.00	0.44
1:A:1589:ALA:O	1:A:1631:ASN:ND2	2.50	0.44
1:A:1625:THR:HG22	1:A:1660:ASN:HD22	1.82	0.44
1:A:2387:ARG:O	1:A:2388:THR:C	2.59	0.44
1:B:688:GLU:CD	1:B:772:GLY:HA3	2.43	0.44
1:B:1286:THR:HA	1:B:1391:ARG:HH21	1.82	0.44
1:B:1428:ILE:HD11	1:B:1451:PHE:HA	1.99	0.44
1:A:518:THR:O	1:A:523:ALA:HB3	2.18	0.44
1:A:1632:ARG:HB2	1:A:1668:TYR:CE1	2.52	0.44
1:A:1717:LYS:HA	1:A:1717:LYS:HD3	1.75	0.44
1:A:448:HIS:ND1	1:A:532:LEU:HD21	2.32	0.44
1:A:1275:PHE:O	1:A:1282:SER:OG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:GLU:O	1:B:1037:PHE:HB3	2.18	0.44
1:B:1732:VAL:HB	1:B:1744:THR:O	2.17	0.44
1:B:493:LEU:O	1:B:497:VAL:HG23	2.17	0.44
1:B:1023:MET:HE3	1:B:1023:MET:O	2.17	0.44
1:B:1632:ARG:HG3	1:B:1668:TYR:CD1	2.52	0.44
1:A:443:PHE:O	1:A:446:THR:OG1	2.30	0.44
1:B:1856:LEU:HD23	1:B:1856:LEU:HA	1.88	0.44
1:A:689:VAL:O	1:A:693:MET:HG2	2.18	0.43
1:A:1290:LYS:N	1:A:1391:ARG:HH22	2.16	0.43
1:B:1179:PHE:CE2	1:B:1183:LEU:HD11	2.52	0.43
1:B:1633:PHE:HB2	1:B:1668:TYR:OH	2.17	0.43
1:A:437:VAL:O	1:A:440:ARG:HG2	2.19	0.43
1:A:533:VAL:HB	1:A:534:PRO:HD3	2.01	0.43
1:A:1722:ALA:HB1	1:A:1734:ILE:HD12	2.00	0.43
1:B:36:THR:O	1:B:40:LYS:N	2.51	0.43
1:B:570:PHE:CE2	1:B:610:PHE:HD2	2.35	0.43
1:B:994:ASN:HA	1:B:997:ARG:HD2	2.00	0.43
1:A:1023:MET:CE	1:A:1026:ARG:HB3	2.48	0.43
1:A:1267:LEU:O	1:A:1269:ASP:N	2.51	0.43
1:A:1561:GLU:HA	1:A:1604:TYR:CE2	2.53	0.43
1:A:3:ALA:HB3	1:A:8:GLU:OE1	2.19	0.43
1:A:678:PRO:HD2	1:A:681:ARG:HD3	2.00	0.43
1:A:1588:VAL:HB	1:A:1591:ARG:HE	1.83	0.43
1:A:2253:ALA:HB2	1:A:2269:LEU:HD22	1.98	0.43
1:B:1517:LYS:HE3	1:B:1521:LEU:HD21	2.01	0.43
1:A:3:ALA:O	1:A:8:GLU:HG3	2.17	0.43
1:A:498:LYS:O	1:A:501:HIS:HB2	2.19	0.43
1:B:1495:GLU:HG2	1:B:1496:LYS:HG2	2.00	0.43
1:B:1578:SER:HB3	1:B:1584:ILE:HD11	2.01	0.43
1:B:175:HIS:C	1:B:177:ILE:H	2.27	0.43
1:B:250:PHE:CE2	1:B:296:LYS:HG2	2.53	0.43
1:B:1172:ASP:O	1:B:1173:LEU:HD23	2.18	0.43
1:B:1354:SER:HB3	1:B:1457:PHE:CE1	2.53	0.43
1:B:1745:SER:O	1:B:1757:PHE:HB3	2.18	0.43
1:A:17:PHE:HD1	1:A:17:PHE:HA	1.62	0.43
1:A:2203:LYS:O	1:A:2207:GLN:HG3	2.17	0.43
1:B:1841:LEU:HD11	1:B:1856:LEU:HD12	2.01	0.43
1:A:442:MET:O	1:A:446:THR:HG23	2.18	0.43
1:A:1841:LEU:HD11	1:A:1856:LEU:HD12	2.00	0.43
1:B:218:LYS:HA	1:B:221:TRP:HB2	2.00	0.43
1:A:570:PHE:CE2	1:A:610:PHE:HD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1921:LYS:O	1:A:1922:HIS:C	2.61	0.43
1:B:442:MET:O	1:B:446:THR:HG23	2.19	0.43
1:B:1389:PHE:HE2	1:B:1458:PHE:CZ	2.36	0.43
1:B:1620:ILE:HG23	1:B:1656:VAL:HG13	2.00	0.43
1:A:577:MET:SD	1:A:578:LEU:HG	2.59	0.43
1:A:1140:SER:O	1:A:1143:HIS:ND1	2.52	0.43
1:A:1269:ASP:HB3	1:A:1273:THR:OG1	2.19	0.43
1:A:1719:PHE:HB3	1:A:1793:HIS:NE2	2.34	0.43
1:A:2073:LEU:O	1:A:2074:ASP:C	2.62	0.43
1:B:1242:VAL:HG23	1:B:1243:LEU:HD22	2.01	0.43
1:A:553:HIS:HD2	1:A:606:CYS:HB2	1.84	0.42
1:A:1804:ILE:HA	1:A:1807:ARG:HG2	2.01	0.42
1:B:384:PHE:CZ	1:B:427:PRO:HB2	2.54	0.42
1:B:518:THR:O	1:B:523:ALA:HB3	2.20	0.42
1:A:1681:GLY:N	1:A:1752:LEU:O	2.52	0.42
1:A:9:TRP:C	1:A:12:ALA:H	2.26	0.42
1:A:175:HIS:C	1:A:177:ILE:H	2.28	0.42
1:A:384:PHE:CZ	1:A:427:PRO:HB2	2.54	0.42
1:A:1771:CYS:SG	1:A:1772:LEU:N	2.92	0.42
1:B:784:TRP:HE1	1:B:841:THR:CG2	2.27	0.42
1:B:832:ASP:O	1:B:836:GLU:HG3	2.19	0.42
1:A:218:LYS:HA	1:A:221:TRP:HB2	2.01	0.42
1:A:493:LEU:HD12	1:A:496:MET:SD	2.59	0.42
1:A:1722:ALA:HA	1:A:1793:HIS:HD2	1.84	0.42
1:A:738:PHE:HA	1:A:741:PHE:CD2	2.50	0.42
1:A:1421:MET:HA	1:A:1424:ILE:HD13	2.00	0.42
1:B:2073:LEU:O	1:B:2074:ASP:C	2.62	0.42
1:A:1575:ALA:HB3	1:A:1586:TYR:HD2	1.84	0.42
1:B:1804:ILE:HA	1:B:1807:ARG:HG2	2.00	0.42
1:A:571:TRP:CH2	1:A:611:LEU:HD12	2.55	0.42
1:B:551:VAL:HA	1:B:554:GLN:OE1	2.19	0.42
1:B:987:SER:HB2	1:B:989:GLU:OE2	2.19	0.42
1:B:1189:GLN:C	1:B:1191:THR:H	2.28	0.42
1:A:17:PHE:HZ	1:A:40:LYS:HA	1.85	0.42
1:A:412:ASN:HB3	1:A:416:ARG:NH1	2.34	0.42
1:A:1736:VAL:HG21	1:A:1799:ILE:HG23	2.02	0.42
1:A:2375:LYS:HD3	1:A:2697:PHE:CE1	2.55	0.42
1:B:1446:PHE:O	1:B:1449:SER:OG	2.35	0.42
1:B:891:VAL:O	1:B:894:PHE:HB3	2.20	0.42
1:A:2084:HIS:HA	1:A:2208:TRP:CZ3	2.54	0.42
1:B:496:MET:O	1:B:499:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1745:SER:N	1:B:1758:LEU:O	2.52	0.42
1:B:1769:GLU:HB2	1:B:1781:THR:HB	2.02	0.42
1:A:1072:SER:O	1:A:1076:VAL:HG23	2.20	0.41
1:B:1275:PHE:HB3	1:B:1282:SER:OG	2.19	0.41
