



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:21 AM UTC

PDB ID : 9J5K / pdb_00009j5k
EMDB ID : EMD-61144
Title : Pathogen effector forms a phosphatase holoenzyme complex with host core enzyme to promote disease
Authors : Wang, J.L.; Wang, Y.L.
Deposited on : 2024-08-12
Resolution : 3.39 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:

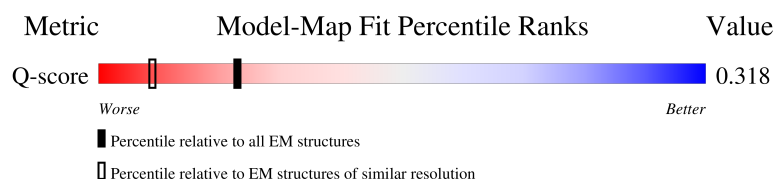
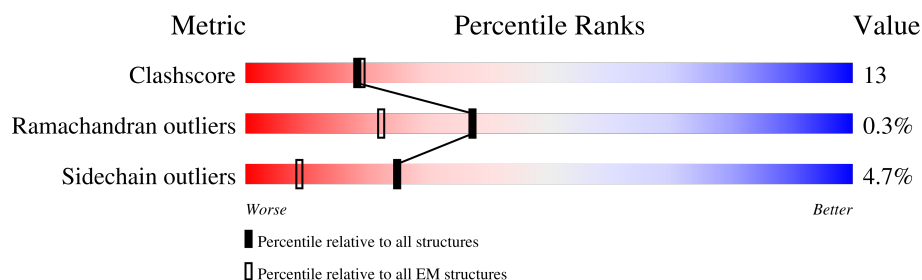
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.39 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	14220 (2.89 - 3.89)

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	C	309	
1	F	309	
2	B	670	
2	E	670	

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Mol	Chain	Length	Quality of chain
3	A	587	<div><div></div><div>21%</div><div>73%</div><div>23%</div><div>..</div></div>
3	D	587	<div><div></div><div>21%</div><div>73%</div><div>22%</div><div>..</div></div>
4	X	6	<div><div></div><div>33%</div><div>17%</div><div>33%</div><div>17%</div></div>
4	Y	6	<div><div></div><div>17%</div><div>17%</div><div>17%</div><div>33%</div><div>17%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19056 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 Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	290	Total	C	N	O	S	0	0
			2320	1469	397	439	15		
1	F	290	Total	C	N	O	S	0	0
			2320	1469	397	439	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	conflict	UNP P67775
F	88	ASN	ASP	conflict	UNP P67775

- Molecule 2 is a protein called RxLR effector protein PSR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	486	Total	C	N	O	S	0	0
			3425	2184	573	661	7		
2	E	486	Total	C	N	O	S	0	0
			3425	2184	573	661	7		

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A beta isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	569	Total	C	N	O	S	0	0
			3742	2359	661	709	13		
3	D	569	Total	C	N	O	S	0	0
			3742	2359	661	709	13		

- Molecule 4 is a protein called random substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	5	Total	C	N	O	P	0	0
			39	21	8	9	1		
4	Y	5	Total	C	N	O	P	0	0
			39	21	8	9	1		

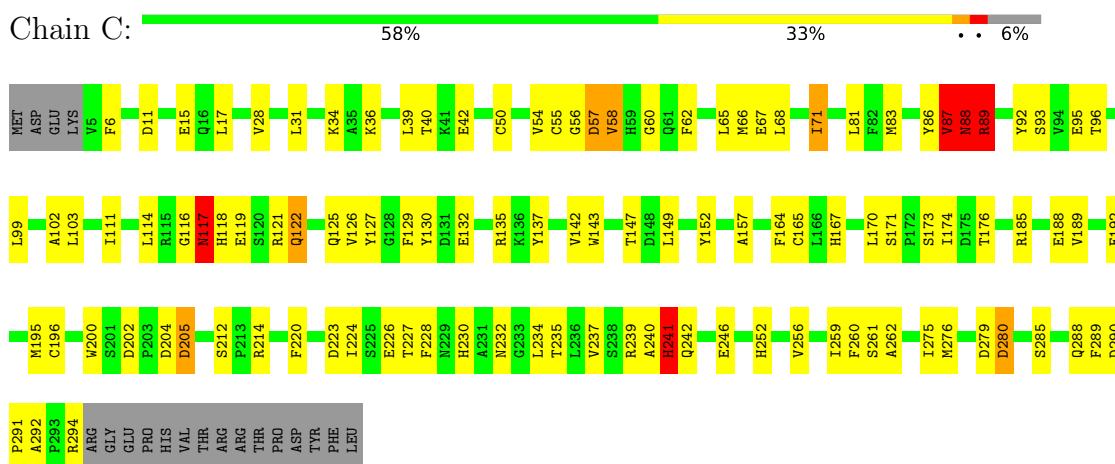
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Mn	0
			2	2	
5	F	2	Total	Mn	0
			2	2	

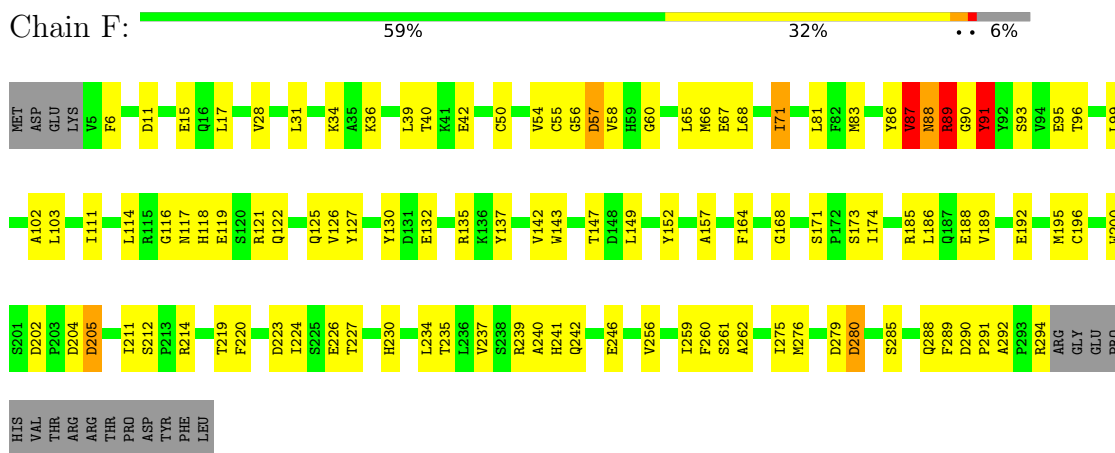
3 Residue-property plots [i](#)

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.

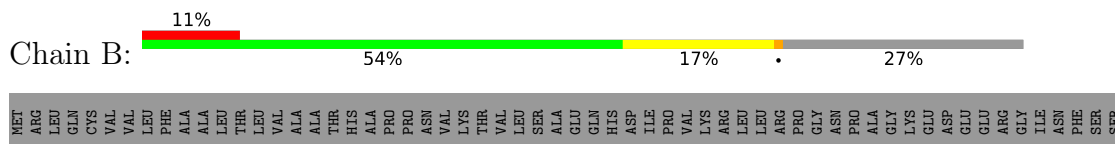
- Molecule 1: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

