



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 07:17 am BST

PDB ID : 9TPJ / pdb_00009tpj
EMDB ID : EMD-56106
Title : Human Cardiac Interacting Heads Motif, E525K mutant
Authors : Lannes, L.; Kikuti, C.M.; Auguin, D.; Robert-Paganin, J.; Houdusse, A.
Deposited on : 2025-12-18
Resolution : 3.02 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:

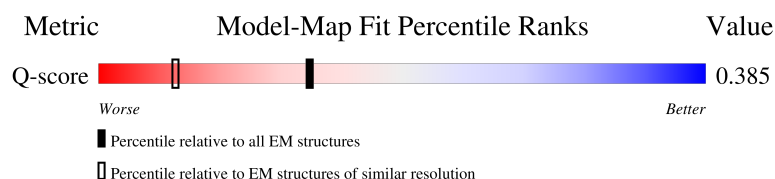
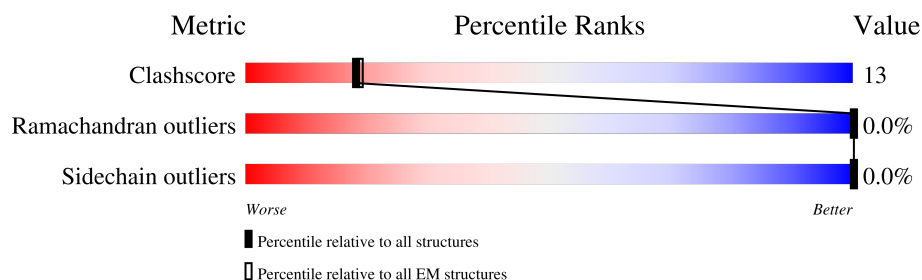
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.02 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	13913 (2.52 - 3.52)

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

Mol	Chain	Length	Quality of chain
1	A	1935	
1	B	1935	
2	C	195	
2	D	195	

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Mol	Chain	Length	Quality of chain
3	E	166	
3	F	166	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19337 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 Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	914	Total	C	N	O	S	0	0
			7384	4711	1267	1366	40		
1	B	881	Total	C	N	O	S	0	0
			7155	4572	1224	1319	40		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	LYS	GLU	engineered mutation	UNP P12883
B	525	LYS	GLU	engineered mutation	UNP P12883

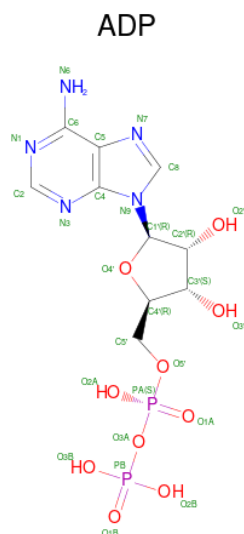
- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	157	Total	C	N	O	S	0	0
			1248	783	209	245	11		
2	D	158	Total	C	N	O	S	0	0
			1256	787	210	248	11		

- Molecule 3 is a protein called Myosin regulatory light chain 2, ventricular/cardiac muscle isoform.

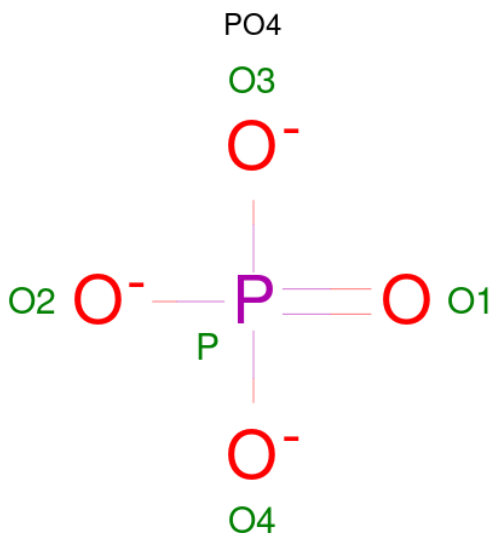
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	137	Total	C	N	O	S	0	0
			1108	706	178	218	6		
3	F	139	Total	C	N	O	S	0	0
			1120	714	183	217	6		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 5	O 4	P 1	0
5	B	1	Total 5	O 4	P 1	0

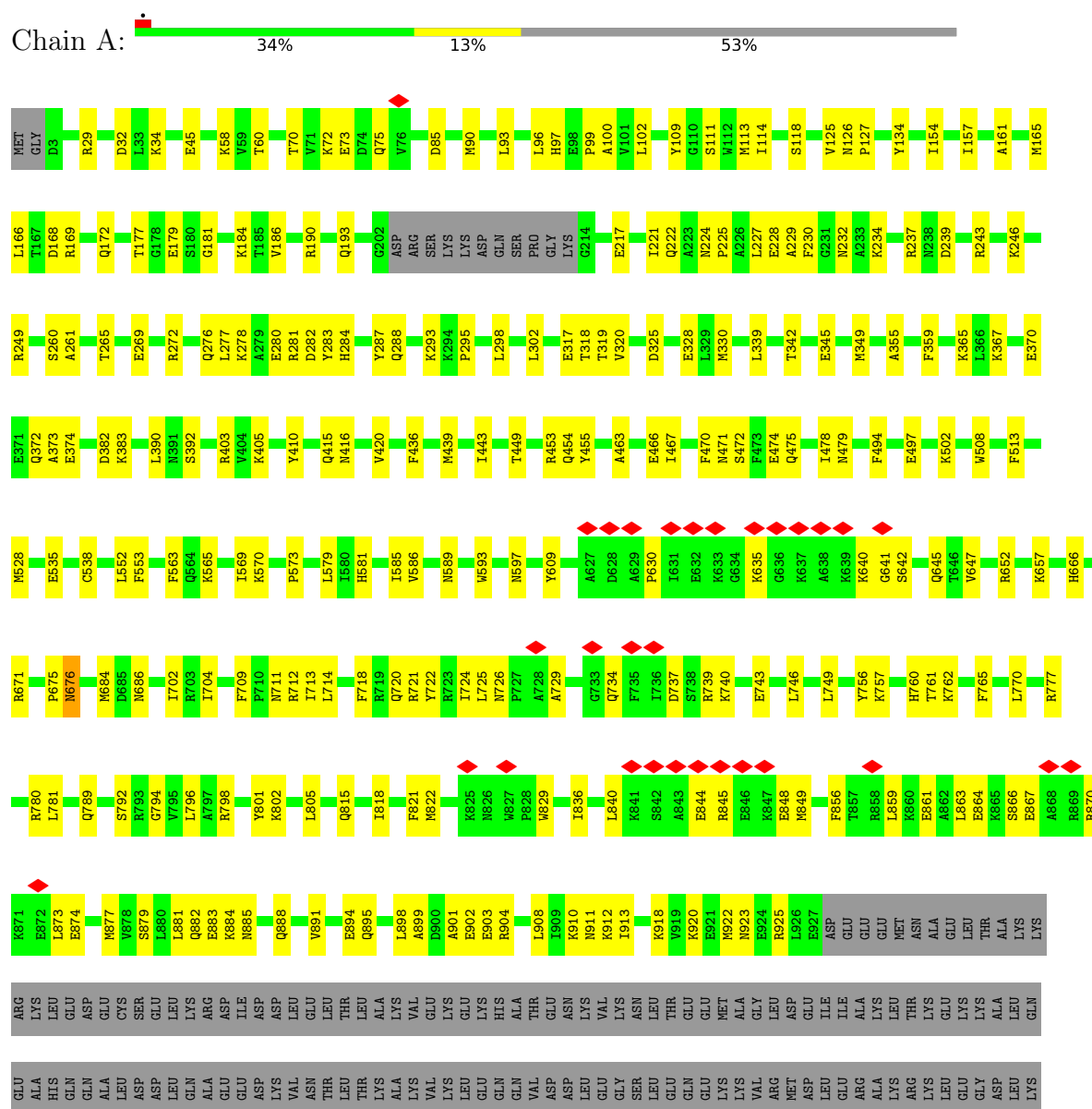
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Mg 1	0
6	B	1	Total 1	Mg 1	0

3 Residue-property plots

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

• Molecule 1: Myosin-7



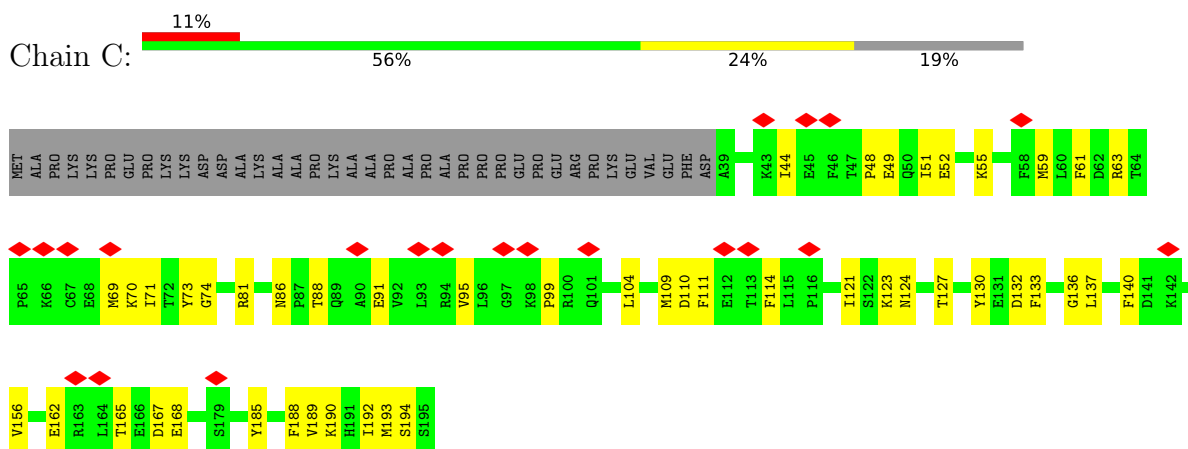
- Molecule 1: Myosin-7

Metabolite	Pathway	Abundance	Significance
R243	L120	Low	
A261	F121	High	
E269	N126	Low	
K270	K129	Low	
S271	W130	High	
R272	Y134	Low	
V273	V139	Low	
I274	R143	Low	
L277	H153	Low	
K278	I157	Low	
A279	M171	Low	
E280	L176	Low	
Y283	E179	Low	
Q288	S180	Low	
L297	G181	Low	
L301	N187	Low	
L302	R190	Low	
T303	Q193	Low	
D325	Y194	Low	
E328	V197	Low	
L329	I198	Low	
T332	ALA	High	
L339	ILE	High	
M349	GLY	High	
L352	ASP	High	
I356	ARG	High	
F364	SER	High	
K366	PRO	High	
L366	GLY	High	
K367	LYS	High	
G371	LYS	High	
ARG	T215	High	
GLU	Q219	High	
E371	P225	High	
Q372	E228	High	
A373	N238	High	
E374			
P375			
T378			
MET	D3	High	
GLY	E20	High	
R23	R23	High	
Q27	Q27	High	
T28	T28	High	
P29	P29	High	
P30	P30	High	
F31	F31	High	
K35	K35	High	
D36	D36	High	
V37	V37	High	
D42	D42	High	
F46	F46	High	
I51	I51	High	
R54	R54	High	
K58	K58	High	
T63	T63	High	
E64	E64	High	
Y65	Y65	High	
K72	K72	High	
E73	E73	High	
D74	D74	High	
Q78	Q78	High	
Q79	Q79	High	
N80	N80	High	
P81	P81	High	
K83	K83	High	
F84	F84	High	
A91	A91	High	
T94	T94	High	
E98	E98	High	
P99	P99	High	
N104	N104	High	
R108	R108	High	
Y109	Y109	High	
Y115	Y115	High	
S118	S118	High	
G119	G119	High	