1:A:1239:LEU:HA	1:A:1242:VAL:HG22	2.02	0.41
1:A:1634:LYS:HD3	1:A:1634:LYS:HA	1.89	0.41
1:A:1745:SER:O	1:A:1757:PHE:HB3	2.19	0.41
1:A:1491:TRP:CE3	1:A:1527:PRO:HD2	2.56	0.41
1:A:1856:LEU:HD23	1:A:1856:LEU:HA	1.91	0.41
1:A:1924:CYS:HA	1:A:1927:TYR:CE2	2.55	0.41
1:A:186:ASP:O	1:A:190:LEU:N	2.35	0.41
1:A:492:LEU:O	1:A:495:SER:OG	2.29	0.41
1:A:1227:LEU:HD23	1:A:1227:LEU:HA	1.95	0.41
1:B:1590:ARG:HA	1:B:1631:ASN:HD21	1.85	0.41
1:A:403:PRO:O	1:A:406:PHE:HB2	2.20	0.41
1:A:526:ILE:O	1:A:530:VAL:HG23	2.21	0.41
1:A:583:LYS:HE2	1:A:686:LYS:HE2	2.03	0.41
1:B:1072:SER:O	1:B:1076:VAL:HG23	2.19	0.41
1:B:1110:PHE:CE2	1:B:1152:LEU:HD11	2.56	0.41
1:B:1387:ALA:HA	1:B:1390:LEU:HG	2.03	0.41
1:A:213:ILE:HG23	1:A:269:LEU:HD22	2.02	0.41
1:A:594:THR:O	1:A:598:LYS:HG3	2.21	0.41
1:B:1719:PHE:HB3	1:B:1793:HIS:NE2	2.36	0.41
1:A:335:ASN:HA	1:A:425:TRP:CH2	2.56	0.41
1:A:901:LEU:HA	1:A:904:CYS:SG	2.60	0.41
1:A:1275:PHE:HB3	1:A:1282:SER:OG	2.21	0.41
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.56	0.41
1:A:2370:VAL:O	1:A:2374:LEU:HG	2.21	0.41
1:B:299:PHE:CZ	1:B:303:LEU:HD11	2.55	0.41
1:B:1257:LEU:HB3	1:B:1261:PHE:CE2	2.56	0.41
1:B:1924:CYS:HA	1:B:1927:TYR:CE2	2.55	0.41
1:A:996:VAL:O	1:A:1000:ARG:HG3	2.21	0.41
1:A:1740:ALA:HA	1:A:1764:ALA:H	1.85	0.41
1:B:303:LEU:H	1:B:303:LEU:HG	1.65	0.41
1:B:696:TRP:NE1	1:B:840:MET:HB2	2.36	0.41
1:B:1267:LEU:O	1:B:1268:ALA:HB3	2.20	0.41
1:A:380:LEU:HA	1:A:380:LEU:HD23	1.86	0.41
1:A:903:VAL:C	1:A:914:ARG:HH21	2.29	0.41
1:A:944:PHE:CE2	1:A:960:PHE:HD2	2.39	0.41
1:A:1304:LEU:HD13	1:A:1403:ALA:HB1	2.03	0.41
1:A:1571:ILE:HG12	1:A:1591:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1736:VAL:HG22	1:A:1741:VAL:HG13	2.03	0.41
1:B:1174:GLN:O	1:B:1178:THR:N	2.54	0.41
1:B:2375:LYS:HD3	1:B:2697:PHE:CE1	2.56	0.41
1:A:790:LEU:O	1:A:794:TYR:HD2	2.04	0.41
1:A:1041:MET:HB2	1:A:1041:MET:HE3	1.77	0.41
1:B:300:LEU:HA	1:B:300:LEU:HD23	1.81	0.41
1:B:556:ASP:OD1	1:B:557:SER:N	2.52	0.41
1:B:897:ARG:HD2	1:B:901:LEU:HD21	2.03	0.40
1:B:1170:HIS:HB3	1:B:1171:LYS:H	1.67	0.40
1:B:1237:ASP:OD1	1:B:1237:ASP:N	2.55	0.40
1:B:1838:LEU:HD23	1:B:1838:LEU:HA	1.95	0.40
1:A:1110:PHE:CE2	1:A:1152:LEU:HD11	2.56	0.40
1:A:1638:LEU:HD23	1:A:1675:LEU:HD13	2.02	0.40
1:A:2634:PRO:O	1:B:5:ARG:NH1	2.51	0.40
1:B:501:HIS:HE1	1:B:547:GLU:CB	2.34	0.40
1:B:684:GLN:O	1:B:688:GLU:HG2	2.21	0.40
1:B:1080:LEU:HD13	1:B:1152:LEU:HD12	2.02	0.40
1:B:1107:PHE:O	1:B:1111:MET:HG2	2.21	0.40
1:B:1612:PRO:O	1:B:1616:LYS:NZ	2.55	0.40
1:B:299:PHE:O	1:B:303:LEU:HG	2.21	0.40
1:B:403:PRO:O	1:B:406:PHE:HB2	2.21	0.40
1:B:834:LEU:O	1:B:838:ILE:HG13	2.21	0.40
1:B:1771:CYS:SG	1:B:1772:LEU:N	2.94	0.40
1:A:440:ARG:HB2	1:A:443:PHE:HE1	1.86	0.40
1:A:1571:ILE:O	1:A:1587:TYR:HA	2.21	0.40
1:B:926:SER:H	1:B:929:LEU:HD12	1.87	0.40
1:B:975:HIS:CE1	1:B:1025:ARG:HH22	2.39	0.40
1:B:1292:TYR:HB3	1:B:1361:LEU:HD21	2.02	0.40
1:B:1347:PHE:O	1:B:1351:ILE:HG12	2.21	0.40
1:B:1495:GLU:O	1:B:1496:LYS:HD2	2.21	0.40
1:B:2082:LEU:HD23	1:B:2082:LEU:HA	1.92	0.40
1:A:601:ARG:CZ	1:A:705:VAL:HA	2.52	0.40
1:A:1183:LEU:C	1:A:1186:ILE:H	2.30	0.40
1:B:740:GLU:C	1:B:742:ALA:H	2.30	0.40
1:B:1588:VAL:HG12	1:B:1590:ARG:HG2	2.03	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	2212/2818 (78%)	2077 (94%)	130 (6%)	5 (0%)	44 73
1	B	2205/2818 (78%)	2093 (95%)	108 (5%)	4 (0%)	44 73
All	All	4417/5636 (78%)	4170 (94%)	238 (5%)	9 (0%)	45 73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	909	VAL
1	B	909	VAL
1	A	4	HIS
1	A	341	VAL
1	A	1379	ASN
1	B	341	VAL
1	B	1273	THR
1	B	1379	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	897/2512 (36%)	887 (99%)	10 (1%)	70 83
1	B	935/2512 (37%)	930 (100%)	5 (0%)	86 93
All	All	1832/5024 (36%)	1817 (99%)	15 (1%)	77 88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	7	VAL
1	A	10	VAL
1	A	17	PHE
1	A	303	LEU
1	A	440	ARG
1	A	1733	SER
1	A	1920	LEU
1	A	1921	LYS
1	A	2387	ARG
1	B	299	PHE
1	B	303	LEU
1	B	304	ARG
1	B	1269	ASP
1	B	1733	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
1	A	614	ASN
1	A	682	GLN
1	A	712	HIS
1	A	781	HIS
1	A	1259	ASN
1	A	1444	ASN
1	A	1660	ASN
1	A	1672	HIS
1	A	1703	GLN
1	A	1759	ASN
1	A	1805	HIS
1	B	293	ASN
1	B	415	HIS
1	B	501	HIS
1	B	510	ASN
1	B	553	HIS
1	B	614	ASN
1	B	712	HIS
1	B	853	GLN
1	B	975	HIS
1	B	1218	GLN