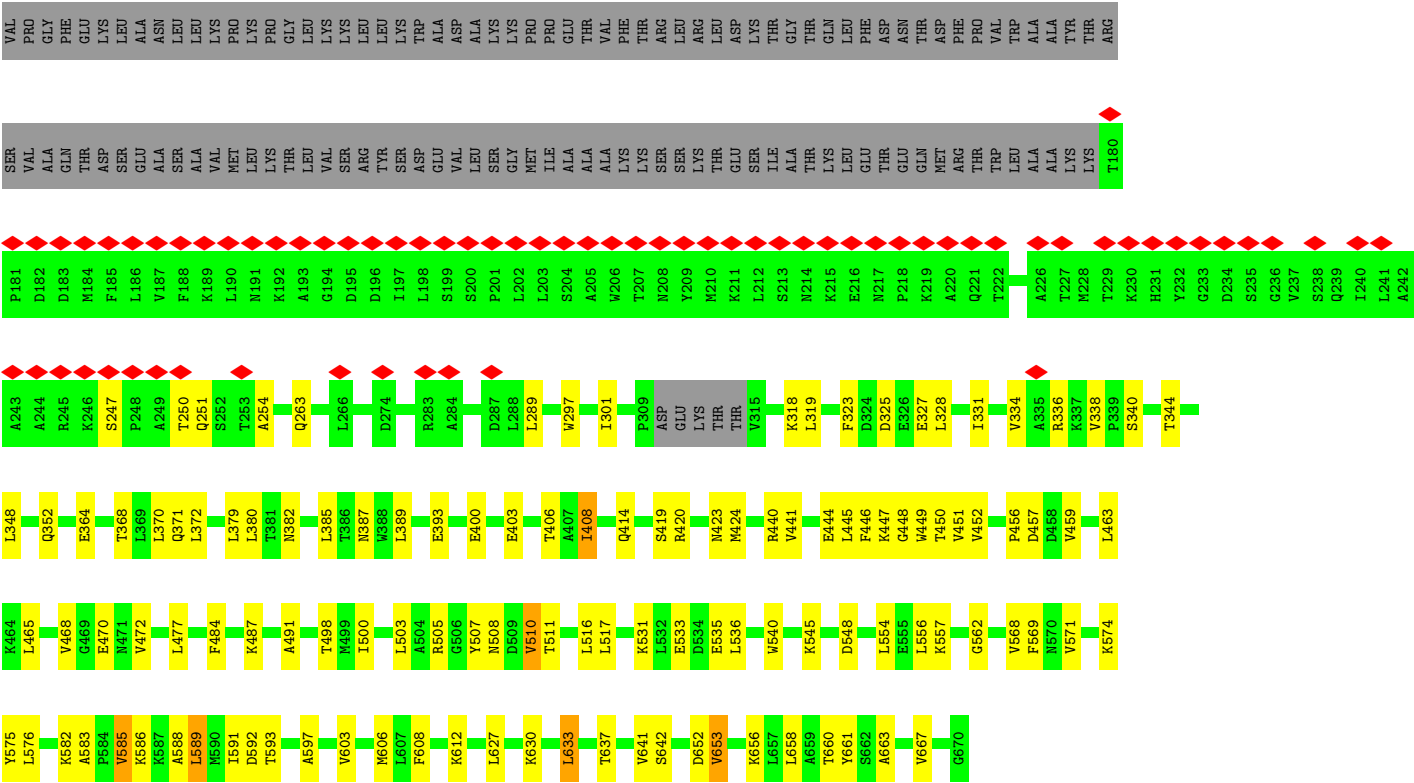


- Molecule 1: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

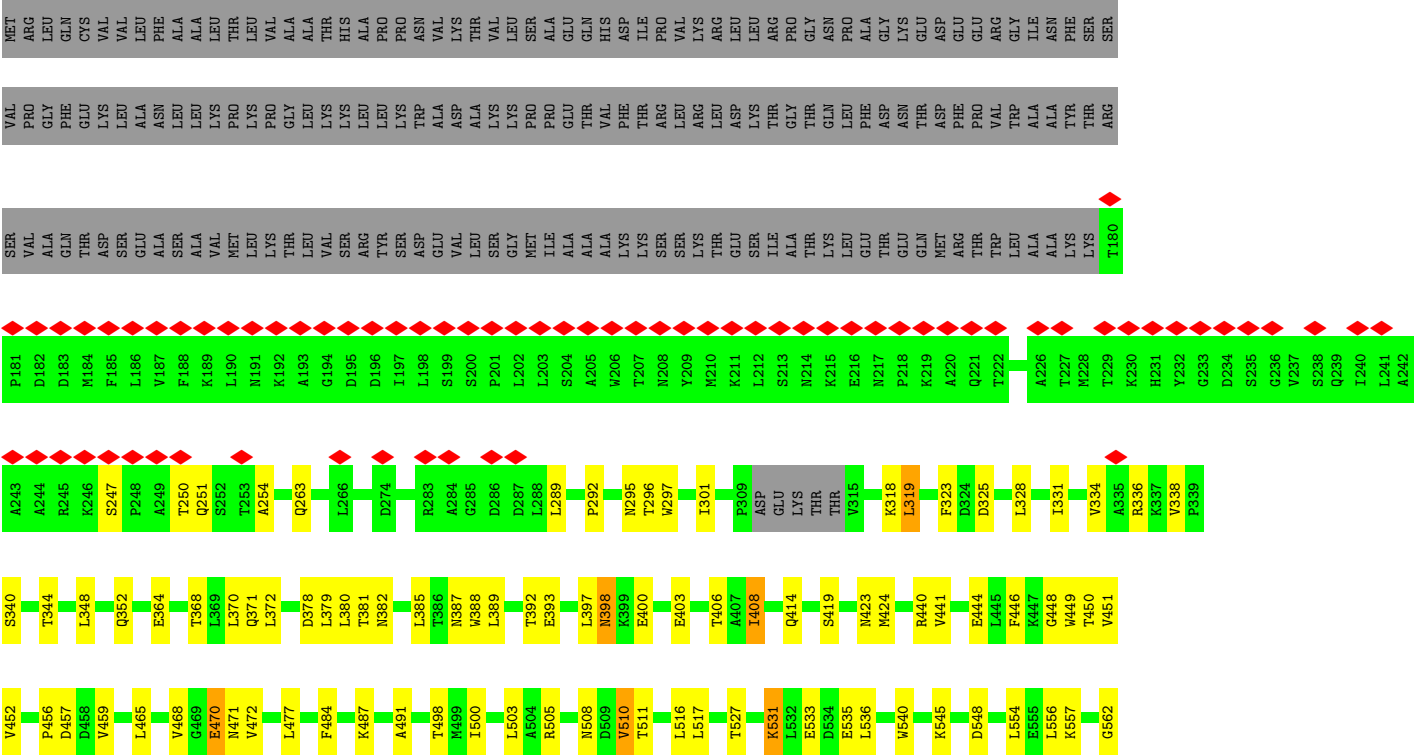


- Molecule 2: RxLR effector protein PSR2



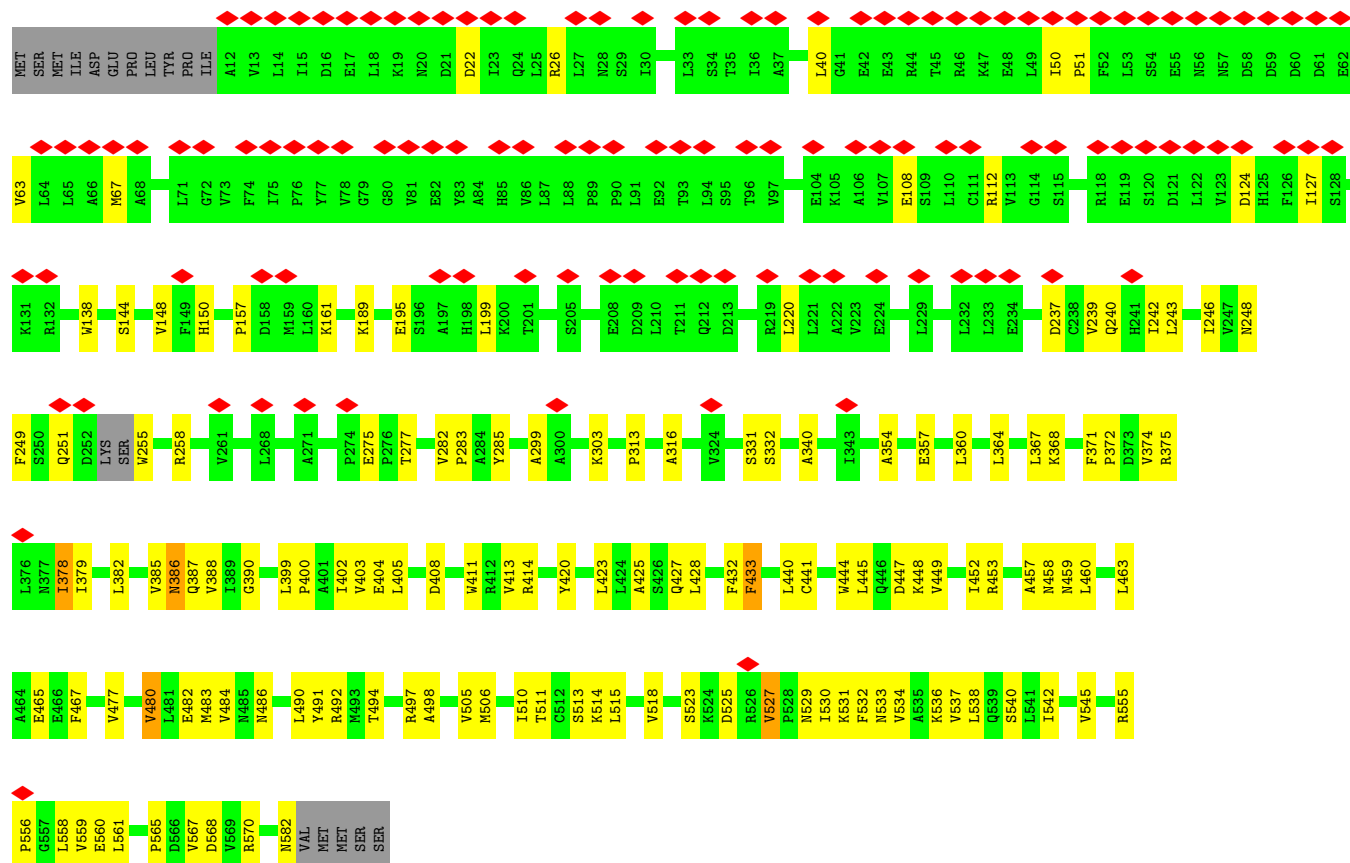
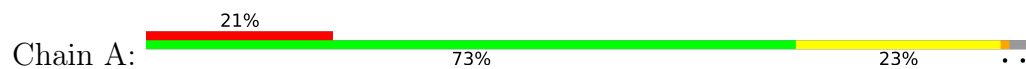


● Molecule 2: RxLR effector protein PSR2

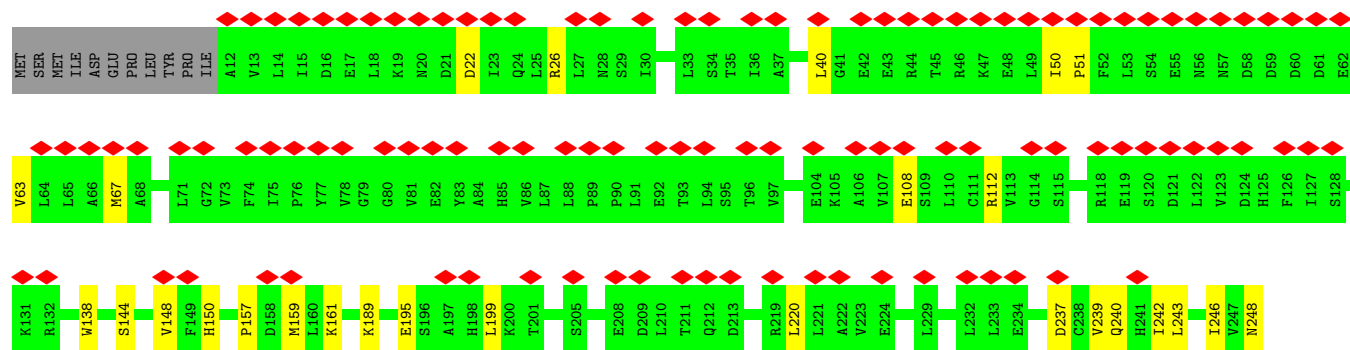
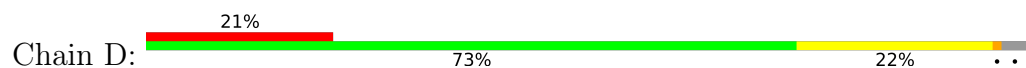


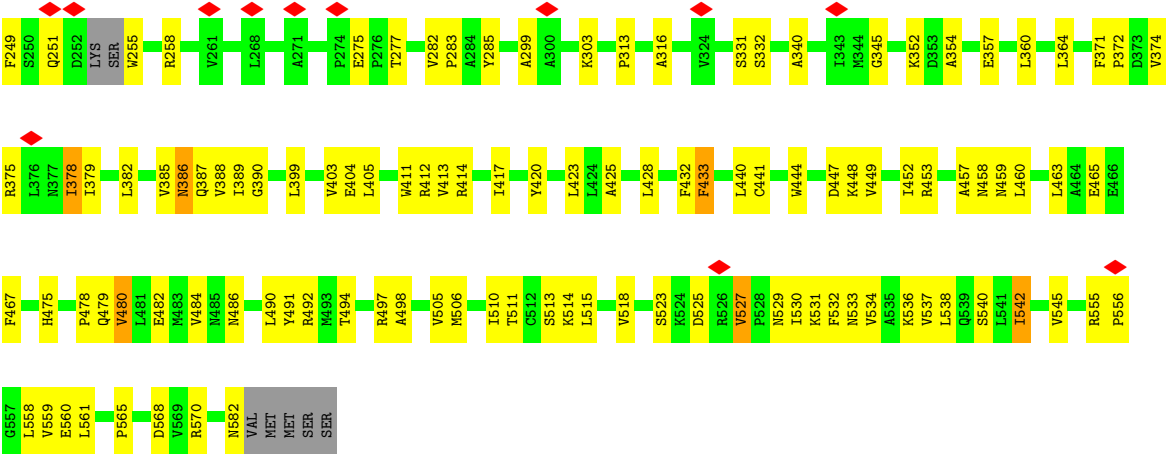


- Molecule 3: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A beta isoform

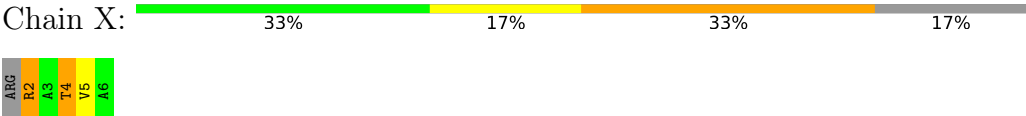


- Molecule 3: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A beta isoform

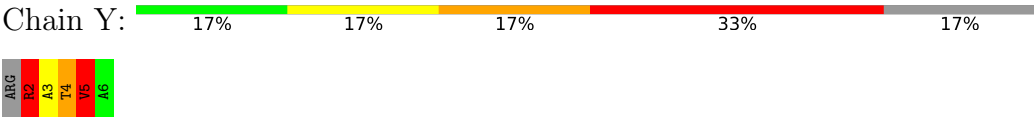




• Molecule 4: random substrate



• Molecule 4: random substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.681	Depositor
Minimum map value	-5.546	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.53	Depositor
Map size (\AA)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, TPO

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	C	0.37	2/2376 (0.1%)	0.56	3/3227 (0.1%)
1	F	0.31	2/2376 (0.1%)	0.52	6/3227 (0.2%)
2	B	0.15	0/3490	0.42	1/4783 (0.0%)
2	E	0.16	0/3490	0.43	1/4783 (0.0%)
3	A	0.15	0/3796	0.43	2/5226 (0.0%)
3	D	0.16	0/3796	0.43	2/5226 (0.0%)
4	X	0.62	0/26	1.25	0/32
4	Y	0.68	0/26	1.10	0/32
All	All	0.22	4/19376 (0.0%)	0.46	15/26536 (0.1%)

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
4	X	0	1
4	Y	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	VAL	C-O	-6.07	1.17	1.24
1	C	87	VAL	C-O	-5.94	1.17	1.24
1	C	117	ASN	C-O	-5.27	1.17	1.24
1	F	90	GLY	C-N	-5.02	1.27	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	ASN	CB-CA-C	-12.42	85.04	110.38
1	C	87	VAL	N-CA-CB	-8.10	100.81	111.82
1	F	87	VAL	CB-CA-C	-7.44	100.37	110.42
1	F	90	GLY	CA-C-N	-7.05	110.85	120.44
1	F	90	GLY	C-N-CA	-7.05	110.85	120.44
1	F	87	VAL	N-CA-CB	-6.68	102.73	111.82
1	F	91	TYR	CA-C-O	-5.75	114.78	120.70
3	A	386	ASN	N-CA-C	-5.43	105.36	111.28
3	D	386	ASN	N-CA-C	-5.41	105.39	111.28
1	F	87	VAL	CA-C-O	-5.37	114.85	120.27
2	B	408	ILE	N-CA-C	-5.33	108.31	113.53
3	A	390	GLY	N-CA-C	5.22	118.56	112.50
3	D	390	GLY	N-CA-C	5.22	118.55	112.50
2	E	408	ILE	N-CA-C	-5.17	108.80	113.71
1	C	117	ASN	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	X	2	ARG	Sidechain
4	Y	2	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	C	2320	0	2208	84	0
1	F	2320	0	2208	78	0
2	B	3425	0	3106	77	0
2	E	3425	0	3106	81	0
3	A	3742	0	3258	83	0
3	D	3742	0	3258	80	0
4	X	39	0	36	4	0
4	Y	39	0	36	6	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	19056	0	17216	475	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 13.