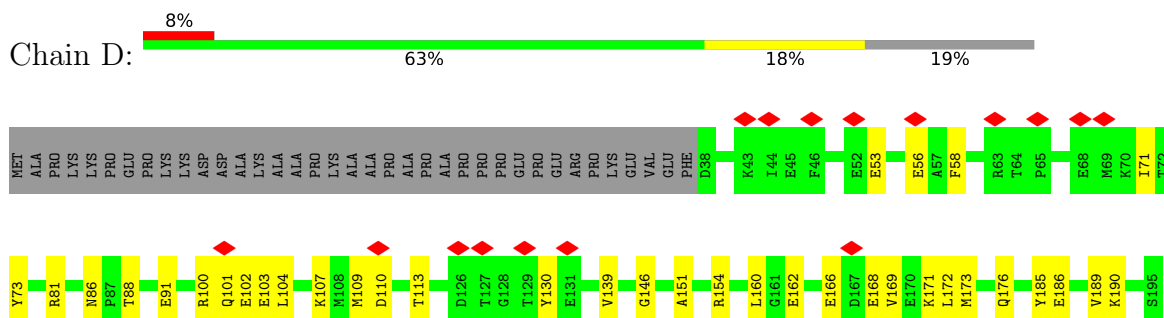


[illegible]

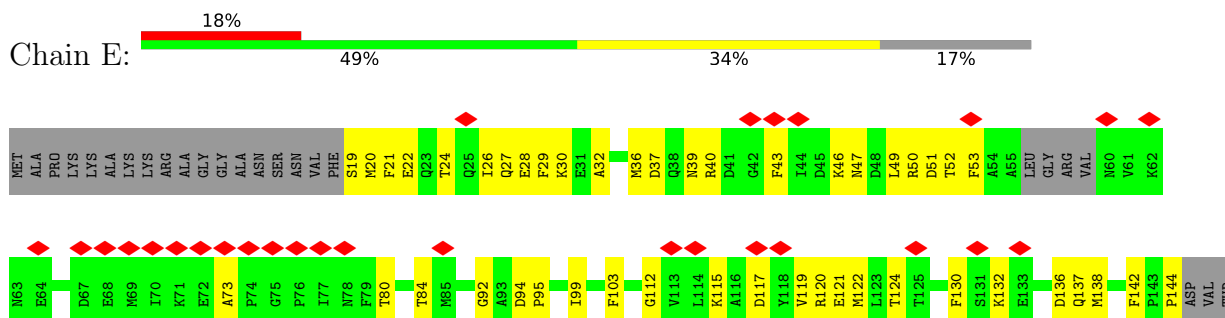
- Molecule 2: Myosin light chain 3



- Molecule 2: Myosin light chain 3

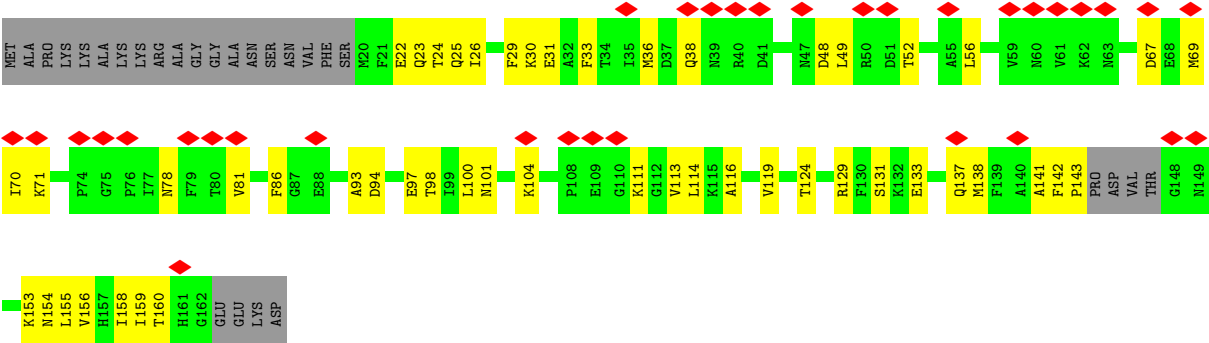


- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform





● Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	680000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.356	Depositor
Minimum map value	-1.352	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.126	Depositor
Map size ($\text{\AA}$)	352.38, 352.38, 352.38	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1746, 1.1746, 1.1746	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, MG, PO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/7505	0.39	0/10097
1	B	0.16	0/7271	0.38	0/9783
2	C	0.12	0/1267	0.37	0/1699
2	D	0.11	0/1275	0.33	0/1710
3	E	0.12	0/1128	0.36	0/1515
3	F	0.11	0/1140	0.32	0/1531
All	All	0.16	0/19586	0.38	0/26335