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Mol	Chain	Res	Type
1	B	1660	ASN
1	B	1703	GLN
1	B	1759	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

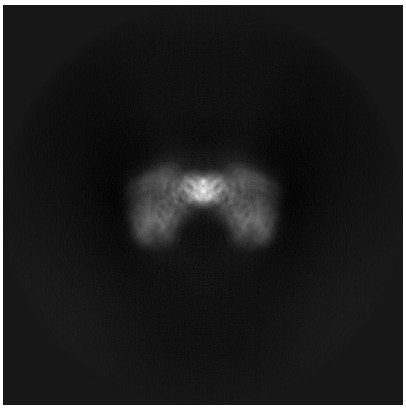
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27826. These allow visual inspection of the internal detail of the map and identification of artifacts.

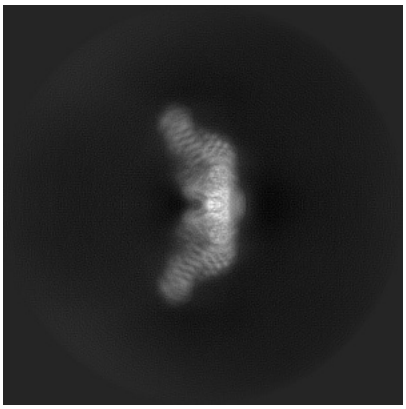
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

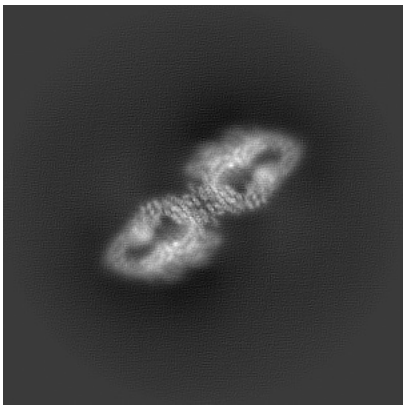
6.1.1 Primary map



X

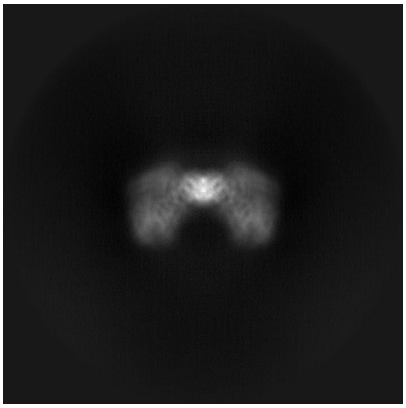


Y

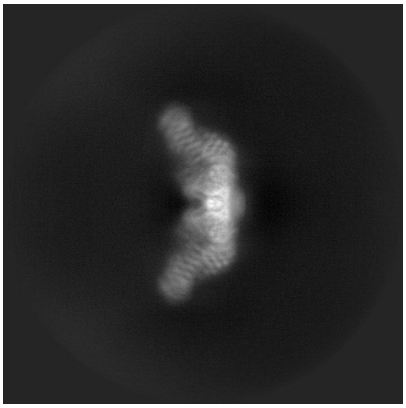


Z

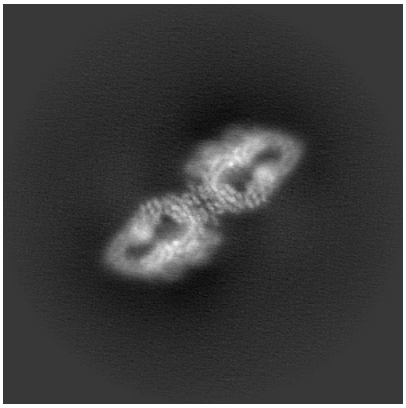
6.1.2 Raw map



X



Y

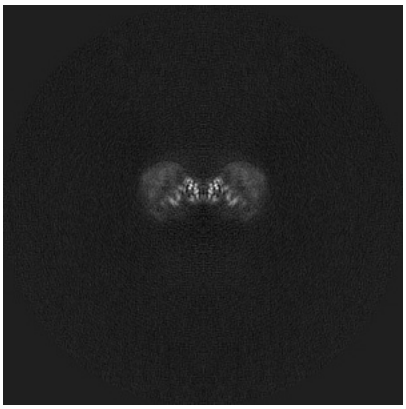


Z

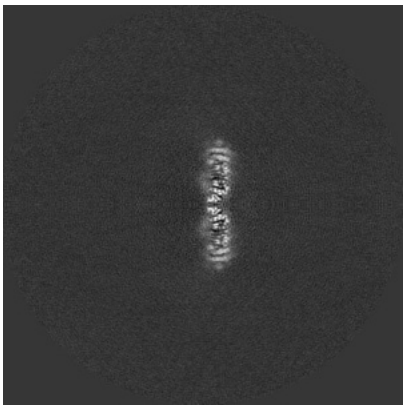
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