All (475) 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:C:117:ASN:HD21	1:C:241:HIS:HE1	1.15	0.89
3:A:50:ILE:HG13	3:A:51:PRO:HD3	1.66	0.78
1:C:117:ASN:HD21	1:C:241:HIS:CE1	2.01	0.78
1:C:83:MET:HE1	1:C:165:CYS:HB3	1.63	0.77
3:D:50:ILE:HG13	3:D:51:PRO:HD3	1.66	0.76
1:C:93:SER:OG	1:C:132:GLU:OE2	2.03	0.75
1:C:164:PHE:HB2	1:C:234:LEU:HD13	1.67	0.75
1:C:42:GLU:O	1:C:185:ARG:NH2	2.20	0.75
1:F:42:GLU:O	1:F:185:ARG:NH2	2.20	0.75
3:D:157:PRO:HD2	3:D:161:LYS:HE3	1.70	0.74
1:C:176:THR:HA	1:C:232:ASN:HD21	1.53	0.74
3:A:157:PRO:HD2	3:A:161:LYS:HE3	1.70	0.73
1:C:152:TYR:O	1:C:185:ARG:NH1	2.23	0.71
3:A:275:GLU:HG3	3:A:277:THR:HG22	1.73	0.71
1:C:280:ASP:N	1:C:280:ASP:OD1	2.24	0.70
1:F:152:TYR:O	1:F:185:ARG:NH1	2.23	0.70
3:D:275:GLU:HG3	3:D:277:THR:HG22	1.73	0.70
1:F:280:ASP:N	1:F:280:ASP:OD1	2.25	0.69
3:A:525:ASP:O	3:A:531:LYS:NZ	2.26	0.68
1:F:164:PHE:HB2	1:F:234:LEU:HD13	1.75	0.68
1:C:54:VAL:HG22	1:C:81:LEU:HD23	1.75	0.68
1:F:89:ARG:NH2	4:Y:4:TPO:O1P	2.27	0.67
1:F:93:SER:HB3	1:F:132:GLU:OE1	1.94	0.67
2:E:642:SER:HA	2:E:658:LEU:HD21	1.75	0.67
1:C:117:ASN:ND2	1:C:241:HIS:HE1	1.90	0.67
3:A:371:PHE:HB3	3:A:374:VAL:HG12	1.76	0.67
1:F:88:ASN:ND2	1:F:127:TYR:HB2	2.10	0.67
2:E:419:SER:O	2:E:423:ASN:ND2	2.29	0.66
1:C:226:GLU:O	1:C:230:HIS:ND1	2.28	0.66
1:C:36:LYS:O	1:C:40:THR:HG23	1.96	0.66
3:D:371:PHE:HB3	3:D:374:VAL:HG12	1.78	0.66
1:F:54:VAL:HB	1:F:276:MET:HB3	1.77	0.65
1:F:95:GLU:N	1:F:95:GLU:OE1	2.29	0.65
1:F:246:GLU:O	1:F:288:GLN:NE2	2.29	0.65
2:E:372:LEU:HD11	2:E:385:LEU:HA	1.78	0.65
1:F:36:LYS:O	1:F:40:THR:HG23	1.96	0.65
3:D:525:ASP:O	3:D:531:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:447:ASP:O	3:D:453:ARG:NH1	2.28	0.65
2:B:642:SER:HA	2:B:658:LEU:HD21	1.78	0.65
3:A:447:ASP:O	3:A:453:ARG:NH1	2.29	0.65
1:C:246:GLU:O	1:C:288:GLN:NE2	2.29	0.64
2:E:516:LEU:HD21	2:E:533:GLU:HB2	1.79	0.64
1:C:292:ALA:O	1:C:294:ARG:NH1	2.30	0.64
3:D:63:VAL:O	3:D:67:MET:HG3	1.98	0.64
1:C:87:VAL:O	1:C:88:ASN:HB2	1.98	0.64
3:A:150:HIS:HA	3:A:189:LYS:HD2	1.80	0.64
3:A:63:VAL:O	3:A:67:MET:HG3	1.98	0.64
1:F:292:ALA:O	1:F:294:ARG:NH1	2.30	0.64
2:B:540:TRP:HB3	2:B:575:TYR:HE2	1.63	0.63
1:F:226:GLU:O	1:F:230:HIS:ND1	2.29	0.63
2:E:540:TRP:HB3	2:E:575:TYR:HE2	1.63	0.63
2:B:372:LEU:HD11	2:B:385:LEU:HA	1.80	0.63
1:F:118:HIS:NE2	4:Y:4:TPO:P	2.72	0.63
3:D:150:HIS:HA	3:D:189:LYS:HD2	1.80	0.63
1:F:87:VAL:O	1:F:88:ASN:HB2	1.98	0.63
2:B:557:LYS:HG2	2:B:597:ALA:HB1	1.81	0.62
2:E:554:LEU:HB3	2:E:556:LEU:HD13	1.81	0.62
1:C:132:GLU:HA	1:C:135:ARG:HB3	1.80	0.62
2:B:419:SER:O	2:B:423:ASN:ND2	2.33	0.62
2:E:378:ASP:OD1	2:E:381:THR:OG1	2.14	0.62
2:B:554:LEU:HB3	2:B:556:LEU:HD13	1.81	0.62
3:D:531:LYS:HG2	3:D:561:LEU:HD11	1.81	0.62
1:C:67:GLU:HB2	1:C:292:ALA:HB2	1.82	0.61
2:B:641:VAL:HG21	2:B:661:TYR:CZ	2.35	0.61
1:F:202:ASP:HA	1:F:239:ARG:NH1	2.16	0.61
1:C:56:GLY:N	1:C:261:SER:OG	2.29	0.61
2:B:516:LEU:HD21	2:B:533:GLU:HB2	1.82	0.61
1:F:223:ASP:O	1:F:227:THR:HG23	2.00	0.61
1:F:58:VAL:HG23	1:F:86:TYR:HA	1.83	0.61
1:F:67:GLU:HB2	1:F:292:ALA:HB2	1.83	0.61
1:F:132:GLU:HA	1:F:135:ARG:HB3	1.81	0.61
2:E:557:LYS:HG2	2:E:597:ALA:HB1	1.81	0.61
1:F:117:ASN:ND2	4:Y:4:TPO:O3P	2.33	0.60
2:E:641:VAL:HG21	2:E:661:TYR:CZ	2.36	0.60
3:D:506:MET:O	3:D:511:THR:OG1	2.18	0.60
1:C:95:GLU:OE1	1:C:95:GLU:N	2.30	0.60
1:C:118:HIS:NE2	4:X:4:TPO:P	2.74	0.60
3:A:531:LYS:HG2	3:A:561:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:456:PRO:HA	2:E:459:VAL:HG12	1.82	0.60
1:F:83:MET:HE3	1:F:240:ALA:HB2	1.82	0.60
1:C:202:ASP:HA	1:C:239:ARG:NH1	2.16	0.60
2:B:642:SER:HB2	2:B:658:LEU:HD11	1.83	0.59
1:C:239:ARG:NH2	1:C:240:ALA:O	2.36	0.59
3:D:494:THR:HG22	3:D:497:ARG:HH21	1.68	0.59
1:C:58:VAL:HG23	1:C:86:TYR:HA	1.84	0.58
3:D:372:PRO:HA	3:D:375:ARG:HH11	1.67	0.58
1:C:205:ASP:OD1	1:C:205:ASP:N	2.37	0.58
2:B:556:LEU:HD21	2:B:569:PHE:HA	1.86	0.58
2:E:642:SER:HB2	2:E:658:LEU:HD11	1.85	0.58
2:E:556:LEU:HD21	2:E:569:PHE:HA	1.86	0.58
1:C:223:ASP:O	1:C:227:THR:HG23	2.04	0.57
3:D:248:ASN:HA	3:D:251:GLN:HG3	1.86	0.57
3:D:352:LYS:HE2	3:D:389:ILE:HD13	1.85	0.57
1:F:117:ASN:HD21	1:F:241:HIS:HE1	1.52	0.57
1:F:196:CYS:HG	1:F:200:TRP:CD1	2.23	0.57
1:C:56:GLY:HA2	1:C:83:MET:HB2	1.86	0.57
1:C:66:MET:HE3	1:C:66:MET:HA	1.87	0.57
3:A:331:SER:OG	3:A:332:SER:N	2.38	0.57
1:F:66:MET:HE3	1:F:66:MET:HA	1.87	0.57
2:E:380:LEU:HD11	2:E:441:VAL:HG11	1.87	0.57
1:F:239:ARG:NH2	1:F:240:ALA:O	2.37	0.56
1:C:121:ARG:N	1:C:188:GLU:OE2	2.38	0.56
2:B:456:PRO:HA	2:B:459:VAL:HG12	1.88	0.56
2:E:591:ILE:HD12	2:E:592:ASP:N	2.21	0.56
2:B:608:PHE:O	2:B:612:LYS:NZ	2.38	0.56
2:E:556:LEU:HD11	2:E:568:VAL:HG12	1.87	0.56
1:F:121:ARG:N	1:F:188:GLU:OE2	2.39	0.56
1:F:205:ASP:N	1:F:205:ASP:OD1	2.36	0.56
3:D:331:SER:OG	3:D:332:SER:N	2.38	0.56
3:D:529:ASN:HA	3:D:532:PHE:CE2	2.42	0.55
2:B:591:ILE:HD12	2:B:592:ASP:N	2.21	0.55
1:C:86:TYR:OH	1:C:114:LEU:O	2.16	0.55
2:B:556:LEU:HD11	2:B:568:VAL:HG12	1.87	0.55
2:E:379:LEU:H	2:E:424:MET:HE1	1.70	0.55
3:A:282:VAL:HA	3:A:285:TYR:HB3	1.89	0.55
1:C:103:LEU:HB3	1:C:111:ILE:HG21	1.88	0.55
1:F:279:ASP:OD1	1:F:279:ASP:N	2.40	0.54
3:A:399:LEU:O	3:A:403:VAL:HG23	2.08	0.54
2:E:380:LEU:HD23	2:E:424:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:LEU:HD11	2:B:441:VAL:HG11	1.89	0.54
3:A:248:ASN:HA	3:A:251:GLN:HG3	1.87	0.54
3:A:529:ASN:HA	3:A:532:PHE:CE2	2.42	0.54
1:C:88:ASN:OD1	1:C:127:TYR:HB2	2.06	0.54
1:C:89:ARG:NH2	4:X:4:TPO:O2P	2.35	0.54
3:A:246:ILE:HA	3:A:249:PHE:HB2	1.90	0.54
2:B:250:THR:O	2:B:254:ALA:N	2.41	0.54
2:B:459:VAL:HG11	2:B:484:PHE:CD2	2.42	0.54
1:F:28:VAL:HG11	1:F:142:VAL:HG23	1.90	0.54
1:C:240:ALA:O	1:C:241:HIS:CB	2.55	0.54
1:F:56:GLY:N	1:F:261:SER:OG	2.31	0.54
3:D:282:VAL:HA	3:D:285:TYR:HB3	1.89	0.54
2:E:446:PHE:HB3	2:E:487:LYS:HE2	1.89	0.54
1:C:57:ASP:OD1	1:C:240:ALA:HB1	2.07	0.54
1:F:68:LEU:HG	1:F:275:ILE:HD11	1.88	0.54
1:C:279:ASP:N	1:C:279:ASP:OD1	2.40	0.53
2:B:459:VAL:HG11	2:B:484:PHE:HD2	1.73	0.53
2:E:459:VAL:HG11	2:E:484:PHE:CD2	2.43	0.53
2:E:370:LEU:O	2:E:371:GLN:HG3	2.09	0.53
1:F:60:GLY:HA2	1:F:96:THR:HG21	1.89	0.53
2:E:459:VAL:HG11	2:E:484:PHE:HD2	1.74	0.53
2:E:562:GLY:HA2	2:E:606:MET:HG3	1.89	0.53
3:D:538:LEU:O	3:D:542:ILE:HD13	2.08	0.53
3:D:399:LEU:O	3:D:403:VAL:HG23	2.09	0.53
3:A:340:ALA:HB3	3:A:378:ILE:HD11	1.91	0.53
1:F:57:ASP:OD1	1:F:240:ALA:HB1	2.09	0.53
3:D:246:ILE:HA	3:D:249:PHE:HB2	1.89	0.53
1:C:173:SER:HA	2:E:637:THR:HG21	1.90	0.52
2:B:370:LEU:O	2:B:371:GLN:HG3	2.09	0.52
2:B:562:GLY:HA2	2:B:606:MET:HG3	1.90	0.52
2:E:328:LEU:HA	2:E:331:ILE:HD12	1.92	0.52
2:B:446:PHE:O	2:B:450:THR:HG22	2.10	0.52
3:A:510:ILE:O	3:A:514:LYS:HG3	2.10	0.52
2:E:250:THR:O	2:E:254:ALA:N	2.41	0.52
2:E:400:GLU:HB3	2:E:403:GLU:HG2	1.90	0.52
3:D:405:LEU:HD23	3:D:440:LEU:HD21	1.91	0.52
3:D:433:PHE:CZ	3:D:463:LEU:HD11	2.45	0.52
3:D:144:SER:O	3:D:148:VAL:HG22	2.10	0.52
2:E:589:LEU:HD13	2:E:589:LEU:H	1.75	0.52
3:A:405:LEU:HD23	3:A:440:LEU:HD21	1.91	0.51
3:D:510:ILE:O	3:D:514:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:397:LEU:O	2:E:398:ASN:HB2	2.11	0.51
2:E:656:LYS:O	2:E:660:THR:HG23	2.10	0.51
3:D:340:ALA:HB3	3:D:378:ILE:HD11	1.92	0.51
3:D:108:GLU:O	3:D:112:ARG:HG3	2.11	0.51
3:A:378:ILE:HG22	3:A:379:ILE:HD13	1.92	0.51
1:C:68:LEU:HG	1:C:275:ILE:HD11	1.91	0.51
3:A:368:LYS:HA	3:A:375:ARG:HH12	1.75	0.51
2:E:652:ASP:OD1	2:E:653:VAL:N	2.43	0.51
2:B:344:THR:O	2:B:348:LEU:HG	2.10	0.51
2:B:652:ASP:OD1	2:B:653:VAL:N	2.44	0.51
3:A:144:SER:O	3:A:148:VAL:HG22	2.10	0.51
1:F:54:VAL:HG22	1:F:81:LEU:HD23	1.92	0.51
1:F:114:LEU:HD21	1:F:157:ALA:HB2	1.91	0.51
3:A:536:LYS:NZ	3:A:540:SER:HB2	2.26	0.51
3:A:382:LEU:HA	3:A:385:VAL:HB	1.94	0.50
2:E:603:VAL:HG12	2:E:627:LEU:HD11	1.93	0.50
3:D:386:ASN:O	3:D:388:VAL:N	2.44	0.50
1:C:117:ASN:ND2	4:X:4:TPO:O1P	2.45	0.50
3:A:480:VAL:O	3:A:484:VAL:HG23	2.12	0.50
3:A:486:ASN:HD21	3:A:491:TYR:HB3	1.77	0.50
2:E:344:THR:O	2:E:348:LEU:HG	2.10	0.50
3:D:378:ILE:HG22	3:D:379:ILE:HD13	1.93	0.50
1:C:28:VAL:HG11	1:C:142:VAL:HG23	1.93	0.50
2:B:589:LEU:HD13	2:B:589:LEU:H	1.75	0.50
3:D:382:LEU:HA	3:D:385:VAL:HB	1.93	0.50
3:D:411:TRP:HB2	3:D:452:ILE:HD11	1.94	0.50
3:A:108:GLU:O	3:A:112:ARG:HG3	2.11	0.50
3:A:386:ASN:O	3:A:388:VAL:N	2.45	0.50
2:E:393:GLU:OE2	2:E:440:ARG:NH1	2.45	0.50
3:D:299:ALA:O	3:D:303:LYS:HG2	2.11	0.50
2:B:603:VAL:HG12	2:B:627:LEU:HD11	1.93	0.50
3:A:299:ALA:O	3:A:303:LYS:HG2	2.11	0.50
3:D:523:SER:HB2	3:D:534:VAL:HG11	1.92	0.50
1:F:137:TYR:CD2	1:F:142:VAL:HG11	2.47	0.50
3:A:523:SER:HB2	3:A:534:VAL:HG11	1.95	0.49
2:E:348:LEU:O	2:E:352:GLN:HG2	2.12	0.49
1:C:137:TYR:CD2	1:C:142:VAL:HG11	2.47	0.49
2:B:445:LEU:HD21	2:B:449:TRP:CZ2	2.47	0.49
3:D:542:ILE:HA	3:D:545:VAL:HG12	1.94	0.49
2:B:500:ILE:HD12	2:B:503:LEU:HB2	1.93	0.49
1:F:57:ASP:OD1	1:F:57:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:457:ASP:HB2	2:E:505:ARG:HD3	1.95	0.49
3:D:313:PRO:HB2	3:D:316:ALA:HB3	1.95	0.49
3:D:480:VAL:O	3:D:484:VAL:HG23	2.12	0.49
3:A:313:PRO:HB2	3:A:316:ALA:HB3	1.95	0.49
1:F:116:GLY:H	1:F:119:GLU:CD	2.21	0.49
2:E:500:ILE:HG12	2:E:536:LEU:HB2	1.94	0.49
3:D:239:VAL:HA	3:D:242:ILE:HD12	1.95	0.49
2:B:468:VAL:HB	2:B:472:VAL:HG12	1.95	0.49
2:E:406:THR:O	2:E:406:THR:OG1	2.31	0.49
2:E:468:VAL:HB	2:E:472:VAL:HG12	1.94	0.49
2:B:400:GLU:HB3	2:B:403:GLU:HG2	1.94	0.49
3:A:494:THR:HG22	3:A:497:ARG:HH21	1.78	0.48
1:F:259:ILE:HD13	1:F:276:MET:HB2	1.93	0.48
1:C:196:CYS:HG	1:C:200:TRP:CD1	2.32	0.48
2:B:637:THR:HG21	1:F:173:SER:HA	1.94	0.48
3:A:428:LEU:HD13	3:A:432:PHE:CG	2.48	0.48
1:F:103:LEU:HB3	1:F:111:ILE:HG21	1.94	0.48
2:B:348:LEU:O	2:B:352:GLN:HG2	2.13	0.48
2:B:393:GLU:OE2	2:B:440:ARG:NH1	2.46	0.48
2:B:457:ASP:OD1	2:B:457:ASP:N	2.44	0.48
1:C:60:GLY:HA2	1:C:96:THR:HG21	1.95	0.48
3:A:378:ILE:HG23	3:A:382:LEU:HD13	1.94	0.48
3:D:486:ASN:HD21	3:D:491:TYR:HB3	1.78	0.48
3:A:457:ALA:HB1	3:A:498:ALA:HB2	1.95	0.48
2:B:500:ILE:HG12	2:B:536:LEU:HB2	1.94	0.48
3:A:411:TRP:HB2	3:A:452:ILE:HD11	1.96	0.48
3:A:433:PHE:CZ	3:A:463:LEU:HD11	2.49	0.48
1:C:125:GLN:HA	1:C:130:TYR:HB2	1.94	0.48
3:A:490:LEU:C	3:A:492:ARG:H	2.22	0.48
3:D:490:LEU:C	3:D:492:ARG:H	2.22	0.48
2:B:406:THR:O	2:B:406:THR:OG1	2.32	0.48
3:A:22:ASP:O	3:A:26:ARG:N	2.44	0.48
3:D:386:ASN:O	3:D:387:GLN:C	2.56	0.48
2:B:379:LEU:HD13	2:B:424:MET:HE1	1.96	0.48
1:F:91:TYR:CD1	1:F:91:TYR:N	2.82	0.48
2:E:608:PHE:O	2:E:612:LYS:NZ	2.40	0.48
3:A:239:VAL:HA	3:A:242:ILE:HD12	1.95	0.47
3:A:482:GLU:OE1	3:A:482:GLU:N	2.35	0.47
2:E:508:ASN:ND2	2:E:511:THR:OG1	2.47	0.47
3:D:378:ILE:HG23	3:D:382:LEU:HD13	1.95	0.47
3:D:536:LYS:NZ	3:D:540:SER:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:PHE:HB2	1:F:224:ILE:HB	1.97	0.47
1:C:11:ASP:O	1:C:15:GLU:HG2	2.15	0.47