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7384	0	7431	201	0
1	B	7155	0	7198	210	0
2	C	1248	0	1231	37	0
2	D	1256	0	1235	25	0
3	E	1108	0	1067	48	0
3	F	1120	0	1089	36	0
4	A	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	2	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	19337	0	19275	509	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 (509) 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:904:ARG:NH1	1:B:905:CYS:SG	2.55	0.80
3:F:137:GLN:HE21	3:F:138:MET:HE3	1.45	0.79
1:A:227:LEU:HD23	1:A:439:MET:HE3	1.66	0.78
1:A:276:GLN:NE2	1:A:282:ASP:OD2	2.20	0.75
1:A:269:GLU:O	1:A:283:TYR:OH	2.04	0.74
1:B:755:GLN:HB2	1:B:769:LEU:HD22	1.68	0.74
1:A:355:ALA:O	1:A:359:PHE:HB2	1.87	0.73
1:A:589:ASN:O	1:A:593:TRP:NE1	2.20	0.73
1:A:792:SER:HB2	2:D:172:LEU:HD11	1.70	0.73
1:B:277:LEU:HB2	1:B:280:GLU:HG3	1.70	0.73
1:A:798:ARG:NH2	2:D:86:ASN:OD1	2.22	0.72
1:A:874:GLU:OE1	1:B:869:ARG:NH2	2.23	0.72
1:A:172:GLN:HG2	1:A:666:HIS:HB3	1.72	0.72
1:A:845:ARG:HA	1:A:849:MET:HE2	1.72	0.71
1:A:277:LEU:HD13	1:A:470:PHE:HE1	1.56	0.70
1:A:863:LEU:O	1:A:867:GLU:HG2	1.91	0.70
2:C:189:VAL:HA	2:C:192:ILE:HG12	1.73	0.70
1:A:870:ARG:NH1	1:A:874:GLU:OE1	2.24	0.70
1:A:184:LYS:N	4:A:2001:ADP:O1B	2.25	0.69
1:A:721:ARG:O	1:A:777:ARG:NH1	2.26	0.69
3:E:39:ASN:ND2	3:E:43:PHE:O	2.27	0.68
1:B:238:ASN:ND2	4:B:2001:ADP:O2A	2.27	0.68
1:A:370:GLU:HG3	1:A:372:GLN:HB3	1.74	0.67
1:B:372:GLN:NE2	1:B:373:ALA:O	2.27	0.67
1:A:845:ARG:NH2	1:B:849:MET:SD	2.69	0.66
2:D:166:GLU:HA	2:D:169:VAL:HG12	1.77	0.66
1:A:403:ARG:NH2	1:B:454:GLN:O	2.28	0.66
1:B:91:ALA:O	1:B:706:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:HE2	1:A:118:SER:HB3	1.76	0.65
1:B:838:PRO:HA	1:B:847:LYS:HZ2	1.60	0.65
1:B:126:ASN:ND2	1:B:181:GLY:O	2.30	0.65
1:B:836:ILE:HA	1:B:840:LEU:HB2	1.78	0.65
1:A:538:CYS:SG	1:A:597:ASN:ND2	2.67	0.65
1:B:486:GLN:OE1	1:B:671:ARG:NH2	2.30	0.65
1:B:793:ARG:HB3	2:C:81:ARG:HD3	1.77	0.64
1:B:845:ARG:NH2	3:E:28:GLU:O	2.31	0.64
1:A:725:LEU:HB3	1:A:749:LEU:HD11	1.80	0.64
1:A:714:LEU:HA	1:A:762:LYS:HD2	1.79	0.63
1:B:827:TRP:HE3	1:B:830:MET:HE1	1.62	0.63
1:B:548:PHE:O	1:B:552:LEU:N	2.31	0.63
1:A:126:ASN:ND2	1:A:181:GLY:O	2.32	0.63
1:A:177:THR:OG1	1:A:671:ARG:NH1	2.31	0.63
1:A:97:HIS:HD2	1:A:99:PRO:HD2	1.64	0.63
1:B:134:TYR:OH	4:B:2001:ADP:N6	2.25	0.63
2:C:189:VAL:HG22	2:C:193:MET:HE3	1.81	0.63
1:B:491:HIS:HA	1:B:495:VAL:HB	1.80	0.63
1:A:597:ASN:HA	1:A:647:VAL:HG22	1.82	0.62
1:A:904:ARG:O	1:A:908:LEU:HG	1.99	0.62
1:B:390:LEU:HD21	1:B:608:LEU:HB3	1.82	0.62
1:A:908:LEU:HB3	1:A:912:LYS:NZ	2.14	0.62
3:F:111:LYS:O	3:F:153:LYS:NZ	2.33	0.62
1:A:470:PHE:HB3	1:A:573:PRO:HB2	1.82	0.62
1:A:794:GLY:HA2	2:D:81:ARG:HB3	1.82	0.62
1:B:272:ARG:NH1	1:B:280:GLU:OE1	2.32	0.62
1:B:269:GLU:O	1:B:283:TYR:OH	2.17	0.61
1:A:724:ILE:HD11	2:D:139:VAL:HG21	1.81	0.61
2:C:137:LEU:HD13	2:C:185:TYR:HB2	1.82	0.61
1:A:102:LEU:HD21	1:A:686:ASN:HD22	1.66	0.61
1:A:90:MET:HA	1:A:93:LEU:HD13	1.82	0.61
1:A:224:ASN:O	1:A:228:GLU:HG2	2.01	0.61
1:A:265:THR:HG21	1:A:436:PHE:HE2	1.63	0.61
1:B:498:GLN:O	1:B:502:LYS:NZ	2.33	0.61
3:E:119:VAL:HG12	3:E:122:MET:HE2	1.81	0.61
1:B:893:ALA:O	1:B:897:ASN:ND2	2.34	0.61
1:A:72:LYS:HG3	1:A:73:GLU:HG2	1.83	0.61
1:A:161:ALA:O	1:A:172:GLN:NE2	2.30	0.61
1:B:522:ASP:O	1:B:526:LYS:HG2	2.01	0.61
1:B:784:ILE:HG21	2:C:136:GLY:HA3	1.83	0.61
1:B:829:TRP:HH2	3:E:73:ALA:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD23	1:B:485:LEU:HD11	1.83	0.60
1:A:114:ILE:HD13	1:A:127:PRO:HG3	1.83	0.60
1:A:293:LYS:HG3	1:A:330:MET:HE2	1.83	0.60
1:A:58:LYS:HA	1:A:72:LYS:HD3	1.83	0.60
2:C:73:TYR:HD1	2:C:109:MET:HG2	1.66	0.60
1:A:269:GLU:HG3	1:A:474:GLU:HG2	1.84	0.60
3:E:144:PRO:O	3:E:149:ASN:N	2.34	0.60
1:B:58:LYS:HG2	1:B:72:LYS:HA	1.83	0.60
1:B:828:PRO:HA	1:B:831:LYS:HD3	1.84	0.60
1:B:567:ARG:HH22	1:B:585:ILE:HG23	1.65	0.60
1:A:895:GLN:HE22	1:B:890:GLN:HE22	1.49	0.60
1:A:179:GLU:O	1:A:184:LYS:NZ	2.35	0.59
1:A:471:ASN:O	1:A:589:ASN:N	2.33	0.59
1:A:879:SER:O	1:A:882:GLN:HG3	2.03	0.59
1:B:171:ASN:HB2	1:B:665:THR:HG22	1.82	0.59
3:F:156:VAL:HA	3:F:159:ILE:HG22	1.85	0.59
1:A:118:SER:HB2	1:A:702:ILE:HG21	1.84	0.59
1:A:463:ALA:HB3	1:A:478:ILE:HD12	1.85	0.59
1:B:98:GLU:HG3	1:B:699:LEU:HD22	1.85	0.58
1:A:234:LYS:HG2	1:A:239:ASP:HA	1.84	0.58
1:A:229:ALA:HA	1:A:284:HIS:HB2	1.85	0.58
1:A:711:ASN:HB3	1:A:770:LEU:HD13	1.86	0.58
1:B:814:ILE:O	1:B:818:ILE:HD12	2.02	0.58
3:F:114:LEU:HD23	3:F:119:VAL:HG11	1.84	0.58
3:E:115:LYS:HA	3:E:149:ASN:HA	1.85	0.58
1:A:760:HIS:O	1:A:761:THR:OG1	2.16	0.58
1:B:449:THR:HG21	1:B:451:GLN:HE21	1.69	0.58
1:B:486:GLN:NE2	1:B:696:ASN:O	2.37	0.58
1:A:166:LEU:HD13	2:D:151:ALA:HB1	1.86	0.58
1:B:761:THR:HG23	1:B:762:LYS:HG3	1.86	0.58
1:A:272:ARG:O	1:A:276:GLN:NE2	2.37	0.57
1:B:905:CYS:O	1:B:909:ILE:HD12	2.02	0.57
1:A:365:LYS:NZ	1:A:374:GLU:OE1	2.37	0.57
2:D:53:GLU:HA	2:D:56:GLU:HG3	1.86	0.57
1:A:881:LEU:O	1:A:885:ASN:HB2	2.03	0.57
1:A:449:THR:O	1:A:453:ARG:NH1	2.36	0.57
1:A:630:PRO:HB3	1:A:640:LYS:HB2	1.86	0.57
1:A:911:ASN:OD1	1:A:912:LYS:HD3	2.05	0.57
2:C:130:TYR:HA	2:C:193:MET:HE1	1.87	0.57
1:B:391:ASN:ND2	1:B:394:ASP:OD2	2.38	0.56
3:E:120:ARG:HE	3:E:138:MET:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ASP:HB3	1:A:740:LYS:HB3	1.88	0.56
1:A:881:LEU:HD22	1:B:880:LEU:HD13	1.87	0.56
1:B:46:PHE:CG	1:B:99:PRO:HG3	2.40	0.56
3:F:23:GLN:O	3:F:26:ILE:N	2.38	0.56
1:A:125:VAL:HG12	1:A:675:PRO:HG3	1.87	0.56
1:A:720:GLN:NE2	2:D:139:VAL:O	2.39	0.56
1:A:765:PHE:HD2	1:A:770:LEU:HB2	1.70	0.56
1:B:597:ASN:OD1	1:B:646:THR:OG1	2.22	0.56
2:C:48:PRO:HA	2:C:51:ILE:HD13	1.87	0.56
2:C:74:GLY:HA2	2:C:104:LEU:HB2	1.88	0.56
1:A:243:ARG:HH12	1:A:466:GLU:CD	2.13	0.56
2:D:103:GLU:O	2:D:107:LYS:NZ	2.33	0.56
1:A:186:VAL:O	1:A:190:ARG:HG2	2.04	0.56
3:E:120:ARG:NH2	3:E:142:PHE:O	2.38	0.56
1:A:724:ILE:HG22	1:A:780:ARG:HB3	1.87	0.56
1:B:698:VAL:O	1:B:702:ILE:HD12	2.06	0.56
2:C:44:ILE:HG21	2:C:123:LYS:HE3	1.87	0.56
1:A:109:TYR:OH	1:A:126:ASN:O	2.15	0.56
1:B:356:ILE:HG23	1:B:428:ALA:HB1	1.88	0.56
3:E:138:MET:HE3	3:E:138:MET:O	2.06	0.56
1:B:755:GLN:HB3	1:B:766:LYS:HB2	1.88	0.56
1:B:787:ARG:HH11	2:C:127:THR:HA	1.71	0.55
1:B:853:LYS:HA	1:B:856:PHE:HD2	1.72	0.55
1:B:901:ALA:O	1:B:904:ARG:HD3	2.07	0.55
1:A:454:GLN:HG3	1:A:455:TYR:CD2	2.42	0.55
1:A:802:LYS:HA	1:A:805:LEU:HD12	1.89	0.54
1:A:318:THR:HG23	1:A:319:THR:HG23	1.88	0.54
1:B:875:GLU:HA	1:B:878:VAL:HG22	1.89	0.54
1:A:154:ILE:HA	1:A:157:ILE:HD12	1.90	0.54
1:A:277:LEU:HD23	1:A:277:LEU:H	1.72	0.54
1:A:467:ILE:HG12	1:A:586:VAL:HG12	1.90	0.54
3:F:26:ILE:O	3:F:30:LYS:HG2	2.07	0.54
1:B:816:TRP:CZ2	3:E:92:GLY:HA2	2.43	0.54
1:B:810:SER:O	1:B:814:ILE:HD12	2.08	0.53
1:B:868:ALA:O	1:B:871:LYS:HG3	2.08	0.53
1:B:676:ASN:ND2	1:B:683:VAL:O	2.41	0.53
1:B:913:ILE:O	1:B:916:GLU:HG3	2.08	0.53
1:A:181:GLY:N	4:A:2001:ADP:O3B	2.37	0.53
1:A:190:ARG:NH1	1:A:193:GLN:OE1	2.42	0.53
1:A:355:ALA:O	1:A:359:PHE:CB	2.57	0.53
1:B:279:ALA:HA	1:B:317:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HD23	1:B:517:LEU:O	2.08	0.53
1:B:886:ASP:O	1:B:890:GLN:HG2	2.08	0.53
1:A:97:HIS:CD2	1:A:99:PRO:HD2	2.44	0.53
1:A:372:GLN:NE2	1:A:373:ALA:O	2.30	0.53
1:A:866:SER:O	1:A:870:ARG:HB2	2.08	0.53
1:B:544:THR:HB	1:B:547:THR:HG23	1.91	0.53
1:A:134:TYR:OH	4:A:2001:ADP:N6	2.39	0.53
2:C:190:LYS:O	2:C:194:SER:OG	2.25	0.53
1:A:228:GLU:HA	1:A:232:ASN:HD22	1.74	0.52
1:B:870:ARG:NH2	1:B:873:LEU:HD23	2.24	0.52
2:C:109:MET:HE1	2:C:114:PHE:HB2	1.90	0.52
3:F:33:PHE:HA	3:F:36:MET:HG3	1.91	0.52
1:B:872:GLU:O	1:B:875:GLU:HG3	2.09	0.52
3:F:131:SER:OG	3:F:133:GLU:OE1	2.26	0.52
3:F:23:GLN:O	3:F:26:ILE:HG22	2.09	0.52
3:F:116:ALA:HA	3:F:119:VAL:HG22	1.91	0.52
1:A:382:ASP:OD1	1:A:383:LYS:N	2.43	0.52
1:B:719:ARG:NH2	1:B:738:SER:O	2.43	0.52
1:B:129:M3L:HB3	1:B:681:PRO:HB3	1.91	0.52
1:B:328:GLU:O	1:B:332:THR:HG23	2.09	0.52
1:A:60:THR:HG22	1:A:70:THR:HB	1.90	0.52
1:B:80:ASN:OD1	1:B:94:THR:OG1	2.25	0.52
1:A:224:ASN:OD1	1:A:246:LYS:NZ	2.34	0.52
1:B:225:PRO:HA	1:B:228:GLU:HB2	1.91	0.52
1:B:814:ILE:HG12	3:E:103:PHE:HE1	1.75	0.52
1:B:827:TRP:CD1	1:B:828:PRO:HD2	2.45	0.52
1:A:295:PRO:HA	1:A:298:LEU:HB2	1.92	0.52
1:B:301:LEU:HA	1:B:387:LEU:HD21	1.92	0.52
1:B:522:ASP:HB3	1:B:526:LYS:HD3	1.91	0.52
1:B:858:ARG:HH12	1:B:862:ALA:HB2	1.73	0.52
1:B:659:MET:HA	1:B:662:LEU:HB2	1.91	0.52
2:C:167:ASP:OD1	2:C:168:GLU:N	2.43	0.52
1:A:277:LEU:HD13	1:A:470:PHE:CE1	2.41	0.51
1:A:365:LYS:O	1:A:374:GLU:N	2.34	0.51
1:B:532:SER:O	1:B:535:GLU:HG3	2.09	0.51
1:A:325:ASP:HA	1:A:328:GLU:HB2	1.92	0.51
1:A:870:ARG:HD2	1:B:869:ARG:CZ	2.41	0.51
3:E:21:PHE:CE2	3:E:84:THR:HA	2.44	0.51
3:E:119:VAL:HA	3:E:122:MET:HG2	1.92	0.51
3:E:121:GLU:OE1	3:E:132:LYS:NZ	2.43	0.51
1:A:111:SER:HB3	1:A:113:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ASN:OD1	1:B:417:VAL:N	2.39	0.51
1:A:714:LEU:O	1:A:718:PHE:N	2.40	0.51
3:F:38:GLN:HE22	3:F:48:ASP:HA	1.76	0.51
1:A:726:ASN:HB3	1:A:729:ALA:HB3	1.92	0.51
1:B:297:LEU:O	1:B:301:LEU:HB2	2.11	0.51
1:B:862:ALA:O	1:B:865:LYS:HG3	2.10	0.51
3:E:47:ASN:HA	3:E:50:ARG:HE	1.74	0.51
3:F:78:ASN:H	3:F:81:VAL:HG22	1.75	0.51
1:A:796:LEU:HD13	2:D:168:GLU:OE1	2.11	0.51
1:B:518:GLN:HA	1:B:521:ILE:HG22	1.93	0.51
1:A:908:LEU:HB3	1:A:912:LYS:HZ3	1.74	0.51
2:C:111:PHE:HA	2:C:114:PHE:HB3	1.92	0.51
1:A:709:PHE:O	1:A:712:ARG:NH2	2.45	0.50
1:A:781:LEU:HD11	2:D:160:LEU:HD23	1.94	0.50
1:B:891:VAL:HG12	1:B:895:GLN:HE22	1.75	0.50
1:A:502:LYS:HZ2	1:A:508:TRP:CD1	2.29	0.50
1:B:365:LYS:NZ	1:B:375:PRO:O	2.45	0.50
1:A:29:ARG:NH2	1:A:85:ASP:OD2	2.42	0.50
1:A:497:GLU:OE1	1:A:712:ARG:NH2	2.45	0.50
2:D:110:ASP:O	2:D:113:THR:HG22	2.12	0.50
2:D:146:GLY:HA2	2:D:185:TYR:HE1	1.76	0.50
1:A:535:GLU:OE2	1:A:652:ARG:NH1	2.41	0.50
1:B:121:PHE:CZ	1:B:698:VAL:HG23	2.47	0.50
1:B:130:TRP:HZ3	1:B:190:ARG:HH12	1.58	0.50
1:B:484:LYS:HG2	1:B:521:ILE:HD11	1.92	0.50
1:B:789:GLN:OE1	2:C:162:GLU:N	2.37	0.50
1:A:734:GLN:HB3	1:A:740:LYS:HE3	1.94	0.50
1:A:884:LYS:HE3	1:B:880:LEU:CD1	2.42	0.50
1:B:835:LYS:HE3	1:B:839:LEU:HD23	1.93	0.50
2:C:91:GLU:O	2:C:95:VAL:HG22	2.12	0.50
2:D:58:PHE:CZ	2:D:71:ILE:HG12	2.46	0.50
3:E:24:THR:HA	3:E:27:GLN:HE22	1.76	0.50
3:E:37:ASP:HB3	3:E:40:ARG:HH21	1.77	0.49
1:A:168:ASP:C	1:A:169:ARG:HD3	2.37	0.49
2:C:55:LYS:NZ	2:C:69:MET:SD	2.77	0.49
1:A:302:LEU:HD13	1:A:383:LYS:HG2	1.95	0.49
1:A:390:LEU:HD11	1:A:609:TYR:HE1	1.78	0.49
1:B:483:GLU:OE2	1:B:582:TYR:N	2.28	0.49
3:E:21:PHE:HD2	3:E:22:GLU:CD	2.20	0.49
2:C:55:LYS:HG3	2:C:59:MET:HE3	1.95	0.49
1:A:821:PHE:CZ	3:F:158:ILE:HD12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HD11	1:B:668:HIS:HB3	1.95	0.49
1:A:278:LYS:O	1:A:317:GLU:HG3	2.12	0.49
1:B:882:GLN:O	1:B:886:ASP:HB2	2.13	0.49
3:F:124:THR:OG1	3:F:129:ARG:NH2	2.45	0.49
1:A:513:PHE:HE2	1:A:704:ILE:HD13	1.77	0.49
1:A:908:LEU:HA	1:A:911:ASN:ND2	2.28	0.49
1:A:922:MET:HA	1:A:925:ARG:CD	2.43	0.49
1:B:461:ASP:N	1:B:461:ASP:OD1	2.45	0.49
2:C:165:THR:OG1	2:C:168:GLU:OE1	2.31	0.48
1:B:821:PHE:CD2	3:E:159:ILE:HG22	2.48	0.48
1:B:845:ARG:O	1:B:849:MET:HG2	2.13	0.48
1:B:876:LYS:HA	1:B:876:LYS:HD3	1.65	0.48
3:E:136:ASP:OD1	3:E:137:GLN:N	2.46	0.48
1:A:32:ASP:C	1:A:34:LYS:H	2.20	0.48
1:A:815:GLN:HA	1:A:818:ILE:HG12	1.95	0.48
2:C:49:GLU:HA	2:C:52:GLU:CD	2.39	0.48
1:A:96:LEU:HD11	1:A:702:ILE:HD11	1.95	0.48
1:A:224:ASN:HB2	1:A:225:PRO:HD3	1.96	0.48
1:A:856:PHE:CE1	1:B:859:LEU:HD22	2.49	0.48
1:B:37:VAL:HG12	1:B:78:GLN:HA	1.95	0.48
2:D:101:GLN:NE2	2:D:102:GLU:HG2	2.29	0.48
3:F:100:LEU:HD21	3:F:156:VAL:HG11	1.96	0.48
1:B:597:ASN:HD21	1:B:648:SER:HB3	1.79	0.48
2:C:140:PHE:CE1	2:C:156:VAL:HG21	2.48	0.48
1:A:228:GLU:O	1:A:232:ASN:HB2	2.14	0.48
1:B:646:THR:HG23	1:B:649:ALA:H	1.78	0.48
2:C:61:PHE:O	2:C:63:ARG:NH1	2.47	0.48
3:E:115:LYS:HG3	3:E:117:ASP:H	1.79	0.48
1:A:870:ARG:HA	1:A:873:LEU:HG	1.96	0.48
1:A:73:GLU:H	1:A:75:GLN:HE22	1.62	0.47
1:A:165:MET:HB2	1:A:172:GLN:NE2	2.29	0.47
1:B:23:ARG:O	1:B:27:GLN:HG2	2.14	0.47