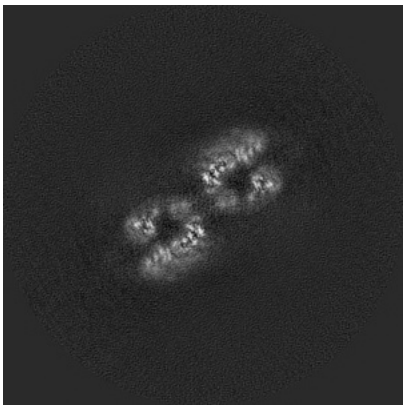
6.2.1 Primary map



X Index: 256

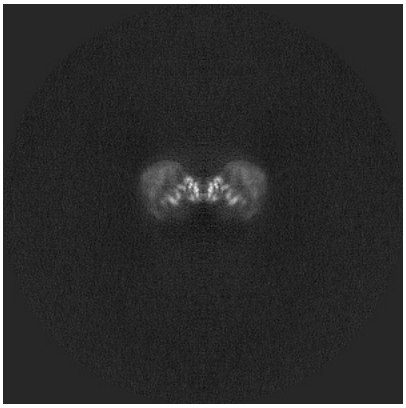


Y Index: 256

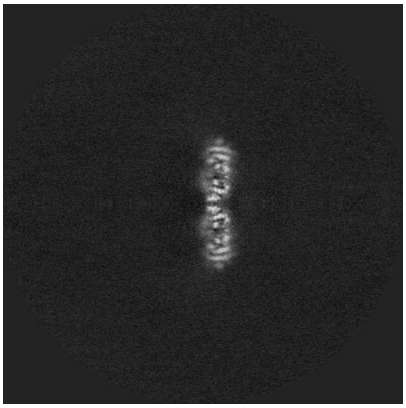


Z Index: 256

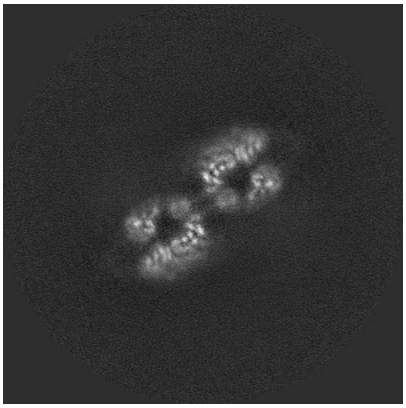
6.2.2 Raw map



X Index: 256



Y Index: 256

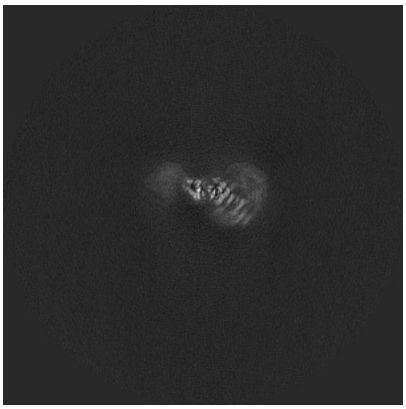


Z Index: 256

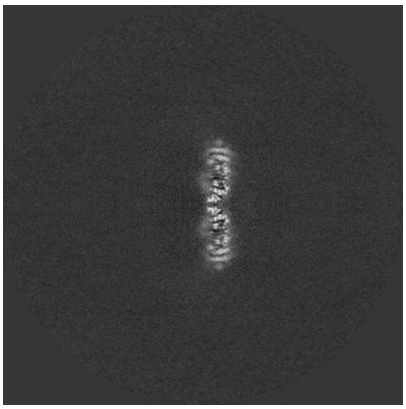
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