1:F:117:ASN:ND2	1:F:241:HIS:HE1	2.11	0.47
3:D:482:GLU:OE1	3:D:482:GLU:N	2.35	0.47
1:C:239:ARG:NH2	1:C:242:GLN:HB2	2.30	0.47
1:F:239:ARG:NH2	1:F:242:GLN:HB2	2.30	0.47
1:C:88:ASN:HD21	1:C:129:PHE:H	1.62	0.47
1:C:114:LEU:HD21	1:C:157:ALA:HB2	1.97	0.47
1:C:116:GLY:H	1:C:119:GLU:CD	2.23	0.47
1:C:119:GLU:OE1	1:C:119:GLU:N	2.47	0.47
2:B:289:LEU:HD21	2:B:348:LEU:HD21	1.96	0.47
2:B:364:GLU:O	2:B:368:THR:HG23	2.15	0.47
2:B:574:LYS:HB2	2:B:574:LYS:HE2	1.57	0.47
3:A:372:PRO:HG3	3:A:413:VAL:HG22	1.96	0.47
3:A:533:ASN:O	3:A:537:VAL:HG12	2.15	0.47
2:E:500:ILE:HD12	2:E:503:LEU:HB2	1.95	0.47
3:D:447:ASP:OD1	3:D:448:LYS:N	2.47	0.47
3:D:556:PRO:HA	3:D:559:VAL:HG22	1.97	0.47
1:C:188:GLU:HG2	2:B:491:ALA:O	2.15	0.47
2:B:328:LEU:HA	2:B:331:ILE:HD12	1.97	0.47
3:A:447:ASP:OD1	3:A:448:LYS:N	2.48	0.47
1:F:126:VAL:HG22	2:E:451:VAL:HG22	1.97	0.47
3:A:386:ASN:O	3:A:387:GLN:C	2.56	0.47
3:A:556:PRO:HA	3:A:559:VAL:HG22	1.96	0.47
1:F:241:HIS:HE1	4:Y:4:TPO:O3P	1.97	0.47
3:A:402:ILE:HG13	3:A:440:LEU:HD22	1.96	0.47
3:A:433:PHE:CE2	3:A:463:LEU:HD11	2.51	0.47
2:E:484:PHE:HD1	2:E:487:LYS:HE3	1.80	0.47
1:C:57:ASP:OD1	1:C:57:ASP:N	2.45	0.46
2:E:364:GLU:O	2:E:368:THR:HG23	2.15	0.46
3:D:404:GLU:OE2	3:D:417:ILE:HD11	2.16	0.46
1:C:117:ASN:OD1	1:C:117:ASN:N	2.44	0.46
1:F:117:ASN:ND2	1:F:241:HIS:CE1	2.83	0.46
2:E:297:TRP:O	2:E:301:ILE:HG22	2.15	0.46
3:D:527:VAL:HG13	3:D:530:ILE:HG22	1.98	0.46
1:F:11:ASP:O	1:F:15:GLU:HG2	2.15	0.46
2:E:289:LEU:HD21	2:E:348:LEU:HD21	1.97	0.46
3:D:433:PHE:CE2	3:D:463:LEU:HD11	2.50	0.46
3:D:533:ASN:O	3:D:537:VAL:HG12	2.15	0.46
3:D:22:ASP:OD1	3:D:22:ASP:N	2.45	0.46
3:D:555:ARG:HH12	3:D:558:LEU:HD23	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:TRP:O	2:B:301:ILE:HG22	2.16	0.46
2:E:540:TRP:HB3	2:E:575:TYR:CE2	2.49	0.46
2:E:582:LYS:HD3	2:E:583:ALA:N	2.31	0.46
2:E:585:VAL:HA	2:E:586:LYS:HA	1.65	0.46
1:C:189:VAL:HA	1:C:195:MET:HE2	1.98	0.46
3:A:565:PRO:O	3:A:570:ARG:NH2	2.49	0.46
1:C:143:TRP:O	1:C:147:THR:OG1	2.32	0.46
2:B:459:VAL:O	2:B:463:LEU:N	2.40	0.46
3:A:527:VAL:HG13	3:A:530:ILE:HG22	1.98	0.46
1:F:125:GLN:HA	1:F:130:TYR:HB2	1.98	0.46
2:E:388:TRP:O	2:E:392:THR:HG22	2.16	0.46
3:D:457:ALA:HB1	3:D:498:ALA:HB2	1.98	0.46
3:A:538:LEU:O	3:A:542:ILE:HD13	2.16	0.46
1:F:58:VAL:HG11	1:F:65:LEU:HD13	1.97	0.46
1:F:143:TRP:O	1:F:147:THR:OG1	2.33	0.46
3:D:195:GLU:O	3:D:199:LEU:CB	2.64	0.46
1:C:290:ASP:HB3	1:C:291:PRO:HD2	1.97	0.46
2:B:334:VAL:O	2:B:338:VAL:HG23	2.16	0.45
3:A:555:ARG:HH12	3:A:558:LEU:HD23	1.80	0.45
1:F:188:GLU:HG2	2:E:491:ALA:O	2.15	0.45
2:E:470:GLU:OE1	2:E:471:ASN:N	2.37	0.45
1:C:67:GLU:HG3	1:C:71:ILE:HD12	1.98	0.45
3:A:440:LEU:HG	3:A:444:TRP:NE1	2.32	0.45
1:F:189:VAL:HA	1:F:195:MET:HE2	1.98	0.45
2:E:508:ASN:HD22	2:E:510:VAL:HG13	1.82	0.45
3:D:565:PRO:O	3:D:570:ARG:NH2	2.49	0.45
3:A:195:GLU:O	3:A:199:LEU:CB	2.64	0.45
1:F:67:GLU:HG3	1:F:71:ILE:HD12	1.98	0.45
2:B:582:LYS:HD3	2:B:583:ALA:N	2.30	0.45
3:D:582:ASN:C	3:D:582:ASN:OD1	2.60	0.45
2:E:334:VAL:O	2:E:338:VAL:HG23	2.16	0.45
3:A:506:MET:O	3:A:511:THR:OG1	2.19	0.45
1:C:87:VAL:HG12	1:C:93:SER:HB2	1.99	0.45
1:C:121:ARG:H	1:C:188:GLU:CD	2.25	0.45
2:E:382:ASN:OD1	2:E:382:ASN:N	2.50	0.45
1:F:119:GLU:OE1	1:F:119:GLU:N	2.48	0.45
1:F:121:ARG:H	1:F:188:GLU:CD	2.25	0.45
2:E:641:VAL:HG12	2:E:645:LEU:HD12	1.99	0.45
4:Y:2:ARG:HB2	4:Y:3:ALA:H	1.47	0.45
2:B:503:LEU:O	2:B:507:TYR:HB2	2.17	0.44
1:C:55:CYS:SG	1:C:68:LEU:HD21	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:ILE:H	2:B:331:ILE:HG13	1.64	0.44
3:A:441:CYS:SG	3:A:460:LEU:HD12	2.58	0.44
3:D:282:VAL:N	3:D:283:PRO:HD2	2.32	0.44
1:C:252:HIS:HB2	1:C:256:VAL:HG12	1.98	0.44
3:A:282:VAL:N	3:A:283:PRO:HD2	2.32	0.44
3:A:441:CYS:HA	3:A:444:TRP:CZ2	2.52	0.44
1:F:122:GLN:O	1:F:126:VAL:HG23	2.17	0.44
1:C:171:SER:HB3	1:C:174:ILE:HG12	1.99	0.44
3:A:427:GLN:HE22	3:A:428:LEU:HG	1.83	0.44
3:A:445:LEU:HD23	3:A:483:MET:HE3	1.99	0.44
3:A:582:ASN:C	3:A:582:ASN:OD1	2.60	0.44
1:F:290:ASP:HB3	1:F:291:PRO:HD2	1.98	0.44
3:A:237:ASP:HA	3:A:240:GLN:HB2	2.00	0.44
1:C:58:VAL:HG11	1:C:65:LEU:HD13	2.00	0.44
1:C:170:LEU:HD22	1:C:228:PHE:CD2	2.53	0.44
2:B:382:ASN:OD1	2:B:382:ASN:N	2.51	0.44
3:A:542:ILE:HA	3:A:545:VAL:HG12	2.00	0.44
2:E:548:ASP:OD1	2:E:593:THR:OG1	2.36	0.44
2:B:457:ASP:HB2	2:B:505:ARG:HD2	1.99	0.44
3:A:360:LEU:O	3:A:364:LEU:HD13	2.18	0.44
1:F:260:PHE:CE2	1:F:262:ALA:HB3	2.53	0.44
1:C:54:VAL:HG13	1:C:83:MET:HE2	2.00	0.44
1:C:260:PHE:CE2	1:C:262:ALA:HB3	2.53	0.44
2:B:247:SER:O	2:B:251:GLN:N	2.51	0.44
1:F:6:PHE:CZ	1:F:34:LYS:HG3	2.53	0.44
1:C:122:GLN:O	1:C:126:VAL:HG23	2.18	0.44
3:D:465:GLU:HB2	3:D:505:VAL:HG21	2.00	0.44
2:B:575:TYR:CD1	2:B:575:TYR:C	2.95	0.43
3:A:465:GLU:HB2	3:A:505:VAL:HG21	2.00	0.43
2:B:548:ASP:OD1	2:B:593:THR:OG1	2.35	0.43
3:D:440:LEU:HG	3:D:444:TRP:NE1	2.33	0.43
2:B:408:ILE:HB	2:B:444:GLU:HG3	1.99	0.43
2:E:292:PRO:O	2:E:296:THR:HG23	2.18	0.43
2:E:575:TYR:CD1	2:E:575:TYR:C	2.95	0.43
2:E:663:ALA:O	2:E:667:VAL:HG13	2.18	0.43
3:D:414:ARG:HB3	3:D:452:ILE:HD13	2.00	0.43
2:B:508:ASN:ND2	2:B:511:THR:OG1	2.52	0.43
2:B:585:VAL:HA	2:B:586:LYS:HA	1.65	0.43
3:A:414:ARG:HB3	3:A:452:ILE:HD13	2.01	0.43
2:E:449:TRP:CE2	2:E:459:VAL:HG23	2.53	0.43
3:D:237:ASP:HA	3:D:240:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASN:ND2	1:C:241:HIS:CE1	2.74	0.43
1:C:192:GLU:OE1	1:C:192:GLU:N	2.52	0.43
3:A:558:LEU:HD12	3:A:558:LEU:HA	1.89	0.43
1:F:31:LEU:HD21	1:F:102:ALA:HB2	2.00	0.43
2:E:247:SER:O	2:E:251:GLN:N	2.52	0.43
2:B:318:LYS:HA	2:B:318:LYS:HD3	1.76	0.43
1:F:39:LEU:HD12	1:F:149:LEU:HD11	2.01	0.43
3:D:515:LEU:O	3:D:518:VAL:HG12	2.19	0.43
1:C:130:TYR:CE2	2:B:447:LYS:HB2	2.54	0.43
2:B:263:GLN:HG2	3:A:138:TRP:O	2.18	0.43
2:B:319:LEU:O	2:B:323:PHE:N	2.51	0.43
2:B:545:LYS:O	2:B:575:TYR:OH	2.34	0.43
2:E:627:LEU:HD23	2:E:627:LEU:HA	1.86	0.43
3:A:40:LEU:HD23	3:A:40:LEU:HA	1.83	0.43
2:E:608:PHE:HE1	2:E:645:LEU:HD23	1.84	0.43
2:B:663:ALA:O	2:B:667:VAL:HG13	2.18	0.43
2:E:448:GLY:O	2:E:452:VAL:HG23	2.19	0.43
2:B:498:THR:HB	2:B:535:GLU:OE2	2.19	0.42
1:F:192:GLU:N	1:F:192:GLU:OE1	2.51	0.42
2:E:498:THR:HB	2:E:535:GLU:OE2	2.19	0.42
3:D:360:LEU:O	3:D:364:LEU:HD13	2.19	0.42
1:C:275:ILE:HG13	1:C:289:PHE:HE1	1.85	0.42
3:A:515:LEU:O	3:A:518:VAL:HG12	2.19	0.42
1:F:55:CYS:SG	1:F:68:LEU:HD21	2.60	0.42
2:E:263:GLN:HG2	3:D:138:TRP:O	2.18	0.42
2:E:319:LEU:O	2:E:323:PHE:N	2.51	0.42
1:C:121:ARG:NH1	1:C:188:GLU:OE1	2.42	0.42
2:E:336:ARG:NH2	2:E:387:ASN:HD21	2.17	0.42
2:B:336:ARG:NH2	2:B:387:ASN:HD21	2.18	0.42
1:C:117:ASN:OD1	1:C:167:HIS:CD2	2.73	0.42
3:A:255:TRP:N	3:A:258:ARG:HH21	2.17	0.42
3:A:367:LEU:HD23	3:A:400:PRO:HB2	2.01	0.42
3:D:255:TRP:N	3:D:258:ARG:HH21	2.17	0.42
1:F:17:LEU:HD13	1:F:99:LEU:HA	2.01	0.42
2:E:408:ILE:HB	2:E:444:GLU:HG3	2.02	0.42
1:F:91:TYR:N	1:F:91:TYR:HD1	2.17	0.42
1:C:17:LEU:HD13	1:C:99:LEU:HA	2.02	0.42
1:F:202:ASP:OD2	1:F:214:ARG:HD2	2.20	0.42
2:E:446:PHE:O	2:E:450:THR:HG22	2.20	0.42
1:C:31:LEU:HD21	1:C:102:ALA:HB2	2.02	0.42
3:A:385:VAL:O	3:A:386:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:441:CYS:HA	3:A:444:TRP:CE2	2.55	0.42
3:D:479:GLN:HA	3:D:482:GLU:CD	2.45	0.42
2:B:465:LEU:HD23	2:B:465:LEU:HA	1.88	0.41
3:A:386:ASN:C	3:A:388:VAL:N	2.78	0.41
3:D:412:ARG:HD2	3:D:412:ARG:HA	1.84	0.41
3:D:458:ASN:OD1	3:D:459:ASN:N	2.53	0.41
1:C:126:VAL:HG22	2:B:451:VAL:HG22	2.01	0.41
1:F:171:SER:HB3	1:F:174:ILE:HG12	2.01	0.41
3:D:441:CYS:HA	3:D:444:TRP:CZ2	2.54	0.41
2:B:554:LEU:HD23	2:B:554:LEU:HA	1.80	0.41
2:E:568:VAL:O	2:E:571:VAL:HG12	2.20	0.41
2:E:574:LYS:HE2	2:E:574:LYS:HB2	1.57	0.41
3:D:428:LEU:HD13	3:D:432:PHE:CG	2.55	0.41
1:C:6:PHE:CZ	1:C:34:LYS:HG3	2.55	0.41
3:D:243:LEU:HA	3:D:246:ILE:HG12	2.01	0.41
1:C:220:PHE:HB2	1:C:224:ILE:HB	2.03	0.41
2:B:420:ARG:HA	2:B:423:ASN:HD22	1.86	0.41
2:B:656:LYS:O	2:B:660:THR:HG23	2.21	0.41
3:A:22:ASP:OD1	3:A:22:ASP:N	2.45	0.41
1:F:93:SER:HA	1:F:96:THR:HG22	2.02	0.41
1:F:168:GLY:O	1:F:239:ARG:HD2	2.20	0.41
1:F:275:ILE:HG13	1:F:289:PHE:HE1	1.85	0.41
2:E:545:LYS:O	2:E:575:TYR:OH	2.35	0.41
3:A:404:GLU:O	3:A:408:ASP:HB2	2.20	0.41
2:E:318:LYS:HA	2:E:318:LYS:HD3	1.76	0.41
1:C:62:PHE:HB2	1:C:92:TYR:HB2	2.03	0.41
2:B:465:LEU:HD21	2:B:477:LEU:HB2	2.02	0.41
3:A:420:TYR:HA	3:A:423:LEU:HD23	2.03	0.41
3:A:458:ASN:OD1	3:A:459:ASN:N	2.54	0.41
2:E:319:LEU:HD12	2:E:319:LEU:HA	1.92	0.41
3:D:345:GLY:HA2	3:D:385:VAL:HG21	2.03	0.41
3:D:386:ASN:C	3:D:388:VAL:N	2.77	0.41
1:F:127:TYR:OH	4:Y:5:VAL:HG12	2.21	0.41
1:F:202:ASP:HA	1:F:239:ARG:HH12	1.85	0.41
3:D:372:PRO:HG3	3:D:413:VAL:HG22	2.02	0.41
1:C:259:ILE:HD13	1:C:276:MET:HB2	2.02	0.41
2:B:327:GLU:O	2:B:331:ILE:HG13	2.21	0.41
2:B:338:VAL:HG12	2:B:340:SER:H	1.86	0.41
2:B:540:TRP:HB3	2:B:575:TYR:CE2	2.49	0.41
1:F:212:SER:OG	1:F:214:ARG:HG3	2.21	0.41
2:E:338:VAL:HG12	2:E:340:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:22:ASP:O	3:D:26:ARG:N	2.44	0.41
3:D:354:ALA:HA	3:D:357:GLU:HG2	2.03	0.41
3:D:405:LEU:HD21	3:D:444:TRP:CD1	2.56	0.41
3:D:420:TYR:HA	3:D:423:LEU:HD23	2.03	0.41
3:D:440:LEU:HG	3:D:444:TRP:CD1	2.56	0.41
1:C:39:LEU:HD12	1:C:149:LEU:HD11	2.02	0.41
1:C:212:SER:OG	1:C:214:ARG:HG3	2.20	0.41
2:B:576:LEU:HD11	2:B:588:ALA:O	2.21	0.41
1:F:202:ASP:O	1:F:219:THR:HA	2.20	0.41
2:E:527:THR:O	2:E:531:LYS:HD2	2.21	0.41
2:B:448:GLY:O	2:B:452:VAL:HG23	2.21	0.40
3:A:425:ALA:HB1	3:A:467:PHE:CZ	2.55	0.40
2:B:630:LYS:O	2:B:633:LEU:HG	2.21	0.40
2:E:465:LEU:HD21	2:E:477:LEU:HB2	2.03	0.40
3:A:243:LEU:HA	3:A:246:ILE:HG12	2.01	0.40
3:A:477:VAL:HG21	3:A:506:MET:HE1	2.03	0.40
2:E:630:LYS:O	2:E:633:LEU:HG	2.21	0.40
3:D:425:ALA:HB1	3:D:467:PHE:CZ	2.56	0.40
3:D:475:HIS:O	3:D:478:PRO:HD2	2.22	0.40
1:C:118:HIS:NE2	4:X:4:TPO:O2P	2.54	0.40
2:B:508:ASN:HD22	2:B:510:VAL:HG13	1.87	0.40
2:B:568:VAL:O	2:B:571:VAL:HG12	2.20	0.40
1:F:152:TYR:CE2	1:F:186:LEU:HD21	2.57	0.40
3:D:40:LEU:HD23	3:D:40:LEU:HA	1.84	0.40
1:C:88:ASN:CG	1:C:127:TYR:HB2	2.46	0.40
3:A:124:ASP:HA	3:A:127:ILE:HG12	2.03	0.40
3:A:354:ALA:HA	3:A:357:GLU:HG2	2.03	0.40
2:E:573:LEU:HD13	2:E:590:MET:HE1	2.03	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	C	288/309 (93%)	282 (98%)	3 (1%)	3 (1%)	12	40
1	F	288/309 (93%)	280 (97%)	6 (2%)	2 (1%)	18	47
2	B	482/670 (72%)	466 (97%)	16 (3%)	0	100	100
2	E	482/670 (72%)	464 (96%)	17 (4%)	1 (0%)	43	71
3	A	565/587 (96%)	532 (94%)	33 (6%)	0	100	100
3	D	565/587 (96%)	533 (94%)	32 (6%)	0	100	100
4	X	2/6 (33%)	2 (100%)	0	0	100	100
4	Y	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	2674/3144 (85%)	2560 (96%)	107 (4%)	7 (0%)	37	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	F	88	ASN
4	Y	5	VAL
1	F	89	ARG
1	C	241	HIS
2	E	398	ASN
1	C	89	ARG