1:B:553:PHE:O	1:B:557:LEU:HG	2.13	0.47
1:B:814:ILE:HG12	3:E:103:PHE:CE1	2.49	0.47
1:A:472:SER:H	1:A:475:GLN:HG3	1.79	0.47
1:B:788:ILE:HD11	2:C:133:PHE:HB3	1.94	0.47
1:B:849:MET:HA	1:B:852:MET:HE2	1.96	0.47
1:B:739:ARG:NH2	1:B:743:GLU:OE2	2.43	0.47
2:D:73:TYR:CD1	2:D:109:MET:HB2	2.49	0.47
1:A:910:LYS:HA	1:A:913:ILE:HG12	1.96	0.47
1:B:139:VAL:HG13	1:B:194:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:98:THR:HA	3:F:101:ASN:HD21	1.80	0.47
1:A:840:LEU:O	1:A:844:GLU:HB2	2.15	0.47
1:A:911:ASN:OD1	1:A:912:LYS:N	2.48	0.47
1:B:179:GLU:HG2	1:B:465:PHE:HB3	1.97	0.47
1:B:569:ILE:HB	1:B:572:LYS:HB2	1.95	0.47
1:B:614:LEU:HD23	1:B:616:LEU:H	1.79	0.47
1:B:692:GLN:HA	1:B:695:CYS:SG	2.55	0.47
1:B:765:PHE:HD2	1:B:769:LEU:HD23	1.79	0.47
2:C:165:THR:OG1	2:C:167:ASP:OD1	2.24	0.47
1:B:3:ASP:N	1:B:20:GLU:OE2	2.47	0.47
1:B:417:VAL:HA	1:B:420:VAL:HG12	1.97	0.47
1:B:869:ARG:HA	1:B:872:GLU:HB3	1.97	0.47
1:B:915:LEU:O	1:B:918:LYS:HB3	2.15	0.47
1:A:96:LEU:HD21	1:A:702:ILE:HG13	1.97	0.47
1:A:836:ILE:HG13	3:F:56:LEU:HD11	1.96	0.47
1:A:845:ARG:HD2	1:A:849:MET:HE3	1.95	0.47
3:E:28:GLU:CD	3:E:28:GLU:H	2.23	0.47
1:B:261:ALA:HB3	1:B:447:LEU:HD13	1.97	0.46
1:A:528:MET:HG3	1:B:910:LYS:HE3	1.98	0.46
1:A:888:GLN:HA	1:A:891:VAL:HG22	1.96	0.46
3:E:24:THR:O	3:E:26:ILE:HD12	2.15	0.46
1:A:873:LEU:HD12	1:A:874:GLU:N	2.29	0.46
1:B:243:ARG:NH2	1:B:466:GLU:OE2	2.34	0.46
1:B:567:ARG:NH2	1:B:585:ILE:HG23	2.29	0.46
1:A:899:ALA:O	1:A:902:GLU:N	2.48	0.46
1:B:63:THR:HG22	1:B:65:TYR:H	1.81	0.46
1:A:552:LEU:HD13	1:A:563:PHE:HZ	1.81	0.46
1:A:32:ASP:HB3	1:A:34:LYS:O	2.16	0.46
1:A:657:LYS:HG3	1:B:896:ASP:OD2	2.15	0.46
1:B:119:GLY:H	1:B:702:ILE:HG13	1.81	0.46
3:F:100:LEU:O	3:F:104:LYS:HG2	2.15	0.46
1:B:84:PHE:CE2	1:B:94:THR:HG23	2.51	0.45
1:B:836:ILE:HD11	3:E:52:THR:HG22	1.98	0.45
1:A:342:THR:OG1	1:A:345:GLU:OE1	2.28	0.45
1:A:870:ARG:HG3	1:B:869:ARG:NH1	2.31	0.45
1:A:881:LEU:HD13	1:B:880:LEU:HD13	1.98	0.45
3:F:156:VAL:O	3:F:160:THR:N	2.42	0.45
1:B:104:ASN:O	1:B:108:ARG:HG2	2.16	0.45
1:B:352:LEU:O	1:B:356:ILE:HG12	2.16	0.45
1:B:544:THR:O	1:B:547:THR:OG1	2.24	0.45
2:D:168:GLU:HA	2:D:171:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:155:LEU:O	3:E:159:ILE:HG23	2.16	0.45
3:E:158:ILE:C	3:E:161:HIS:H	2.24	0.45
3:F:25:GLN:HG3	3:F:29:PHE:CE2	2.52	0.45
1:B:301:LEU:HB3	1:B:303:ILE:HG12	1.98	0.45
1:B:845:ARG:NH1	3:E:28:GLU:HB3	2.31	0.45
1:B:31:PHE:CD2	1:B:82:PRO:HG3	2.51	0.45
1:B:582:TYR:O	1:B:695:CYS:HB2	2.17	0.45
1:B:662:LEU:O	1:B:665:THR:OG1	2.30	0.45
1:B:800:GLU:OE1	1:B:800:GLU:N	2.50	0.45
1:B:317:GLU:C	1:B:319:THR:H	2.24	0.45
1:B:339:LEU:CD2	1:B:443:ILE:HG12	2.47	0.45
3:E:46:LYS:O	3:E:49:LEU:HG	2.17	0.45
3:E:157:HIS:O	3:E:162:GLY:N	2.46	0.45
1:A:281:ARG:HD2	1:A:320:VAL:HG23	1.99	0.45
1:B:115:TYR:CG	1:B:153:HIS:HA	2.52	0.45
1:B:193:GLN:O	1:B:197:VAL:HG22	2.17	0.45
1:B:513:PHE:HZ	1:B:704:ILE:HD13	1.82	0.45
3:F:113:VAL:C	3:F:114:LEU:HD12	2.41	0.45
1:B:783:ARG:HH12	1:B:787:ARG:NE	2.15	0.45
1:B:825:LYS:O	1:B:831:LYS:HD2	2.17	0.45
1:B:834:PHE:CD1	1:B:838:PRO:HG3	2.51	0.45
1:A:217:GLU:O	1:A:221:ILE:HG12	2.17	0.45
1:B:84:PHE:HE2	1:B:94:THR:HG23	1.82	0.45
1:B:339:LEU:HD23	1:B:443:ILE:HG12	1.98	0.45
2:C:71:ILE:HG12	2:C:111:PHE:HE1	1.82	0.45
1:A:877:MET:O	1:A:881:LEU:HD23	2.17	0.45
1:A:901:ALA:O	1:A:904:ARG:HG3	2.17	0.45
1:B:35:LYS:HA	1:B:51:ILE:HD12	1.99	0.45
1:B:684:MET:HE3	1:B:689:VAL:HG11	1.98	0.45
1:B:789:GLN:O	1:B:793:ARG:NE	2.32	0.45
3:E:94:ASP:OD1	3:E:95:PRO:HD2	2.17	0.45
1:A:879:SER:O	1:A:882:GLN:N	2.50	0.44
1:A:920:LYS:HA	1:A:923:ASN:ND2	2.31	0.44
1:B:615:LYS:O	1:B:618:SER:OG	2.25	0.44
3:F:49:LEU:HA	3:F:52:THR:HG22	1.99	0.44
3:F:69:MET:HG3	3:F:70:ILE:N	2.31	0.44
1:A:642:SER:HA	1:A:645:GLN:HG2	2.00	0.44
1:B:118:SER:OG	1:B:121:PHE:O	2.27	0.44
1:A:713:ILE:HD13	1:A:722:TYR:HE2	1.82	0.44
1:A:829:TRP:HE1	3:F:86:PHE:HE1	1.65	0.44
1:B:454:GLN:N	1:B:454:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:ARG:HH22	1:B:873:LEU:HD23	1.83	0.44
1:A:339:LEU:HD13	1:A:443:ILE:HG12	1.98	0.44
1:B:791:GLN:OE1	2:C:86:ASN:ND2	2.50	0.44
2:C:188:PHE:O	2:C:192:ILE:HG23	2.17	0.44
1:B:500:GLU:HG2	1:B:764:PHE:HZ	1.81	0.44
1:B:576:HIS:CE1	1:B:590:ILE:HG12	2.53	0.44
2:D:88:THR:HG23	2:D:91:GLU:H	1.83	0.44
3:F:22:GLU:OE1	3:F:24:THR:HG22	2.17	0.44
1:A:918:LYS:O	1:A:922:MET:HG3	2.17	0.44
1:B:442:ARG:NH1	1:B:446:THR:HB	2.32	0.44
1:B:724:ILE:HG22	1:B:780:ARG:HG3	1.99	0.44
2:D:73:TYR:HB3	2:D:104:LEU:HD12	1.98	0.44
1:A:676:ASN:N	1:A:676:ASN:ND2	2.66	0.44
1:B:35:LYS:HA	1:B:51:ILE:HB	1.99	0.44
1:B:109:TYR:CD2	1:B:684:MET:HB2	2.52	0.44
2:D:100:ARG:O	2:D:104:LEU:N	2.51	0.44
3:E:49:LEU:O	3:E:52:THR:OG1	2.19	0.44
1:A:739:ARG:O	1:A:743:GLU:HG2	2.17	0.43
1:A:641:GLY:O	1:A:645:GLN:HG2	2.18	0.43
1:A:870:ARG:HG3	1:B:869:ARG:HH12	1.82	0.43
1:B:115:TYR:OH	1:B:187:ASN:OD1	2.36	0.43
1:B:483:GLU:OE2	1:B:581:HIS:HB3	2.18	0.43
1:B:513:PHE:CZ	1:B:704:ILE:HD13	2.53	0.43
3:F:67:ASP:HA	3:F:70:ILE:HG12	1.99	0.43
3:F:97:GLU:O	3:F:101:ASN:ND2	2.51	0.43
1:A:746:LEU:HD13	1:A:756:TYR:CE2	2.54	0.43
1:B:791:GLN:HB3	2:C:192:ILE:HD12	2.00	0.43
1:A:709:PHE:HZ	1:A:757:LYS:HE2	1.83	0.43
1:B:426:ALA:HA	1:B:429:LYS:HE3	2.00	0.43
1:B:836:ILE:HG12	1:B:840:LEU:HD12	2.00	0.43
1:B:837:LYS:HG3	3:E:32:ALA:HB1	2.00	0.43
2:C:49:GLU:HA	2:C:52:GLU:OE2	2.18	0.43
3:F:155:LEU:HD13	3:F:158:ILE:HD11	2.00	0.43
1:A:725:LEU:HD23	1:A:780:ARG:HG3	2.00	0.43
1:A:789:GLN:HE22	2:D:162:GLU:H	1.66	0.43
2:D:154:ARG:NE	2:D:173:MET:SD	2.92	0.43
3:E:112:GLY:HA3	3:E:150:LEU:O	2.18	0.43
1:B:857:THR:O	1:B:861:GLU:HG3	2.19	0.43
2:C:121:ILE:HA	2:C:124:ASN:OD1	2.19	0.43
3:E:47:ASN:HA	3:E:50:ARG:NE	2.33	0.43
1:A:288:GLN:NE2	1:A:328:GLU:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:GLU:HA	1:A:864:GLU:CD	2.44	0.43
1:B:435:MET:HB2	1:B:620:LEU:HD21	2.01	0.43
1:B:480:PHE:O	1:B:484:LYS:HG3	2.19	0.43
1:B:719:ARG:O	1:B:723:ARG:HB2	2.19	0.43
1:B:834:PHE:CZ	3:E:161:HIS:HB2	2.54	0.43
1:B:28:THR:O	1:B:30:PRO:HD3	2.19	0.43
1:B:215:THR:O	1:B:219:GLN:N	2.45	0.43
2:C:73:TYR:HE2	2:C:99:PRO:HB3	1.83	0.43
3:E:29:PHE:O	3:E:32:ALA:HB3	2.19	0.43
1:A:97:HIS:NE2	1:A:100:ALA:HB2	2.34	0.42
1:A:382:ASP:HA	1:A:392:SER:HB2	2.01	0.42
1:B:349:MET:HE1	1:B:435:MET:HG2	2.00	0.42
1:B:480:PHE:CE2	1:B:484:LYS:HD2	2.54	0.42
1:A:45:GLU:H	1:A:686:ASN:HB3	1.85	0.42
1:A:494:PHE:HD2	1:A:513:PHE:CD2	2.37	0.42
1:A:894:GLU:O	1:A:898:LEU:HD12	2.18	0.42
1:B:749:LEU:HD23	1:B:749:LEU:HA	1.93	0.42
1:A:184:LYS:HB2	1:A:184:LYS:HE2	1.86	0.42
1:A:403:ARG:HH21	1:A:410:TYR:HB2	1.84	0.42
1:A:836:ILE:HG23	1:A:840:LEU:HD21	2.02	0.42
1:B:375:PRO:HB3	1:B:378:THR:HG21	2.01	0.42
1:B:724:ILE:HD12	1:B:724:ILE:H	1.84	0.42
1:B:904:ARG:HA	1:B:907:GLN:HG3	2.00	0.42
2:C:70:LYS:NZ	2:C:110:ASP:HB3	2.34	0.42
3:E:19:SER:OG	3:E:20:MET:N	2.53	0.42
3:E:30:LYS:NZ	3:E:80:THR:O	2.53	0.42
1:A:230:PHE:HB2	1:A:439:MET:HE1	2.02	0.42
1:B:705:CYS:O	1:B:767:ALA:HB2	2.19	0.42
3:F:22:GLU:H	3:F:93:ALA:HB3	1.85	0.42
1:A:249:ARG:O	1:A:261:ALA:HA	2.19	0.42
1:B:143:ARG:HD2	1:B:198:ILE:HD12	2.02	0.42
1:B:899:ALA:HA	1:B:902:GLU:OE1	2.20	0.42
3:F:154:ASN:O	3:F:158:ILE:HG12	2.20	0.42
1:A:237:ARG:NH2	1:A:467:ILE:O	2.50	0.42
1:A:282:ASP:OD1	1:A:283:TYR:N	2.42	0.42
1:A:479:ASN:HB3	1:A:581:HIS:CE1	2.55	0.42
1:A:848:GLU:HG2	1:A:849:MET:SD	2.60	0.42
1:B:273:VAL:HG23	1:B:274:ILE:HG23	2.02	0.42
1:B:784:ILE:HD13	1:B:784:ILE:HA	1.91	0.42
2:C:88:THR:OG1	2:C:162:GLU:OE2	2.38	0.42
1:A:513:PHE:CE2	1:A:704:ILE:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LYS:HA	1:A:903:GLU:CD	2.44	0.42
1:B:3:ASP:N	1:B:3:ASP:OD1	2.52	0.42
2:C:73:TYR:HD2	2:C:104:LEU:HA	1.84	0.42
3:F:94:ASP:N	3:F:94:ASP:OD1	2.51	0.42
1:A:260:SER:HB2	1:A:453:ARG:HD3	2.01	0.42
1:B:804:LEU:HA	1:B:807:ARG:HB2	2.02	0.42
1:B:822:MET:SD	3:E:137:GLN:NE2	2.91	0.42
3:F:97:GLU:HA	3:F:100:LEU:HD12	2.02	0.42
1:A:908:LEU:HB3	1:A:912:LYS:HZ1	1.82	0.41
1:B:837:LYS:NZ	3:E:36:MET:HB3	2.35	0.41
1:B:841:LYS:NZ	3:E:51:ASP:O	2.53	0.41
3:E:22:GLU:HA	3:E:26:ILE:HB	2.02	0.41
1:A:281:ARG:HH21	1:A:287:TYR:HB2	1.86	0.41
1:A:859:LEU:O	1:A:863:LEU:HG	2.19	0.41
1:B:655:LEU:HB3	1:B:659:MET:HE1	2.02	0.41
1:B:615:LYS:O	1:B:619:THR:HG23	2.20	0.41
1:B:83:LYS:HD2	1:B:84:PHE:CD1	2.55	0.41
1:B:773:LEU:HD23	1:B:773:LEU:HA	1.88	0.41
3:E:50:ARG:HG3	3:E:53:PHE:CE2	2.56	0.41
1:A:840:LEU:HB3	3:F:31:GLU:OE2	2.20	0.41
1:B:576:HIS:CG	1:B:590:ILE:HG23	2.56	0.41
2:D:173:MET:HB3	2:D:176:GLN:HB2	2.02	0.41
1:A:416:ASN:O	1:A:420:VAL:HG22	2.20	0.41
1:B:442:ARG:HH12	1:B:446:THR:HB	1.86	0.41
1:A:75:GLN:H	1:A:75:GLN:CD	2.28	0.41
1:A:272:ARG:HH12	1:A:280:GLU:HB3	1.85	0.41
1:A:553:PHE:HE2	1:A:565:LYS:HG2	1.86	0.41
1:A:367:LYS:O	1:A:370:GLU:HG2	2.20	0.41
1:A:579:LEU:O	1:A:585:ILE:HG23	2.21	0.41
1:A:676:ASN:N	1:A:676:ASN:HD22	2.17	0.41
1:B:418:GLN:NE2	1:B:419:GLN:HG3	2.35	0.41
1:B:709:PHE:HB3	1:B:764:PHE:HB3	2.01	0.41
1:B:719:ARG:HD3	1:B:730:ILE:HG21	2.02	0.41
1:B:914:GLN:O	1:B:918:LYS:HB2	2.21	0.41
1:A:281:ARG:HH21	1:A:287:TYR:CB	2.34	0.41
1:A:349:MET:HE1	1:A:439:MET:SD	2.61	0.41
1:A:405:LYS:HB2	1:A:410:TYR:CE1	2.56	0.41
1:A:415:GLN:HB3	1:A:420:VAL:HG13	2.03	0.41
1:A:801:TYR:O	1:A:805:LEU:HG	2.20	0.41
1:A:874:GLU:CD	1:B:869:ARG:HH21	2.23	0.41
1:A:879:SER:O	1:A:883:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD21	1:A:686:ASN:ND2	2.34	0.41
1:A:234:LYS:HB3	1:A:281:ARG:HB2	2.02	0.41
1:A:818:ILE:O	1:A:822:MET:HG2	2.21	0.41
3:F:67:ASP:C	3:F:71:LYS:HZ3	2.29	0.41
1:A:222:GLN:C	1:A:225:PRO:HD2	2.46	0.40
1:B:270:LYS:HB3	1:B:429:LYS:HD3	2.03	0.40
1:B:288:GLN:HA	1:B:325:ASP:HB3	2.02	0.40
1:B:524:ILE:HG22	1:B:531:MET:HE2	2.03	0.40
1:B:580:ILE:HG12	1:B:585:ILE:HD13	2.03	0.40
1:B:727:PRO:HG2	2:C:132:ASP:HA	2.02	0.40
2:C:133:PHE:N	2:C:133:PHE:CD1	2.88	0.40
1:A:109:TYR:CD2	1:A:684:MET:HE3	2.56	0.40
1:A:390:LEU:HD11	1:A:609:TYR:CE1	2.55	0.40
1:B:272:ARG:HB3	1:B:283:TYR:CE2	2.56	0.40
1:B:364:PHE:HB2	1:B:417:VAL:HG23	2.02	0.40
1:B:421:ILE:HA	1:B:424:THR:HG22	2.02	0.40
2:D:130:TYR:CE1	2:D:190:LYS:HE3	2.56	0.40
3:E:95:PRO:O	3:E:99:ILE:HG12	2.22	0.40
3:F:142:PHE:CG	3:F:143:PRO:HD3	2.56	0.40
1:B:288:GLN:O	1:B:329:LEU:HD22	2.22	0.40
1:B:915:LEU:HD23	1:B:918:LYS:HD3	2.02	0.40
3:E:151:ASP:O	3:E:154:ASN:ND2	2.55	0.40
1:A:75:GLN:OE1	1:A:75:GLN:N	2.51	0.40
1:A:535:GLU:OE1	1:A:652:ARG:NH2	2.38	0.40
1:A:569:ILE:HG23	1:A:570:LYS:HG2	2.04	0.40
1:B:849:MET:O	1:B:853:LYS:HG2	2.21	0.40
2:D:186:GLU:HA	2:D:189:VAL:HG12	2.03	0.40
3:E:39:ASN:OD1	3:E:39:ASN:N	2.51	0.40
3:F:116:ALA:HB3	3:F:141:ALA:HB2	2.02	0.40
3:E:124:THR:HG23	3:E:130:PHE:H	1.87	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	908/1935 (47%)	880 (97%)	28 (3%)	0	100	100
1	B	869/1935 (45%)	834 (96%)	34 (4%)	1 (0%)	48	79
2	C	155/195 (80%)	152 (98%)	3 (2%)	0	100	100
2	D	156/195 (80%)	154 (99%)	2 (1%)	0	100	100
3	E	131/166 (79%)	123 (94%)	8 (6%)	0	100	100
3	F	135/166 (81%)	125 (93%)	10 (7%)	0	100	100
All	All	2354/4592 (51%)	2268 (96%)	85 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	792/1693 (47%)	791 (100%)	1 (0%)	88	92
1	B	772/1693 (46%)	772 (100%)	0	100	100
2	C	137/167 (82%)	137 (100%)	0	100	100
2	D	138/167 (83%)	138 (100%)	0	100	100
3	E	120/141 (85%)	120 (100%)	0	100	100
3	F	120/141 (85%)	120 (100%)	0	100	100
All	All	2079/4002 (52%)	2078 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	676	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	97	HIS
1	A	232	ASN
1	A	288	GLN
1	A	306	ASN
1	A	645	GLN
1	A	895	GLN
1	B	288	GLN
1	B	292	ASN
1	B	372	GLN
1	B	482	ASN
1	B	518	GLN
1	B	576	HIS
1	B	651	HIS
1	B	666	HIS
1	B	755	GLN
2	C	50	GLN
2	D	101	GLN
2	D	124	ASN
3	F	25	GLN
3	F	63	ASN
3	F	78	ASN
3	F	137	GLN
3	F	161	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
1	M3L	B	129	1	10,11,12	0.53	0	9,14,16	0.46	0
1	M3L	A	129	1	10,11,12	0.51	0	9,14,16	0.48	0
1	M3L	A	549	1	10,11,12	0.55	0	9,14,16	0.51	0
1	M3L	B	549	1	10,11,12	0.53	0	9,14,16	0.47	0