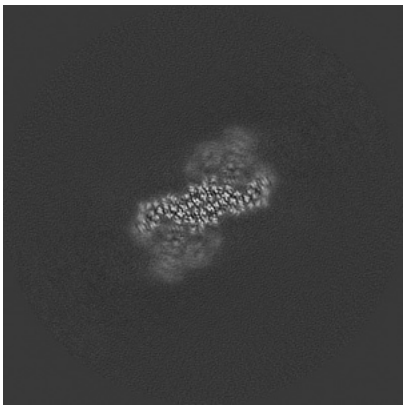
6.3.1 Primary map



X Index: 268

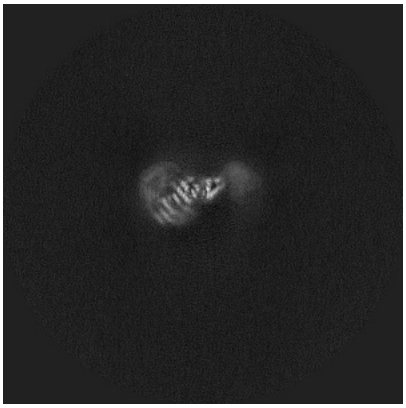


Y Index: 256

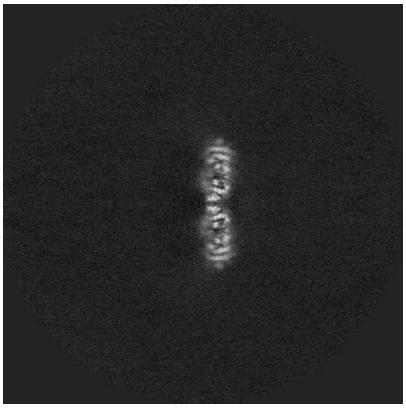


Z Index: 276

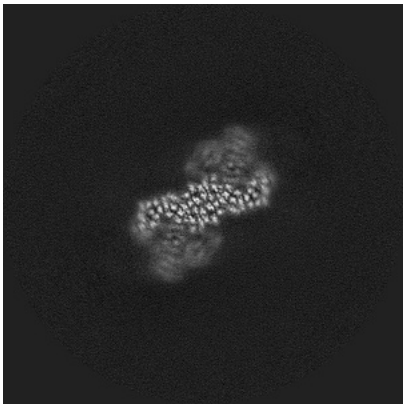
6.3.2 Raw map



X Index: 244



Y Index: 256

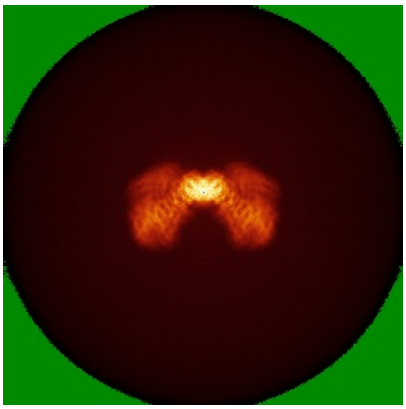


Z Index: 276

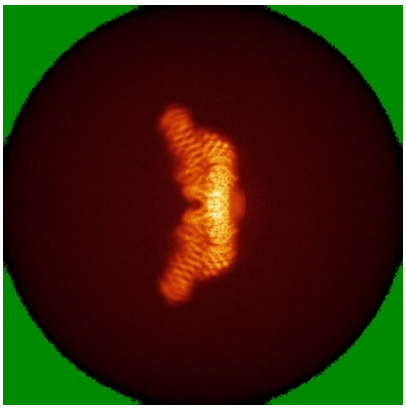
The images above show the largest variance slices of the map in three orthogonal directions.

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

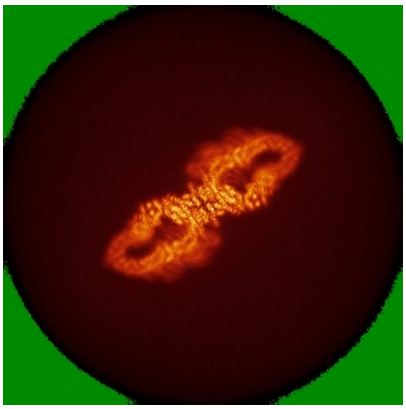
6.4.1 Primary map



X

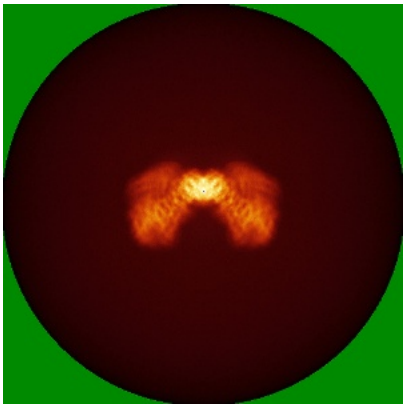


Y

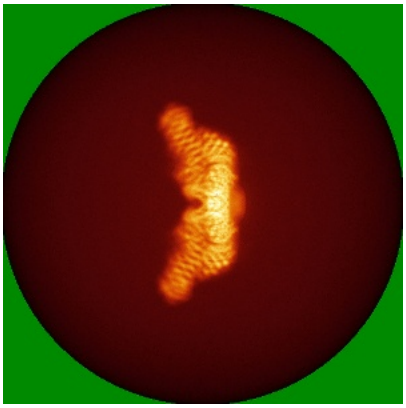


Z

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 0.0133. 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.

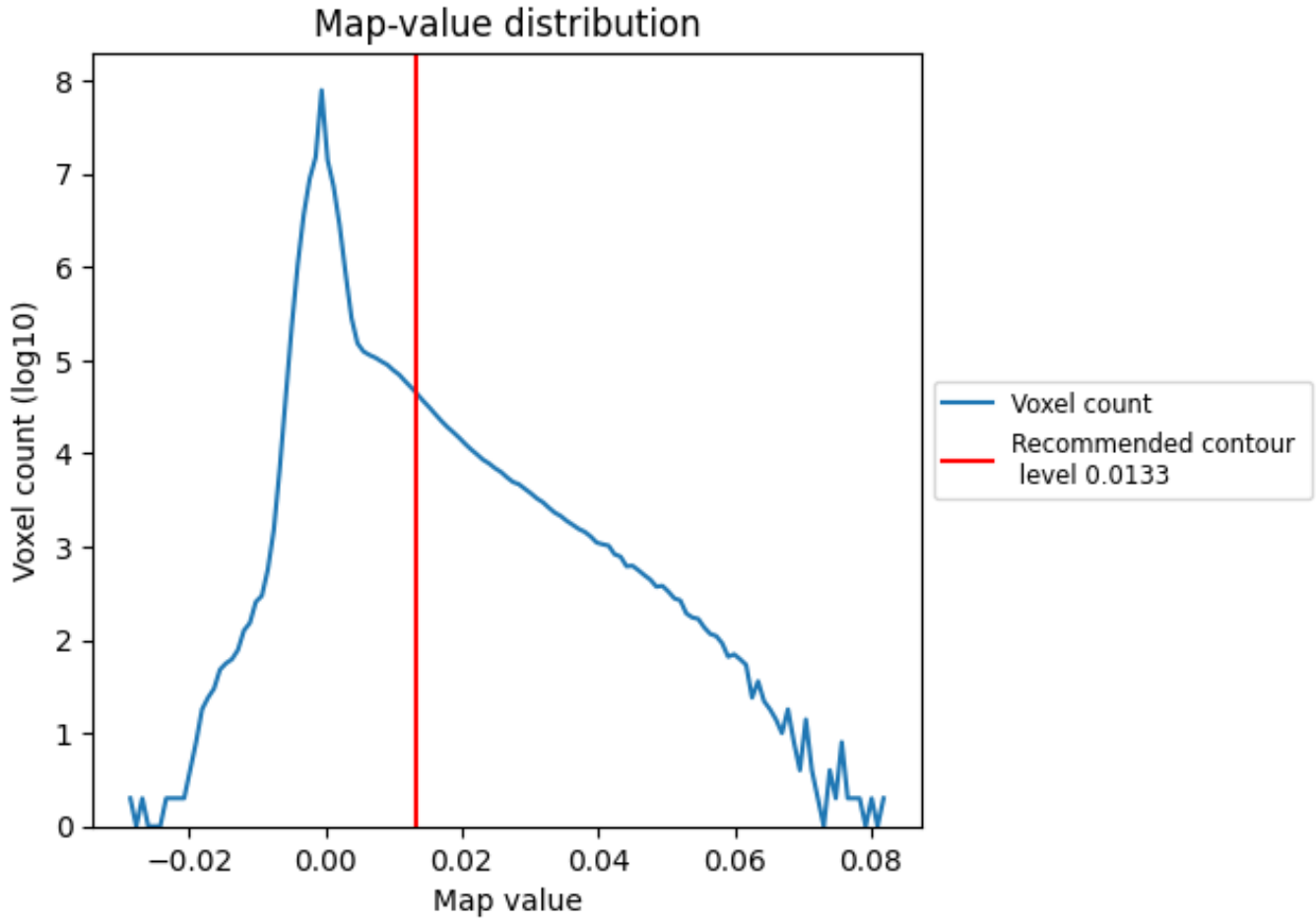
6.6 Mask visualisation (i)