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	C	251/274 (92%)	235 (94%)	16 (6%)	16	42
1	F	251/274 (92%)	237 (94%)	14 (6%)	19	46
2	B	307/573 (54%)	295 (96%)	12 (4%)	28	53
2	E	307/573 (54%)	294 (96%)	13 (4%)	26	52
3	A	305/516 (59%)	295 (97%)	10 (3%)	33	57
3	D	305/516 (59%)	293 (96%)	12 (4%)	28	53
4	X	2/3 (67%)	0	2 (100%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	2/3 (67%)	0	2 (100%)	0	0
All	All	1730/2732 (63%)	1649 (95%)	81 (5%)	25	50

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	50	CYS
1	C	57	ASP
1	C	58	VAL
1	C	71	ILE
1	C	87	VAL
1	C	88	ASN
1	C	89	ARG
1	C	117	ASN
1	C	122	GLN
1	C	204	ASP
1	C	205	ASP
1	C	235	THR
1	C	237	VAL
1	C	241	HIS
1	C	280	ASP
1	C	285	SER
2	B	325	ASP
2	B	389	LEU
2	B	414	GLN
2	B	470	GLU
2	B	487	LYS
2	B	510	VAL
2	B	517	LEU
2	B	531	LYS
2	B	585	VAL
2	B	589	LEU
2	B	633	LEU
2	B	653	VAL
3	A	220	LEU
3	A	378	ILE
3	A	433	PHE
3	A	449	VAL
3	A	480	VAL
3	A	513	SER
3	A	527	VAL
3	A	560	GLU

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Mol	Chain	Res	Type
3	A	567	VAL
3	A	568	ASP
4	X	2	ARG
4	X	5	VAL
1	F	50	CYS
1	F	57	ASP
1	F	71	ILE
1	F	87	VAL
1	F	89	ARG
1	F	91	TYR
1	F	204	ASP
1	F	205	ASP
1	F	211	ILE
1	F	235	THR
1	F	237	VAL
1	F	256	VAL
1	F	280	ASP
1	F	285	SER
2	E	295	ASN
2	E	319	LEU
2	E	325	ASP
2	E	389	LEU
2	E	414	GLN
2	E	470	GLU
2	E	510	VAL
2	E	517	LEU
2	E	531	LYS
2	E	585	VAL
2	E	589	LEU
2	E	633	LEU
2	E	653	VAL
3	D	159	MET
3	D	220	LEU
3	D	378	ILE
3	D	433	PHE
3	D	449	VAL
3	D	460	LEU
3	D	480	VAL
3	D	513	SER
3	D	527	VAL
3	D	542	ILE
3	D	560	GLU

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Mol	Chain	Res	Type
3	D	568	ASP
4	Y	2	ARG
4	Y	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	C	122	GLN
1	C	187	GLN
1	C	232	ASN
1	C	252	HIS
1	C	272	GLN
2	B	423	ASN
3	A	28	ASN
3	A	240	GLN
3	A	377	ASN
1	F	187	GLN
1	F	252	HIS
1	F	272	GLN
2	E	462	ASN
3	D	28	ASN
3	D	240	GLN
3	D	377	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TPO	X	4	5,4	8,10,11	0.98	1 (12%)	10,14,16	3.29	2 (20%)
4	TPO	Y	4	5,4	8,10,11	1.05	1 (12%)	10,14,16	3.68	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPO	X	4	5,4	-	1/9/11/13	-
4	TPO	Y	4	5,4	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	4	TPO	P-OG1	-2.07	1.55	1.59
4	X	4	TPO	P-OG1	-2.03	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	4	TPO	P-OG1-CB	-10.81	93.96	123.33
4	X	4	TPO	P-OG1-CB	-9.49	97.53	123.33
4	Y	4	TPO	O-C-CA	-3.24	116.43	124.77
4	X	4	TPO	O-C-CA	-3.00	117.05	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	4	TPO	N-CA-CB-CG2
4	Y	4	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	4	TPO	4	0
4	Y	4	TPO	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

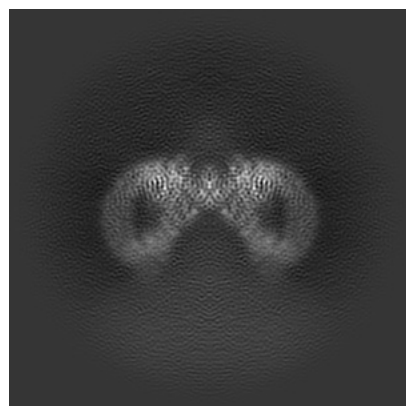
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61144. These allow visual inspection of the internal detail of the map and identification of artifacts.