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
1	M3L	B	129	1	-	4/9/10/12	-
1	M3L	A	129	1	-	0/9/10/12	-
1	M3L	A	549	1	-	1/9/10/12	-
1	M3L	B	549	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	129	M3L	N-CA-CB-CG
1	B	129	M3L	C-CA-CB-CG
1	B	129	M3L	CG-CD-CE-NZ
1	B	129	M3L	CA-CB-CG-CD
1	A	549	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	129	M3L	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	ADP	B	2001	6	27,29,29	1.34	4 (14%)	42,45,45	2.00	10 (23%)
5	PO4	B	2002	6	4,4,4	1.02	0	6,6,6	0.39	0
4	ADP	A	2001	6	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
5	PO4	A	2002	6	4,4,4	1.11	0	6,6,6	0.38	0

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	ADP	B	2001	6	-	4/16/32/32	0/3/3/3
4	ADP	A	2001	6	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	ADP	C5-C4	4.36	1.47	1.39
4	B	2001	ADP	C5-C4	4.34	1.47	1.39
4	A	2001	ADP	C5-C6	2.69	1.48	1.41
4	B	2001	ADP	C5-C6	2.55	1.48	1.41
4	B	2001	ADP	C5-N7	-2.33	1.34	1.39
4	A	2001	ADP	C5-N7	-2.30	1.34	1.39
4	B	2001	ADP	C8-N7	2.29	1.35	1.31
4	A	2001	ADP	C8-N7	2.22	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ADP	C5-C4-N3	-6.39	118.41	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	ADP	C5-C4-N3	-6.22	118.64	126.75
4	B	2001	ADP	N3-C4-N9	4.96	135.25	127.08
4	A	2001	ADP	N3-C4-N9	4.90	135.16	127.08
4	B	2001	ADP	PA-O3A-PB	-4.01	119.06	132.83
4	A	2001	ADP	C2-N3-C4	3.92	121.02	111.75
4	B	2001	ADP	C2-N3-C4	3.81	120.76	111.75
4	A	2001	ADP	C4-C5-N7	-3.34	106.55	110.62
4	B	2001	ADP	C4-C5-N7	-3.10	106.84	110.62
4	B	2001	ADP	N3-C2-N1	-3.03	123.86	128.60
4	A	2001	ADP	N3-C2-N1	-3.02	123.89	128.60
4	A	2001	ADP	PA-O3A-PB	-2.83	123.13	132.83
4	A	2001	ADP	C5-N7-C8	2.76	107.44	103.51
4	A	2001	ADP	C3'-C2'-C1'	2.72	106.59	101.43
4	B	2001	ADP	C5-N7-C8	2.68	107.32	103.51
4	B	2001	ADP	C4-N9-C8	2.65	108.60	105.73
4	B	2001	ADP	C3'-C2'-C1'	2.47	106.11	101.43
4	A	2001	ADP	C4-N9-C8	2.36	108.29	105.73
4	A	2001	ADP	C6-C5-N7	2.15	136.03	132.02
4	A	2001	ADP	O3B-PB-O2B	2.06	115.49	107.64
4	B	2001	ADP	N9-C8-N7	-2.04	111.12	113.91