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

7 Map analysis

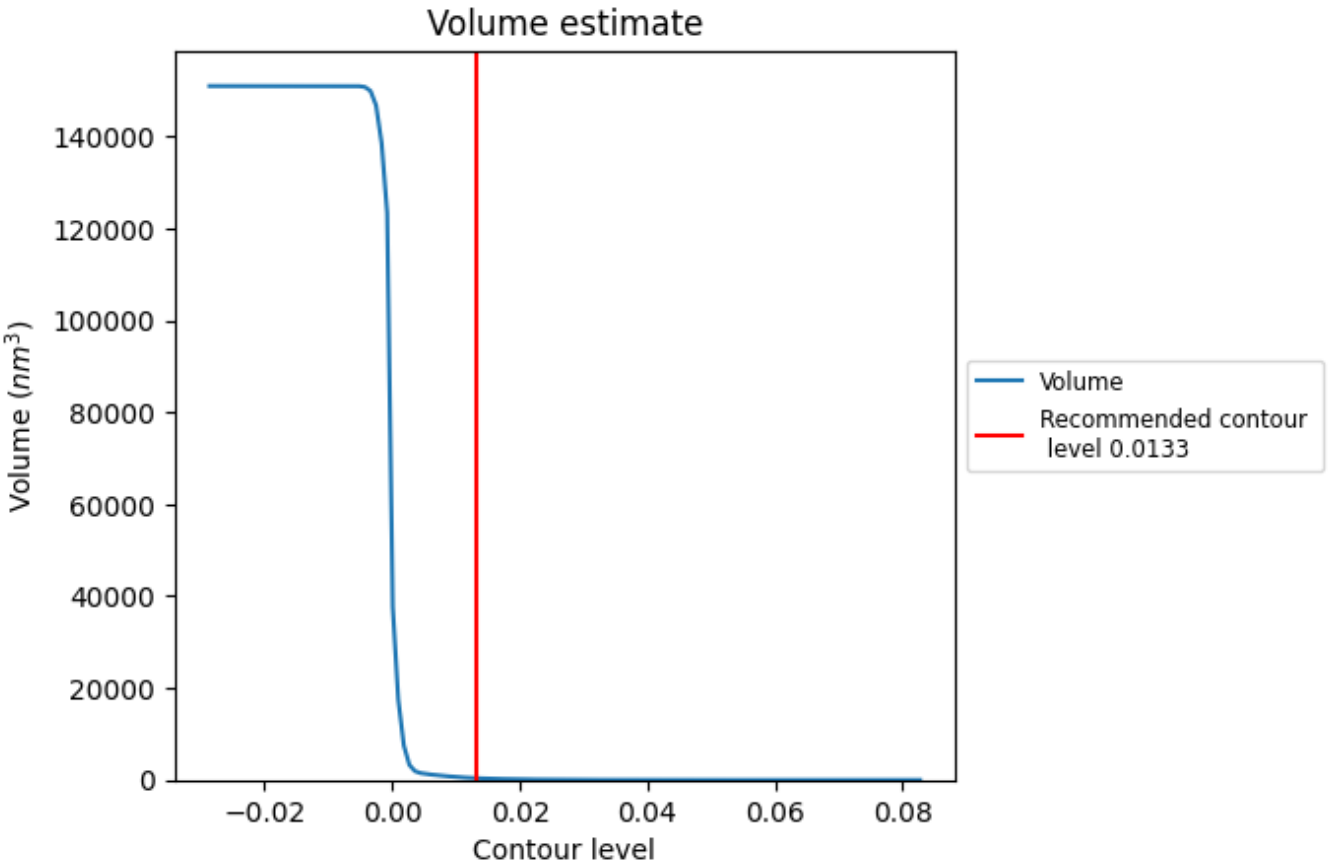
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

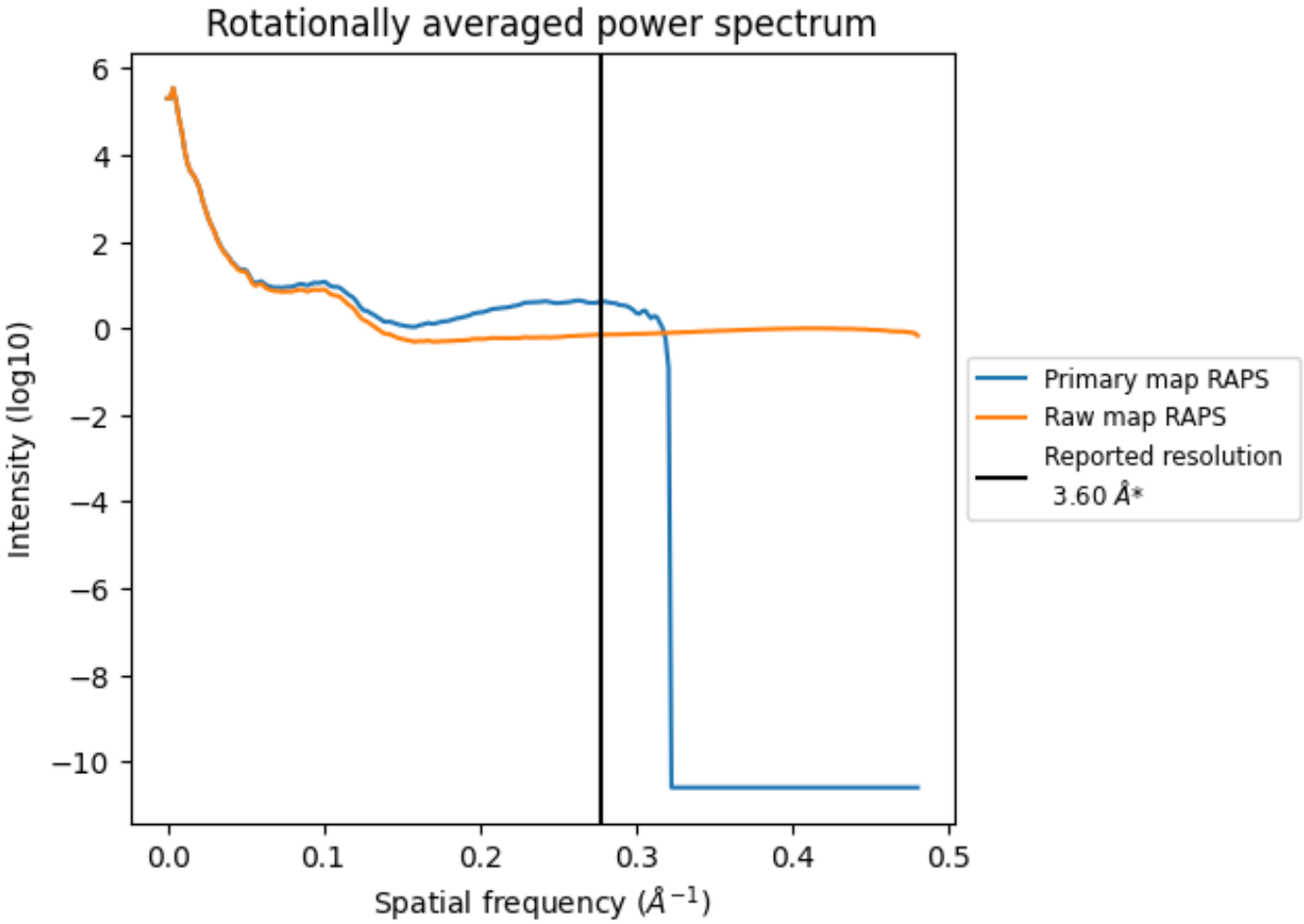
7.2 Volume estimate



The volume at the recommended contour level is 381 nm^3; this corresponds to an approximate mass of 345 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