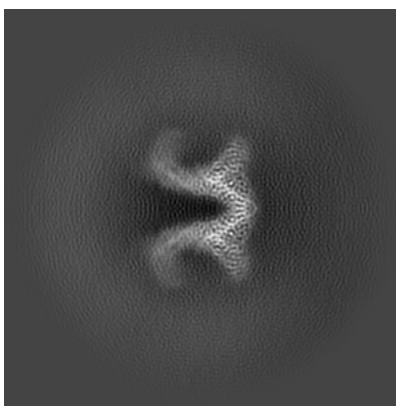
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

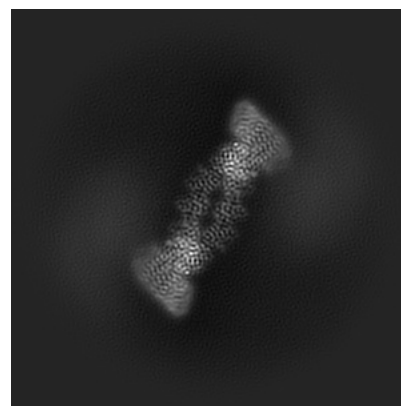
6.1.1 Primary map



X

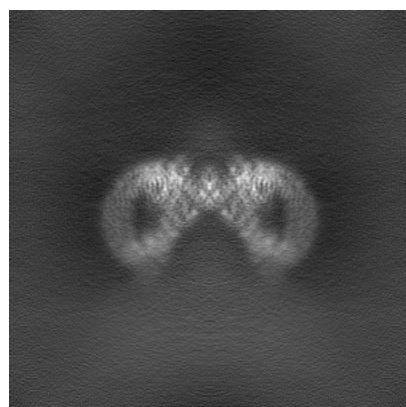


Y

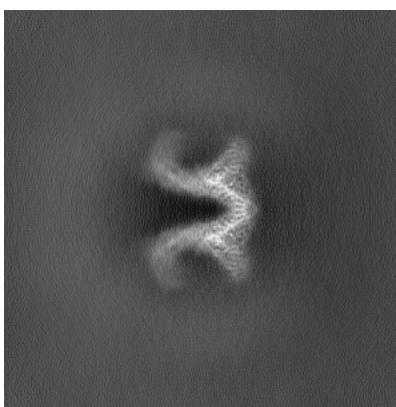


Z

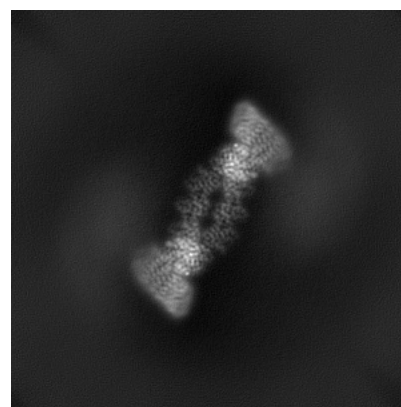
6.1.2 Raw map



X



Y

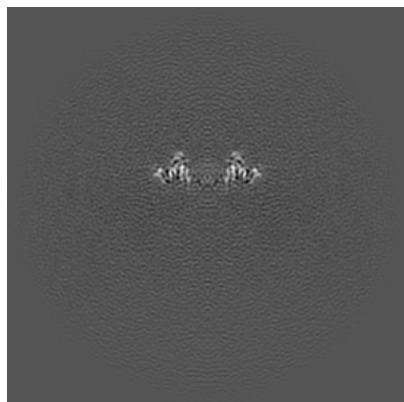


Z

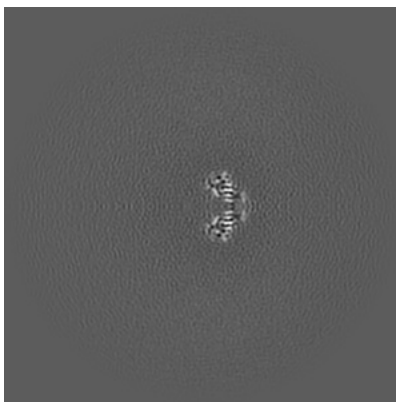
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

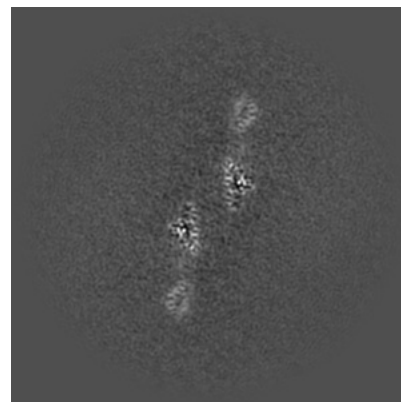
6.2.1 Primary map



X Index: 180

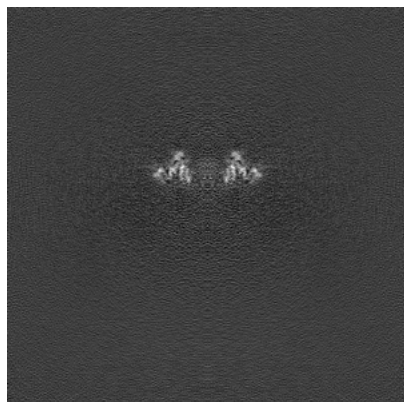


Y Index: 180



Z Index: 180

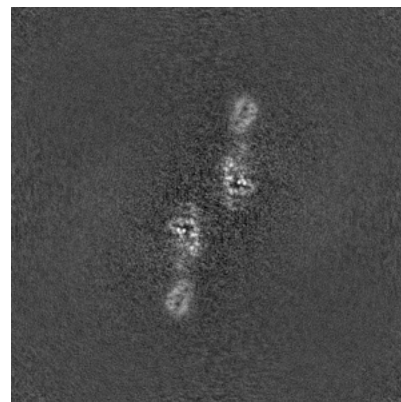
6.2.2 Raw map



X Index: 180



Y Index: 180

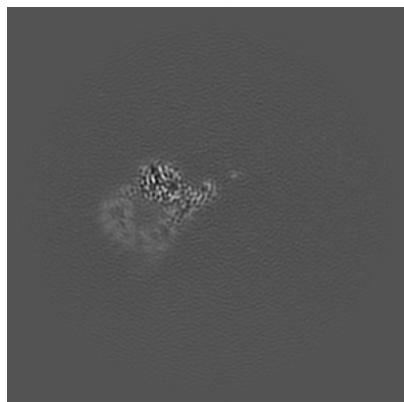


Z Index: 180

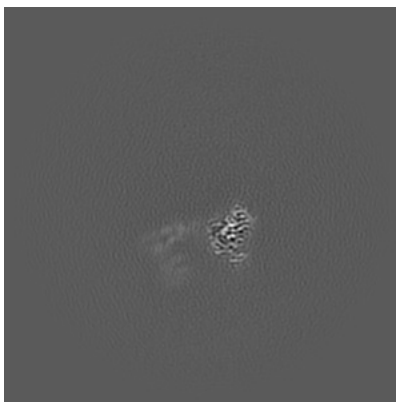
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

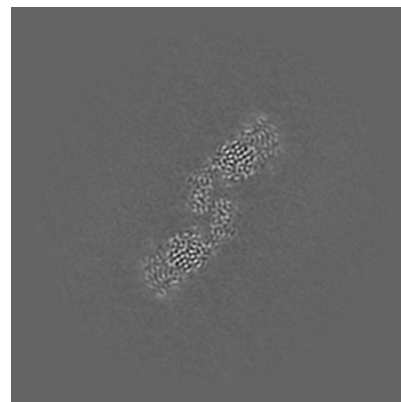
6.3.1 Primary map



X Index: 156

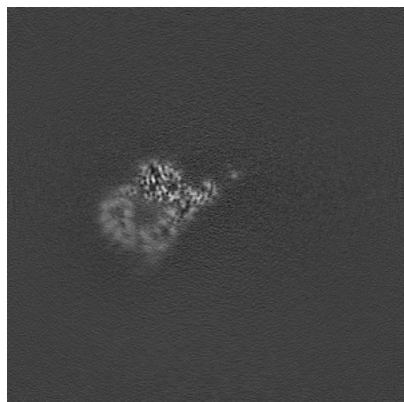


Y Index: 135

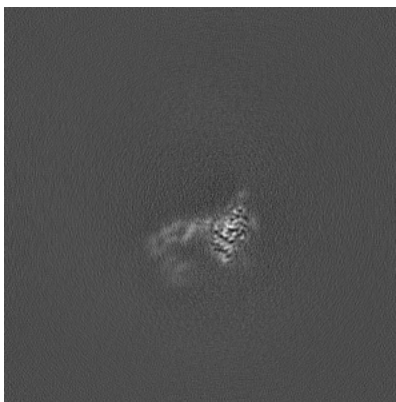


Z Index: 205

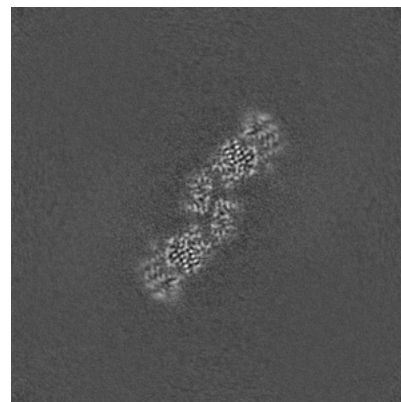
6.3.2 Raw map



X Index: 156



Y Index: 140

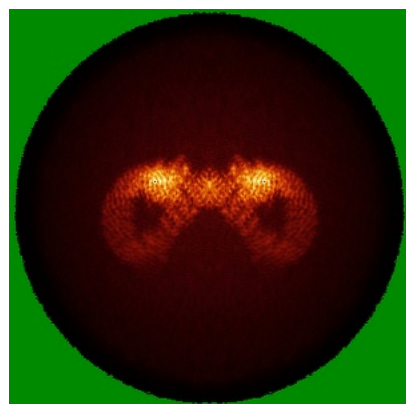


Z Index: 204

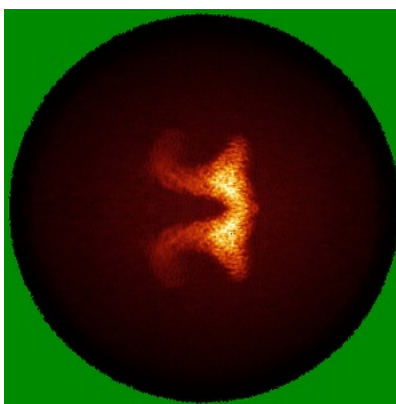
The images above show the largest variance slices of the map in three orthogonal directions.

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

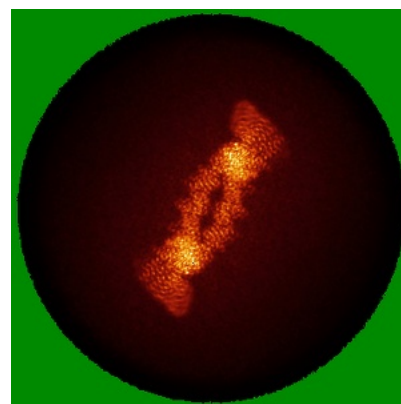
6.4.1 Primary map



X

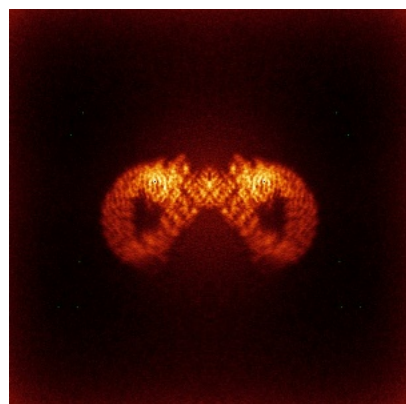


Y

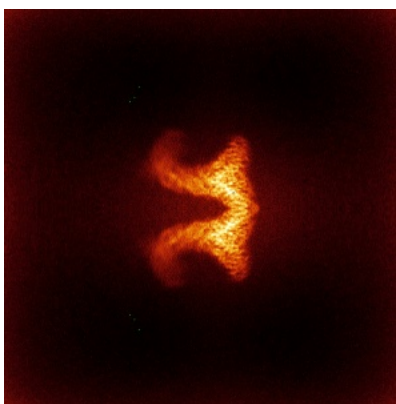


Z

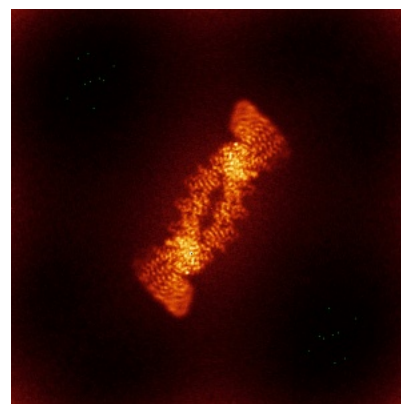
6.4.2 Raw map



X



Y

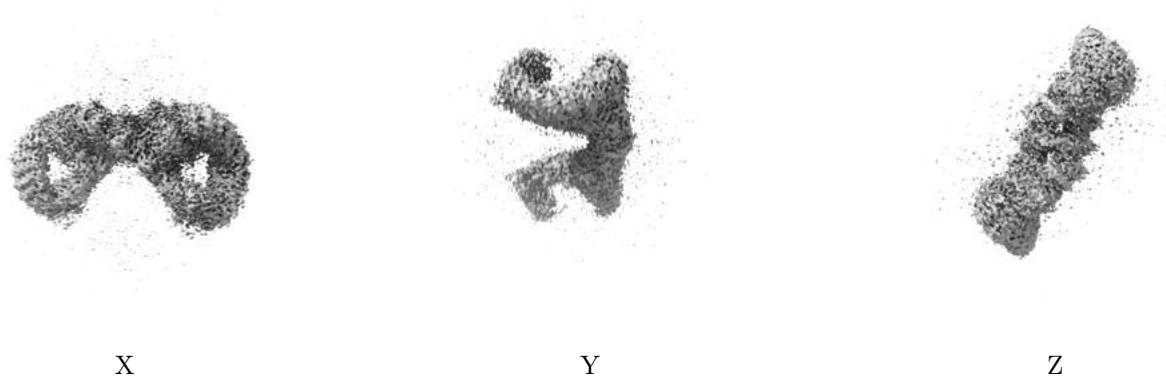


Z

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.