There are no chirality outliers.

All (8) torsion outliers are listed below:

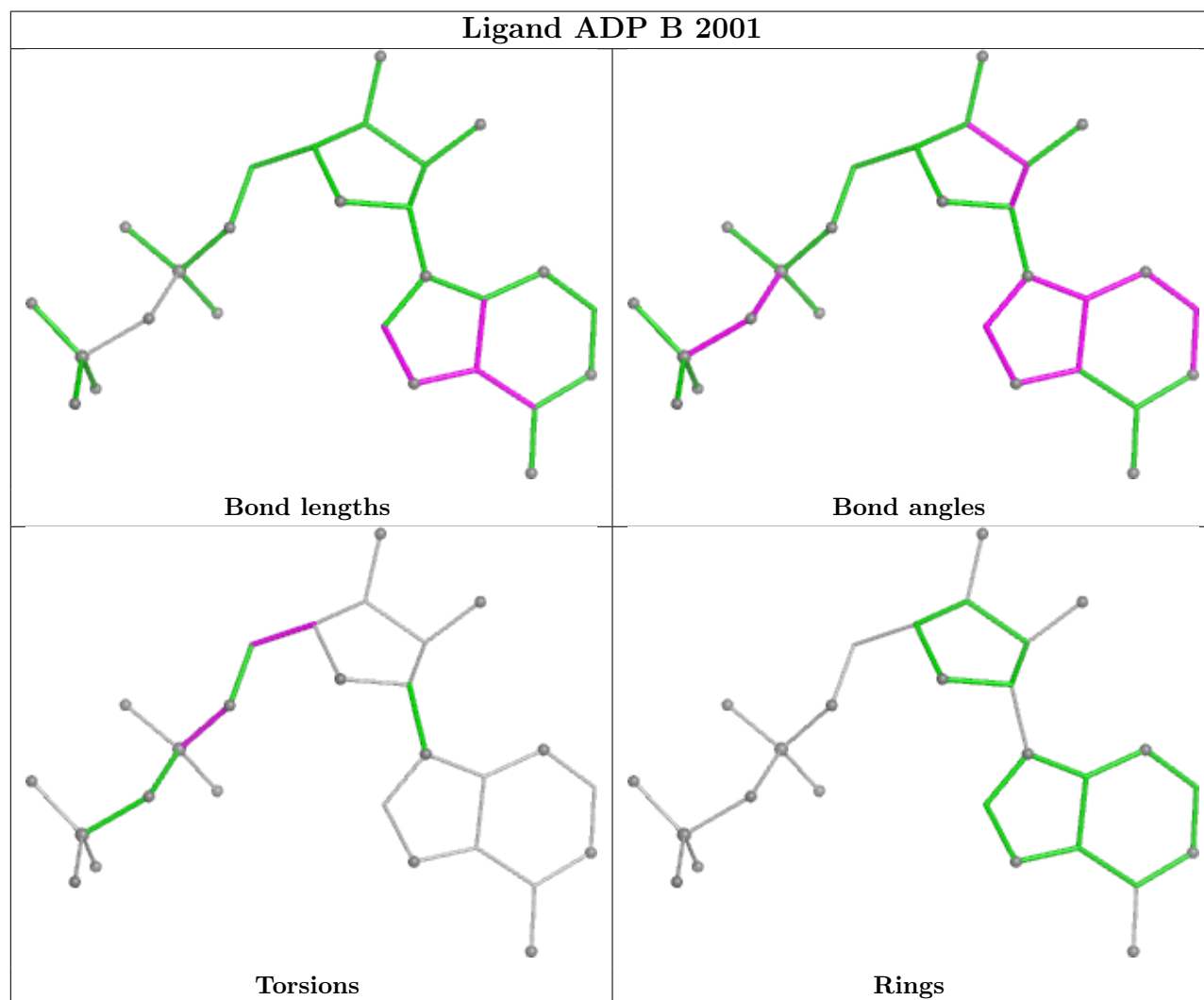
Mol	Chain	Res	Type	Atoms
4	A	2001	ADP	C5'-O5'-PA-O3A
4	A	2001	ADP	O4'-C4'-C5'-O5'
4	A	2001	ADP	C3'-C4'-C5'-O5'
4	B	2001	ADP	C5'-O5'-PA-O1A
4	B	2001	ADP	O4'-C4'-C5'-O5'
4	B	2001	ADP	C3'-C4'-C5'-O5'
4	A	2001	ADP	C5'-O5'-PA-O1A
4	B	2001	ADP	C5'-O5'-PA-O3A