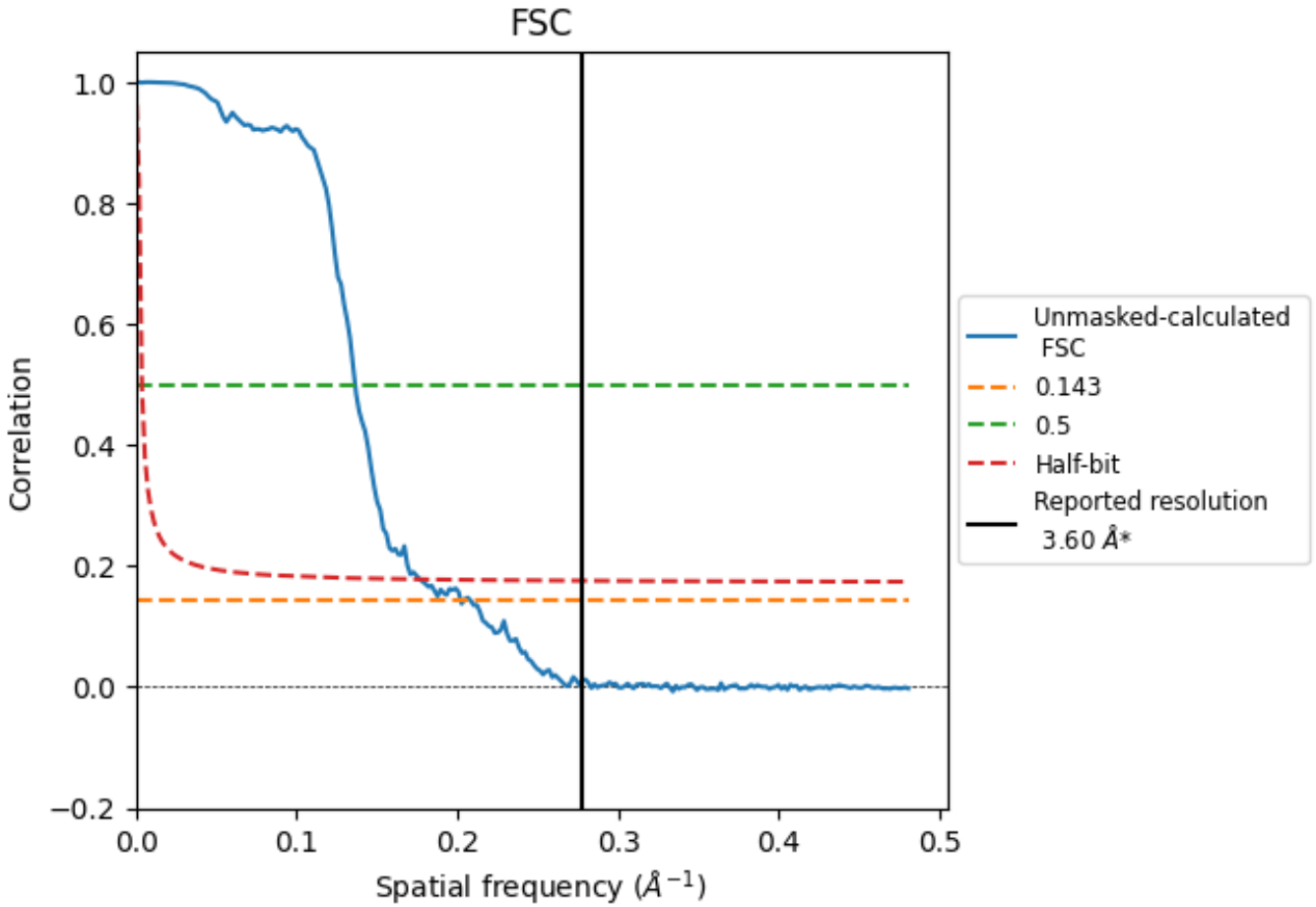


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

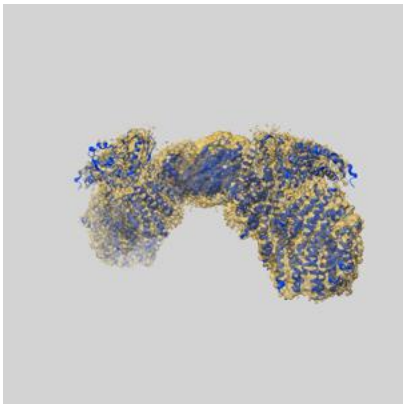
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.94	7.33	5.66

*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 4.94 differs from the reported value 3.6 by more than 10 %

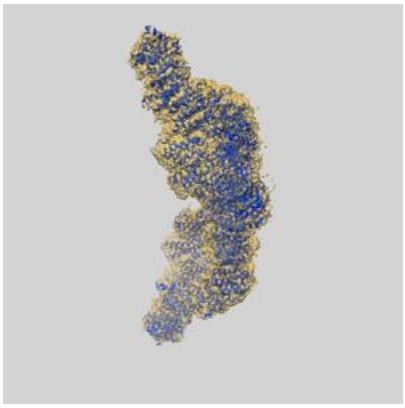
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27826 and PDB model 8E20. Per-residue inclusion information can be found in section 3 on page 4.