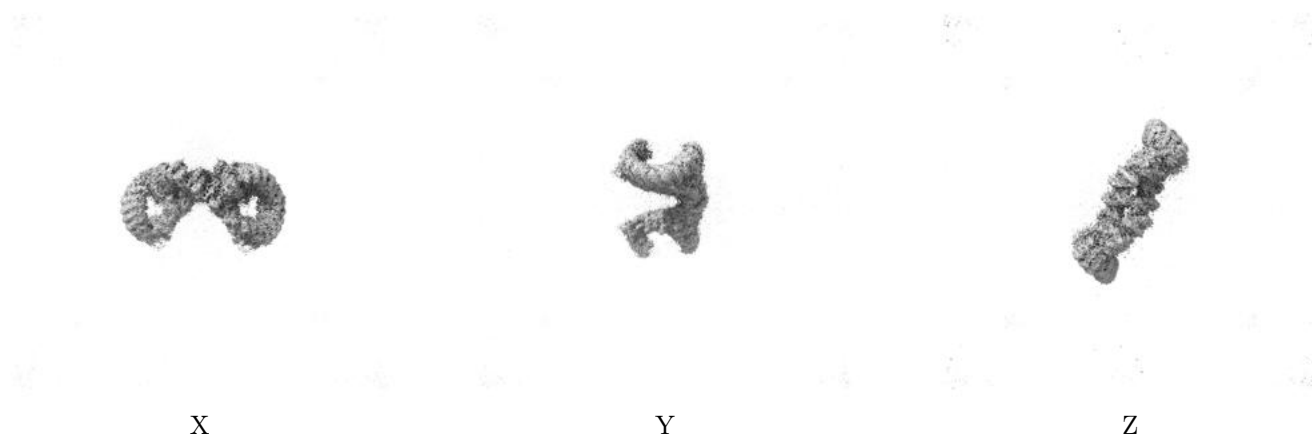
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.53. 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.

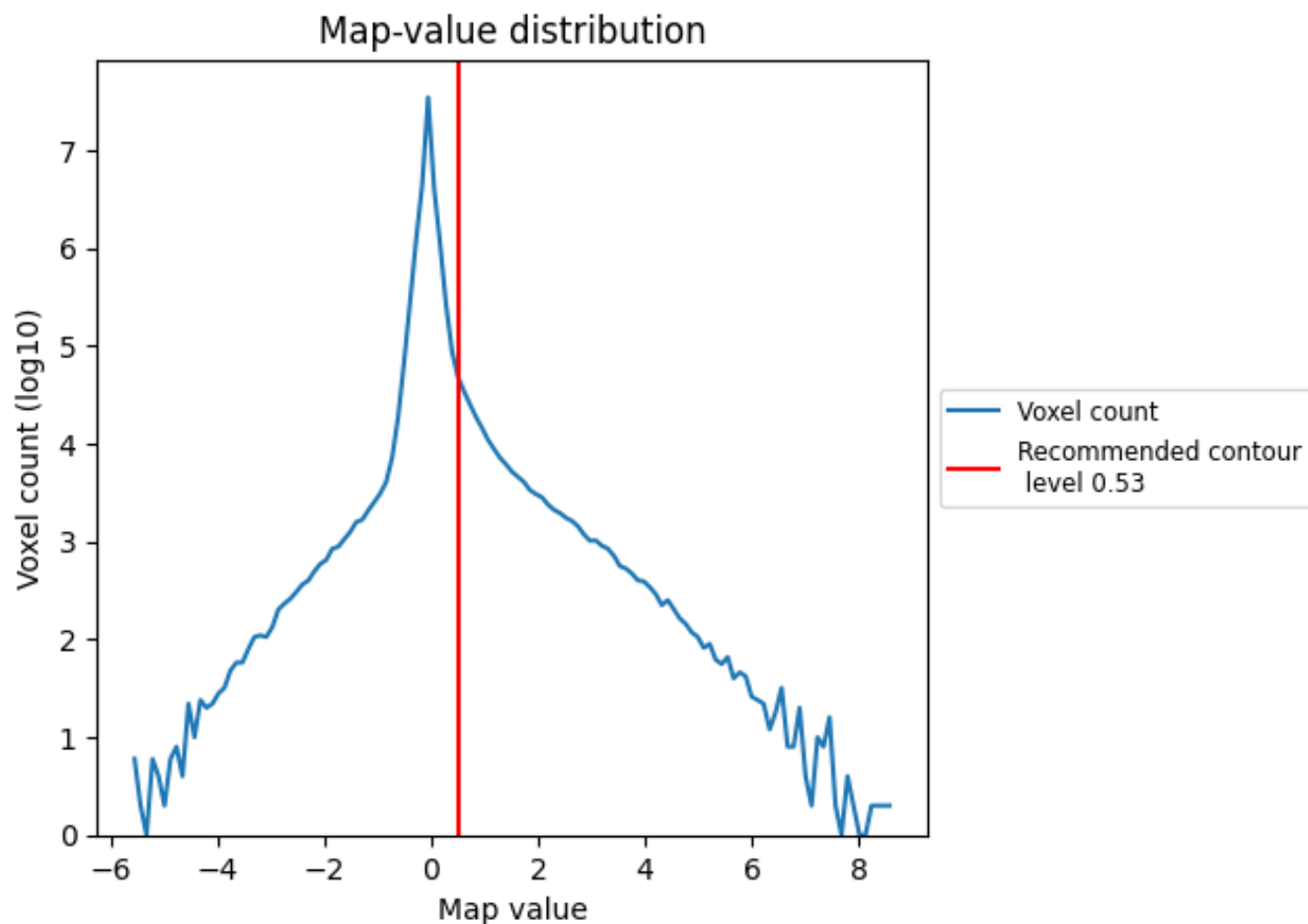
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

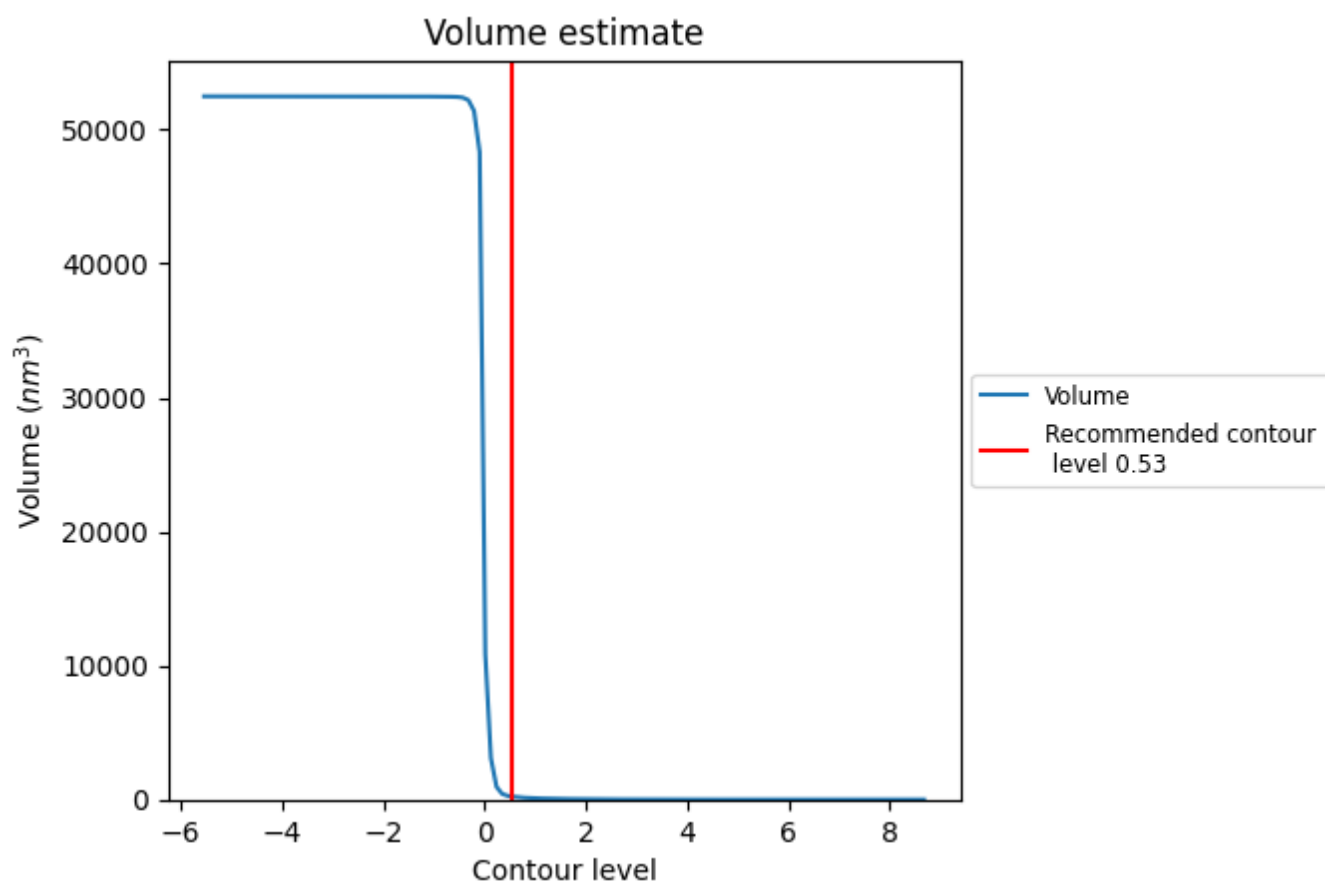
This section contains the results of statistical analysis of the map.

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.

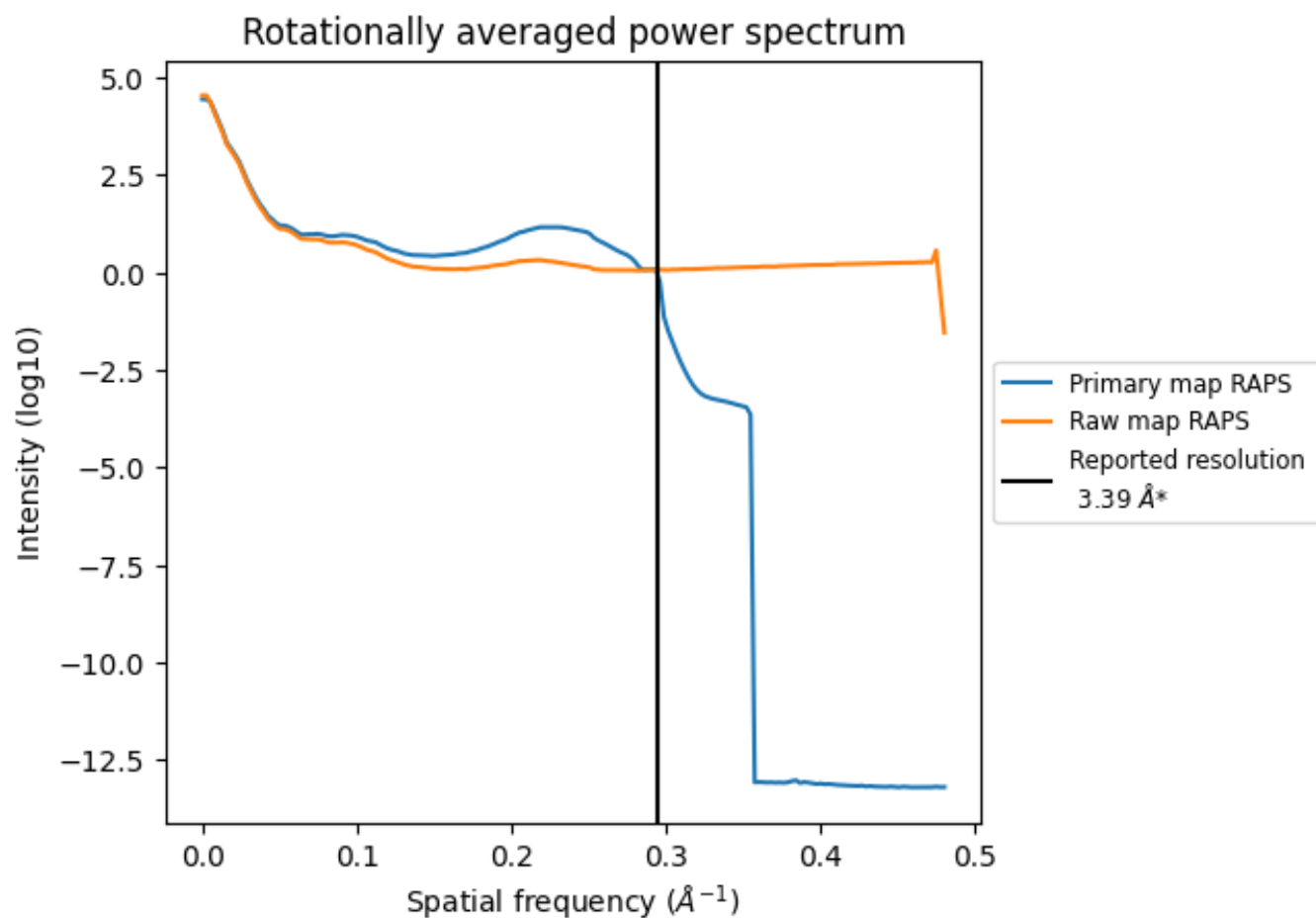
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm³; this corresponds to an approximate mass of 212 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 ⓘ