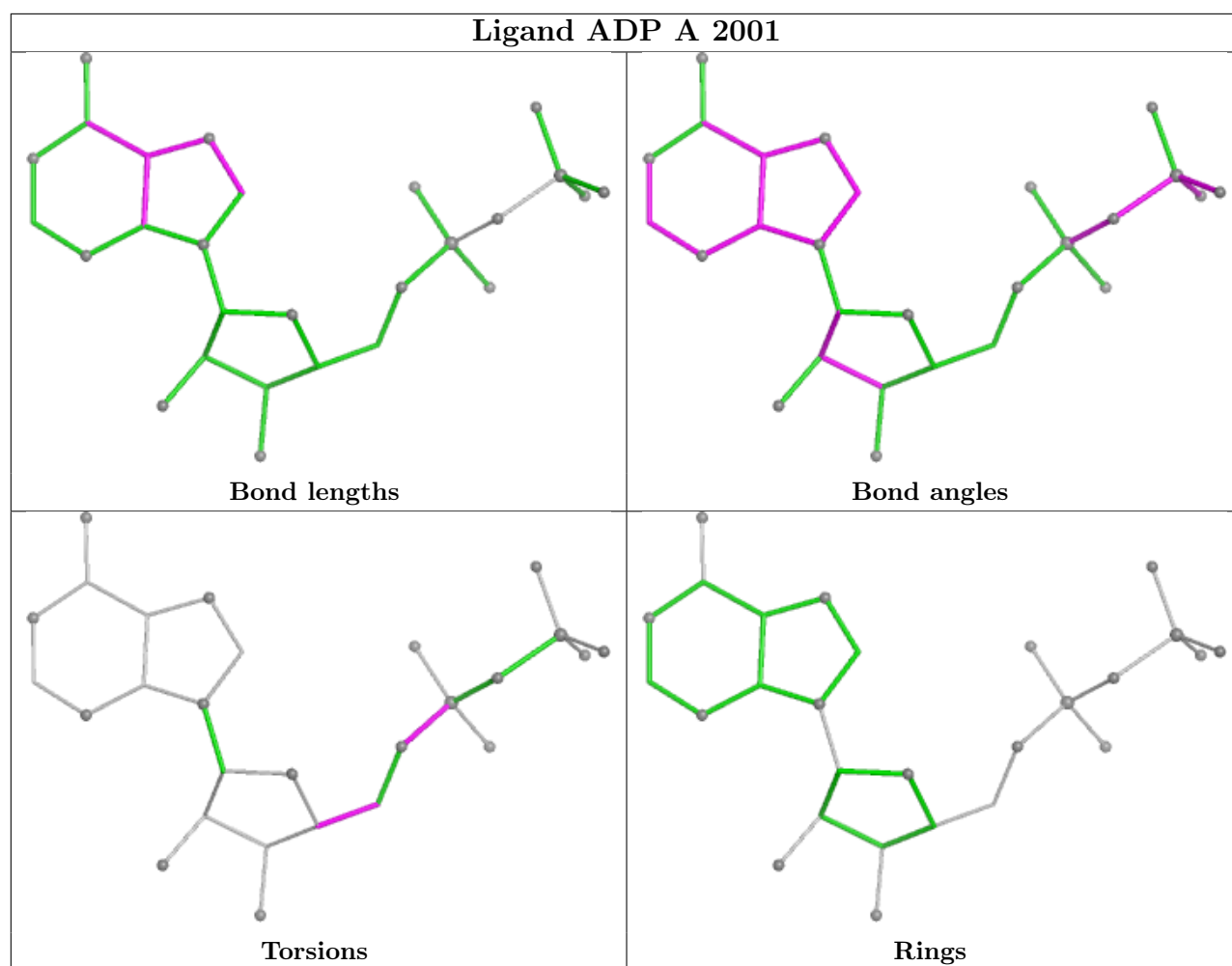
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	ADP	2	0
4	A	2001	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

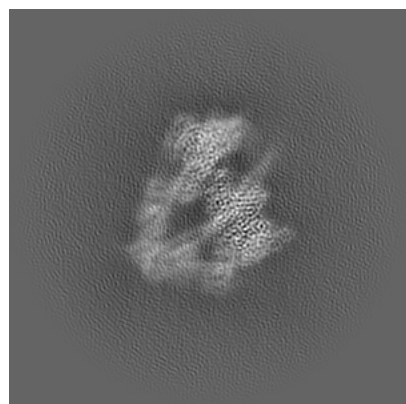
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56106. These allow visual inspection of the internal detail of the map and identification of artifacts.

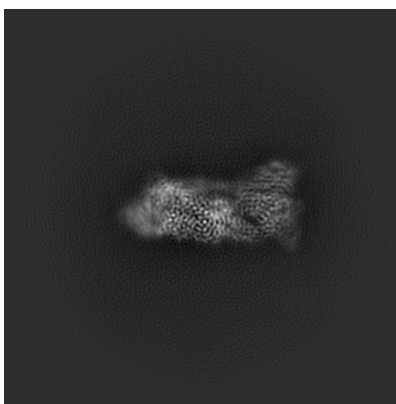
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

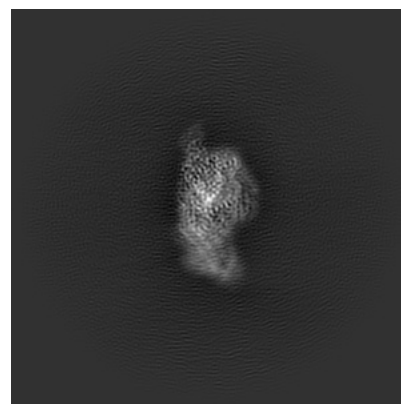
6.1.1 Primary map



X

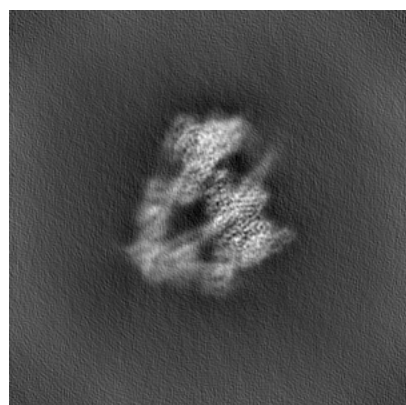


Y

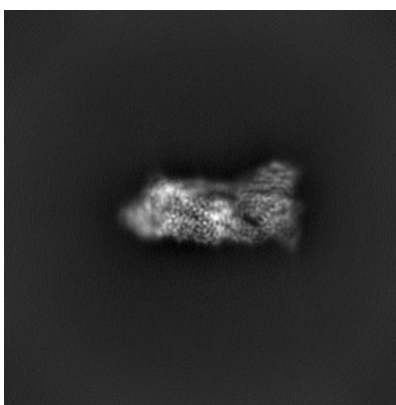


Z

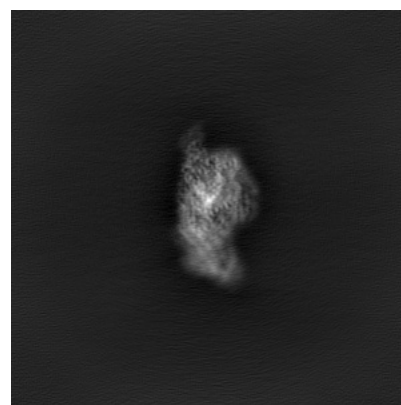
6.1.2 Raw map



X



Y

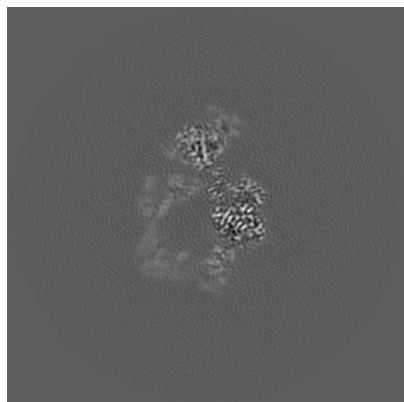


Z

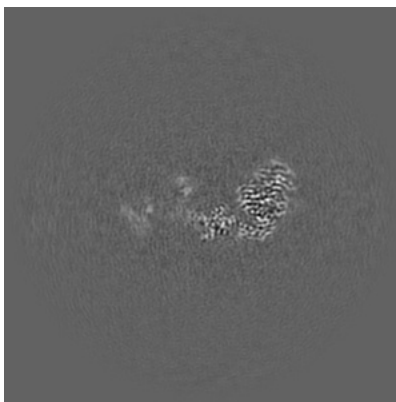
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