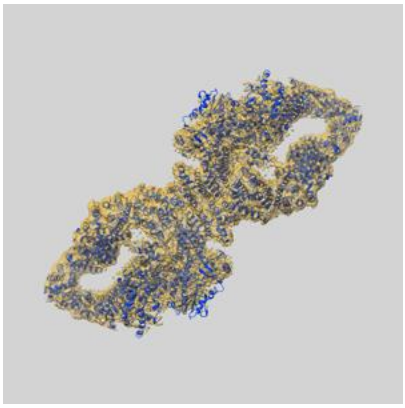
9.1 Map-model overlay



X



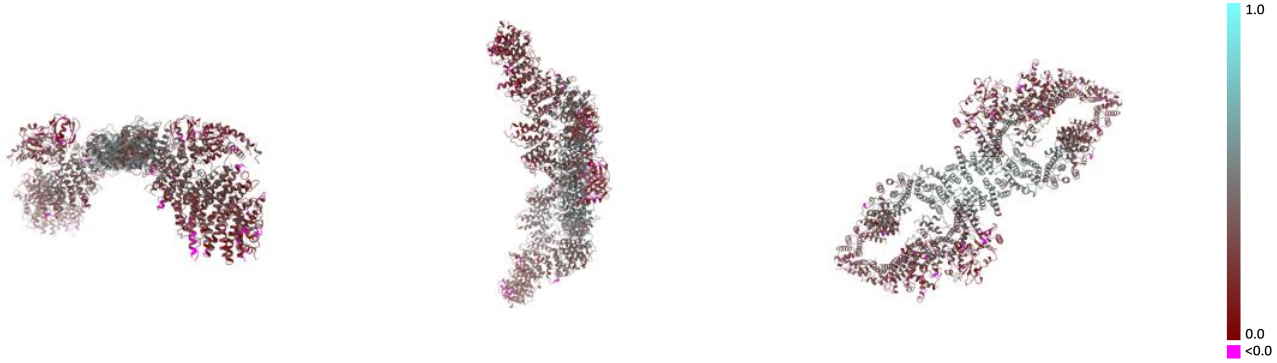
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

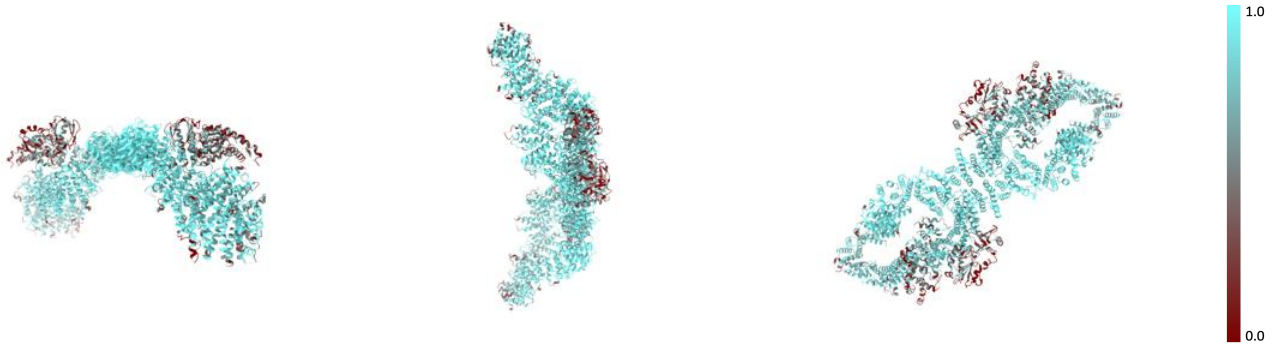
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

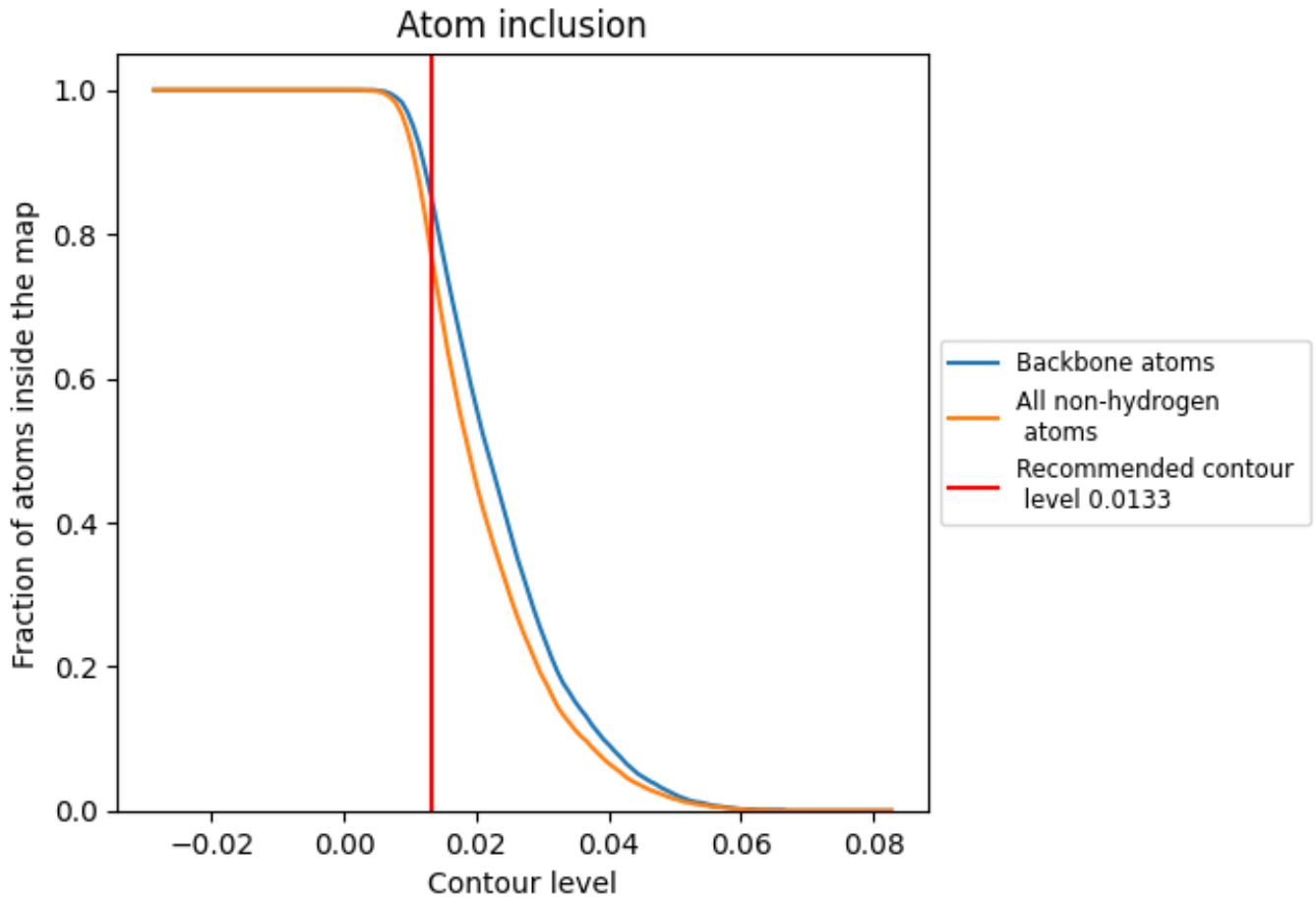
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0133).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.3230
A	0.7700	0.3250
B	0.7650	0.3200