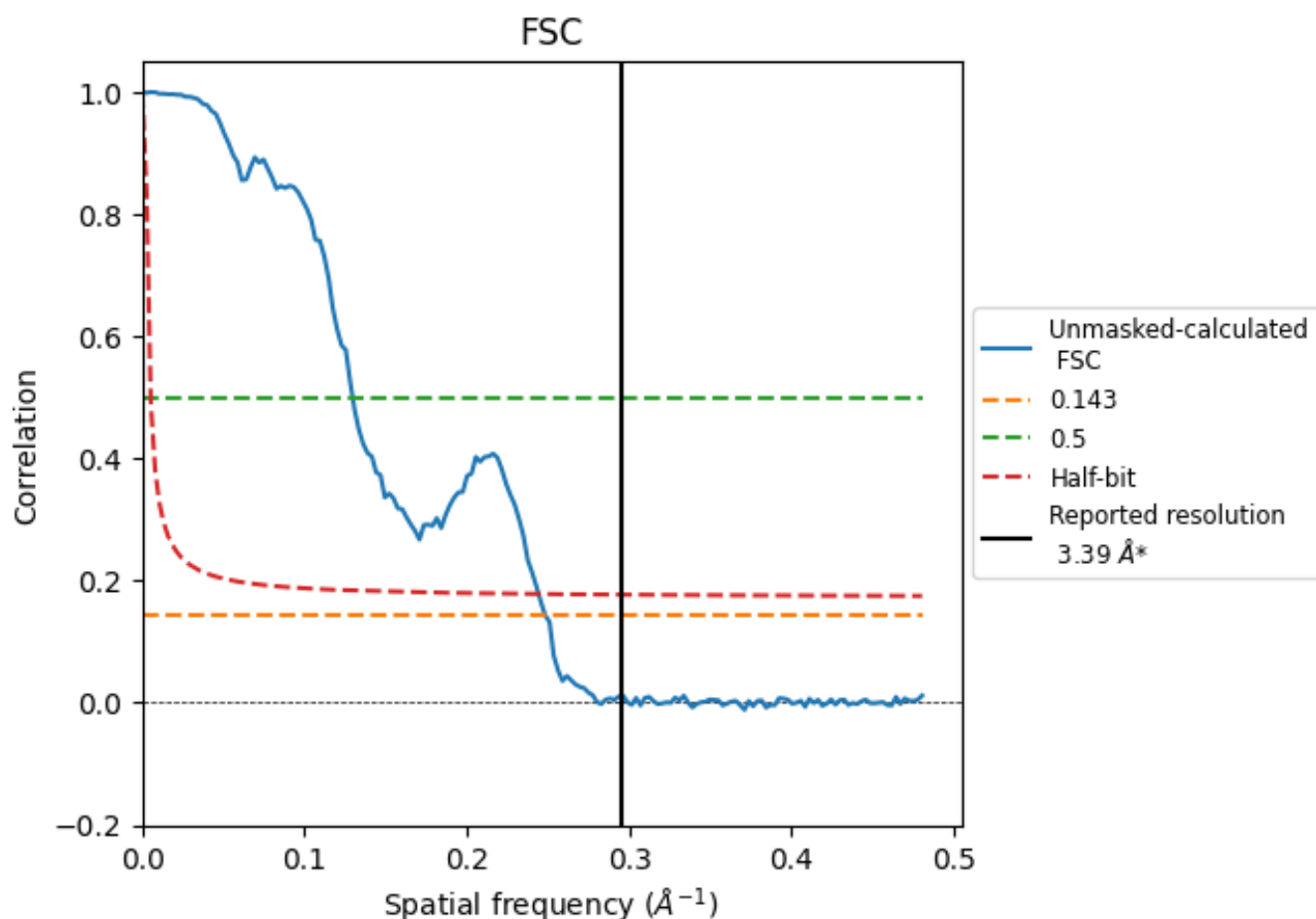


*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

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 0.295 \AA^{-1}

8.2 Resolution estimates [i](#)

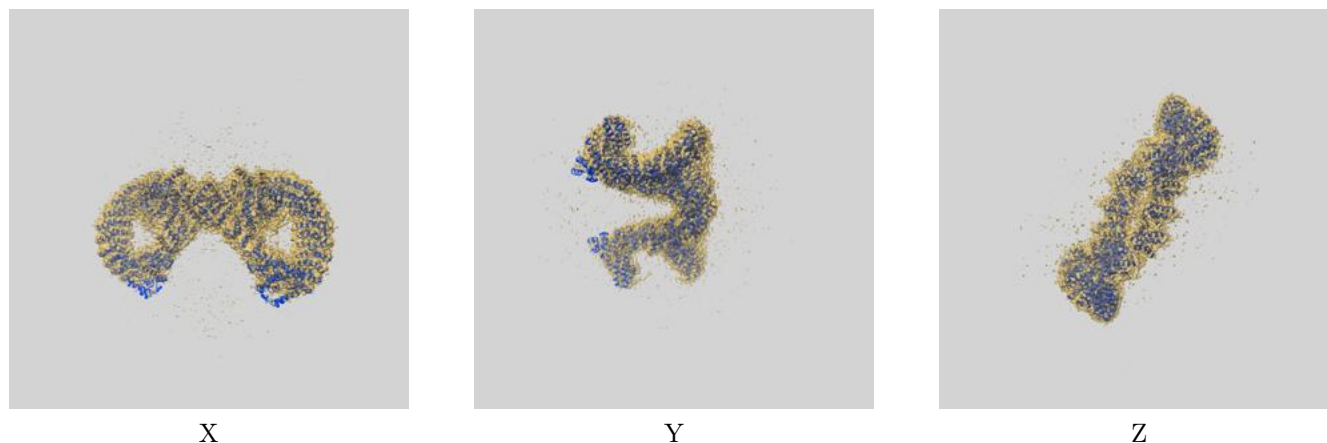
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.71	4.09

*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 4.03 differs from the reported value 3.39 by more than 10 %

9 Map-model fit [i](#)

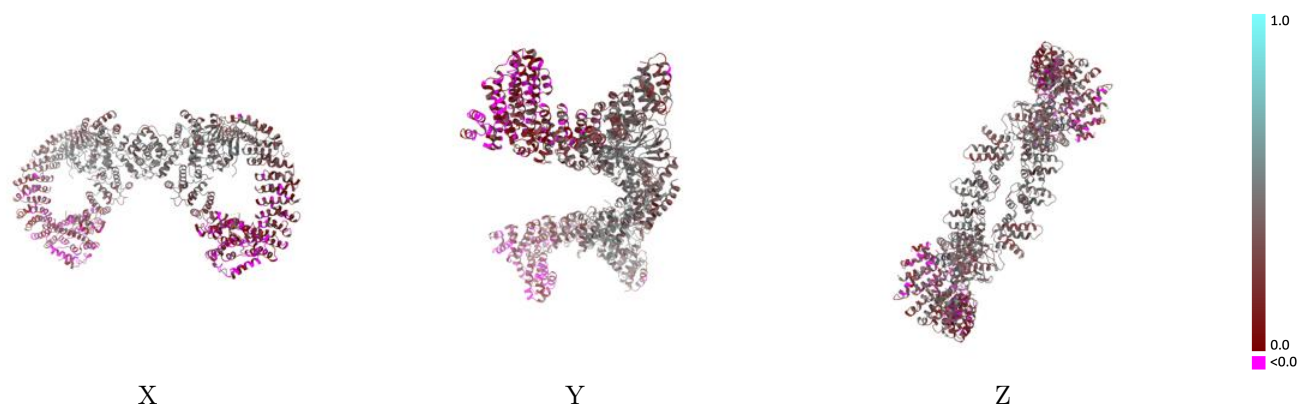
This section contains information regarding the fit between EMDB map EMD-61144 and PDB model 9J5K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



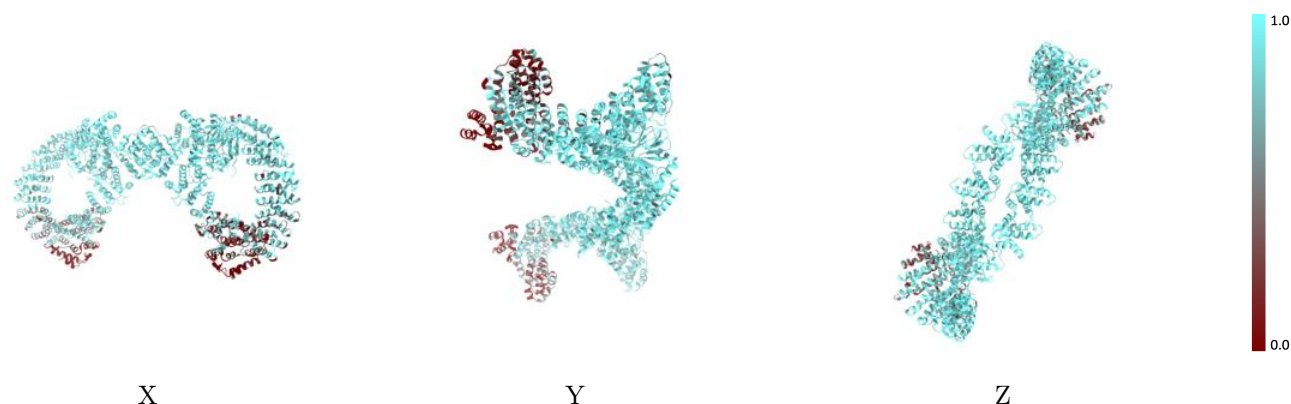
The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



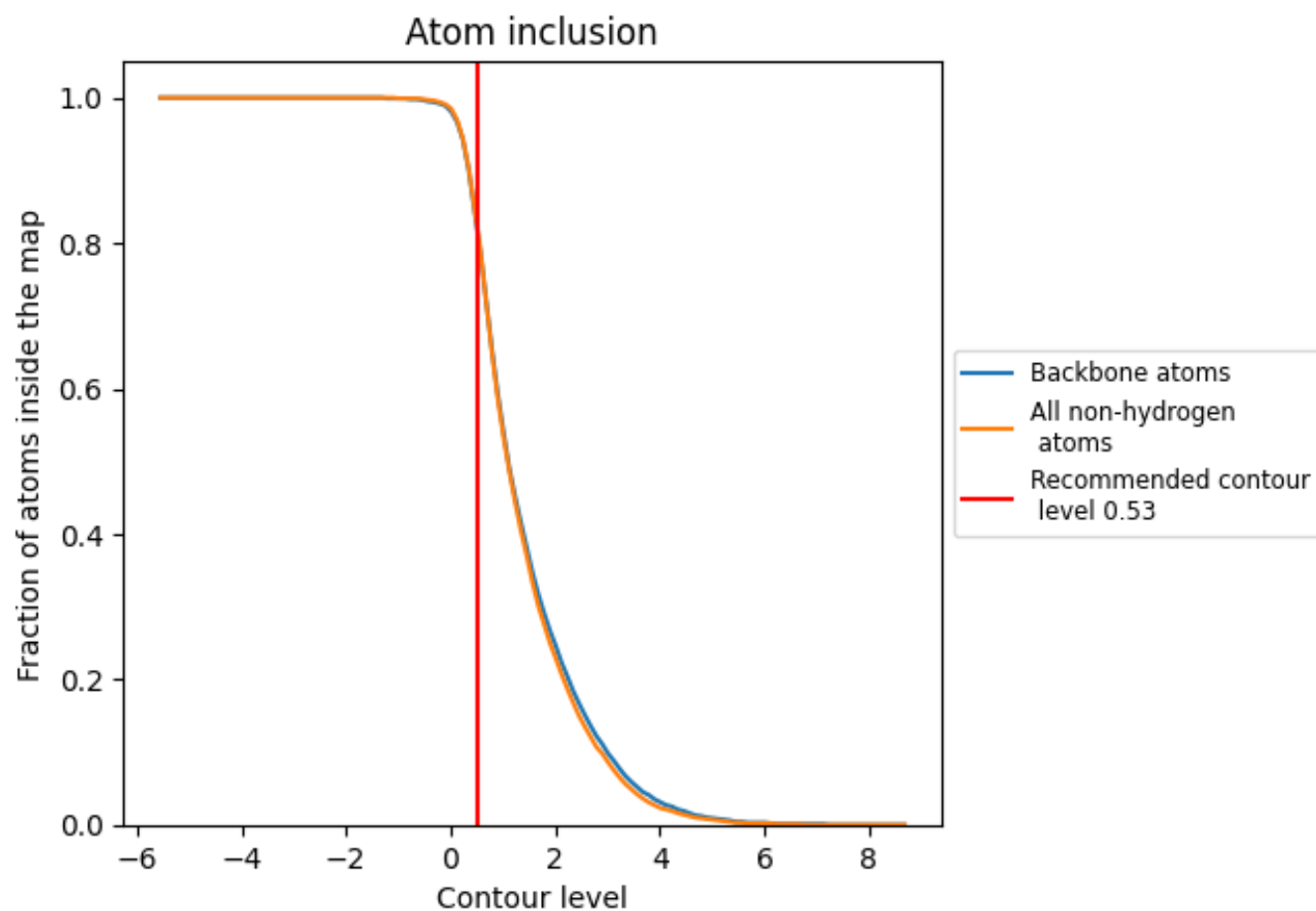
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.53).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8130	<div></div> 0.3180
A	<div></div> 0.7310	<div></div> 0.2160
B	<div></div> 0.8250	<div></div> 0.3410
C	<div></div> 0.9290	<div></div> 0.4480
D	<div></div> 0.7310	<div></div> 0.2170
E	<div></div> 0.8240	<div></div> 0.3400
F	<div></div> 0.9320	<div></div> 0.4490
X	<div></div> 0.8380	<div></div> 0.4240
Y	<div></div> 0.7840	<div></div> 0.4110

1.0

0.0

<0.0