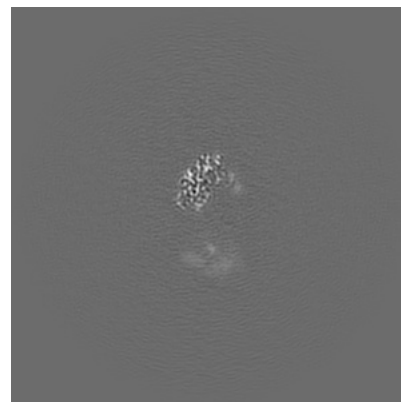
6.2.1 Primary map



X Index: 150

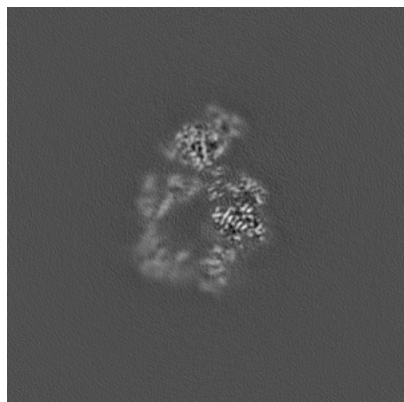


Y Index: 150

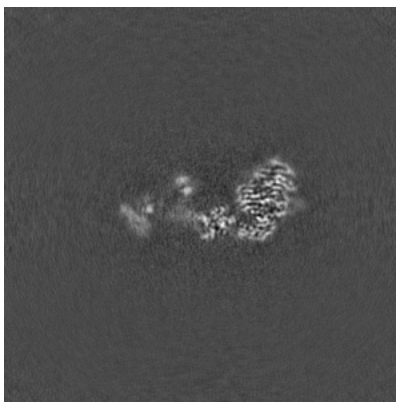


Z Index: 150

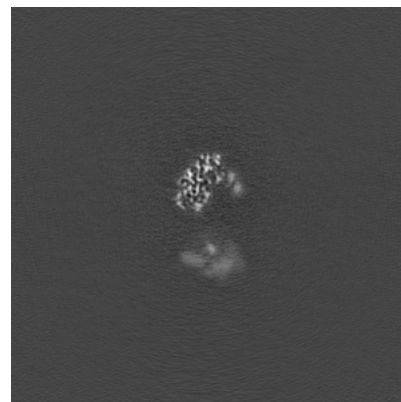
6.2.2 Raw map



X Index: 150



Y Index: 150

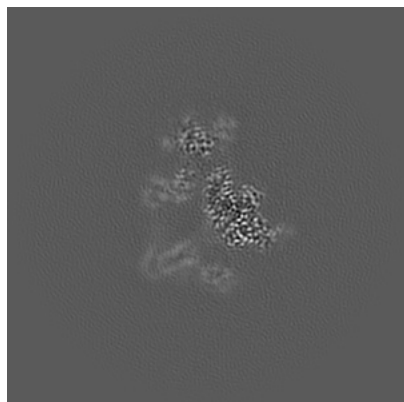


Z Index: 150

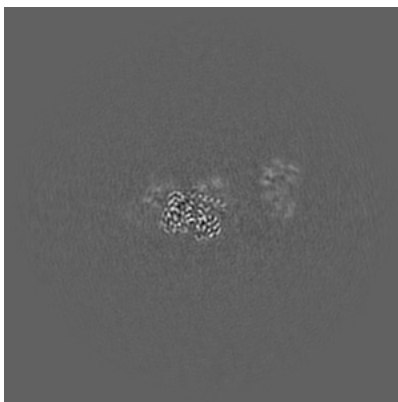
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

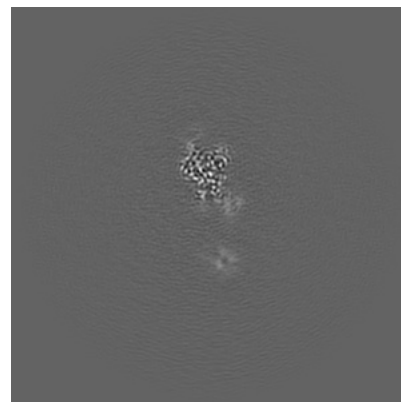
6.3.1 Primary map



X Index: 142

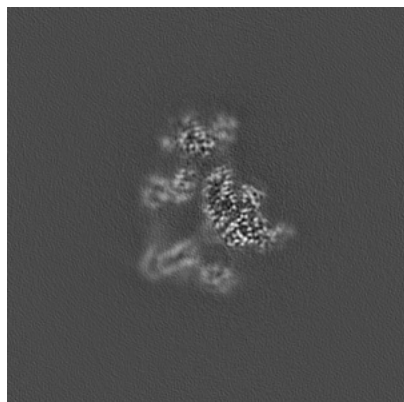


Y Index: 170

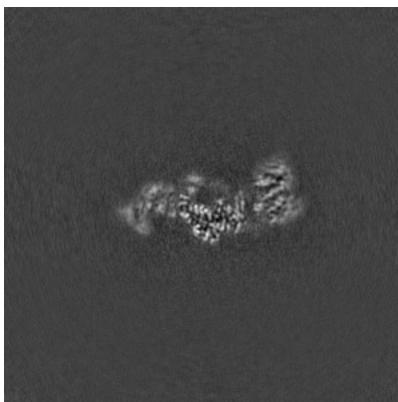


Z Index: 137

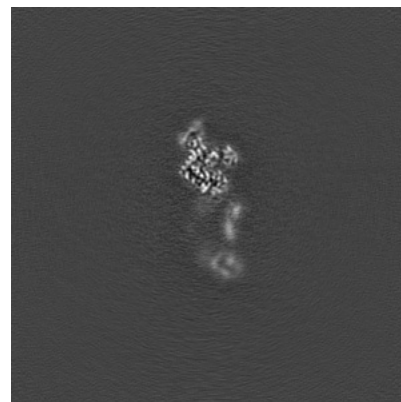
6.3.2 Raw map



X Index: 142



Y Index: 158

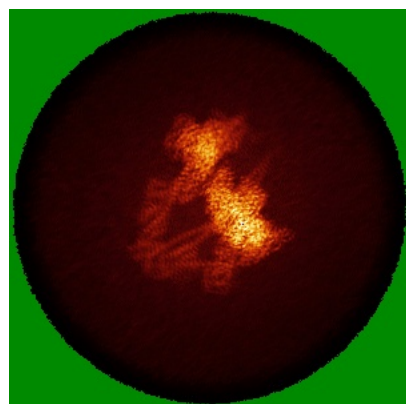


Z Index: 130

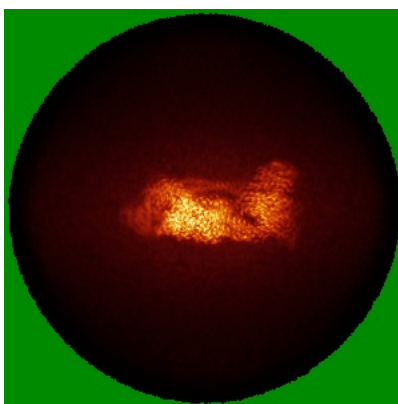
The images above show the largest variance slices of the map in three orthogonal directions.

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

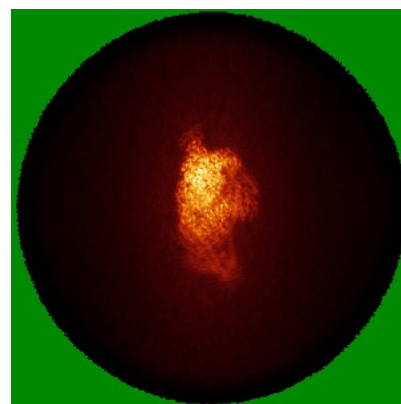
6.4.1 Primary map



X

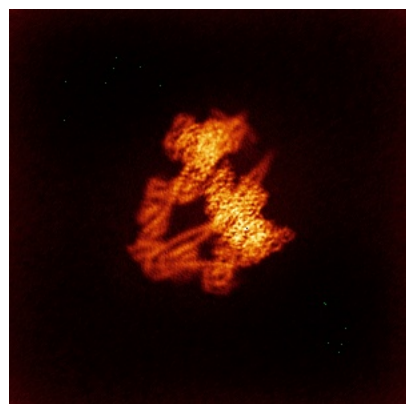


Y

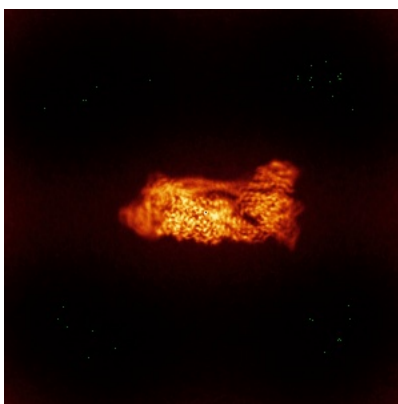


Z

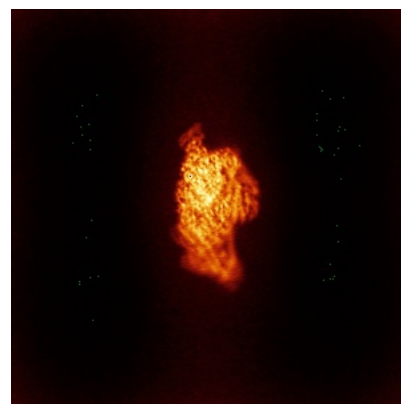
6.4.2 Raw map



X



Y

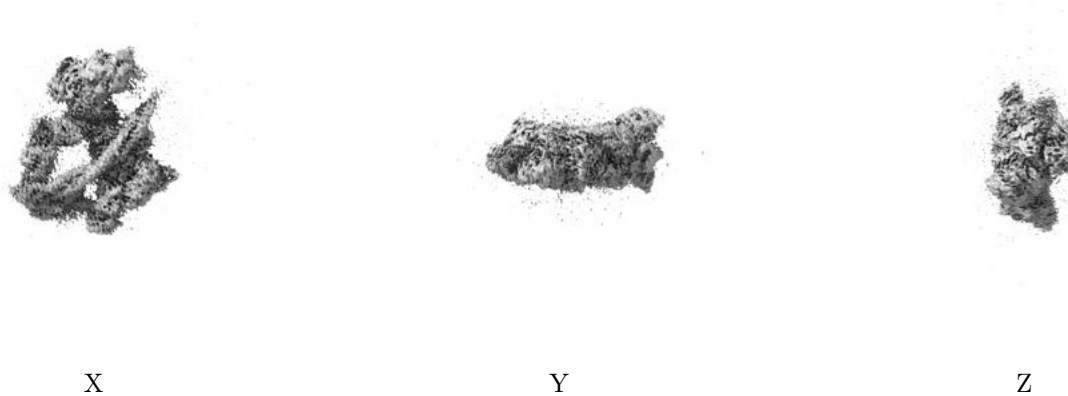


Z

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

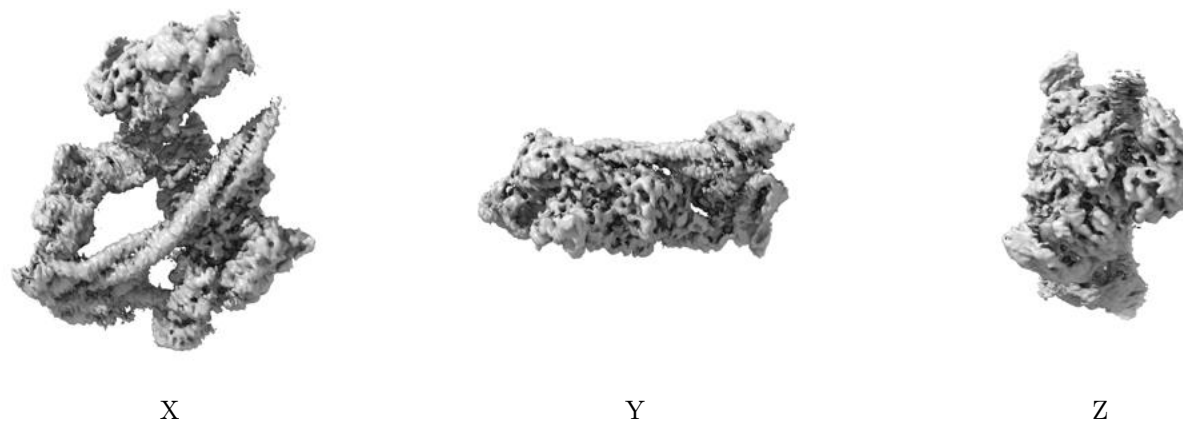
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.126. 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.

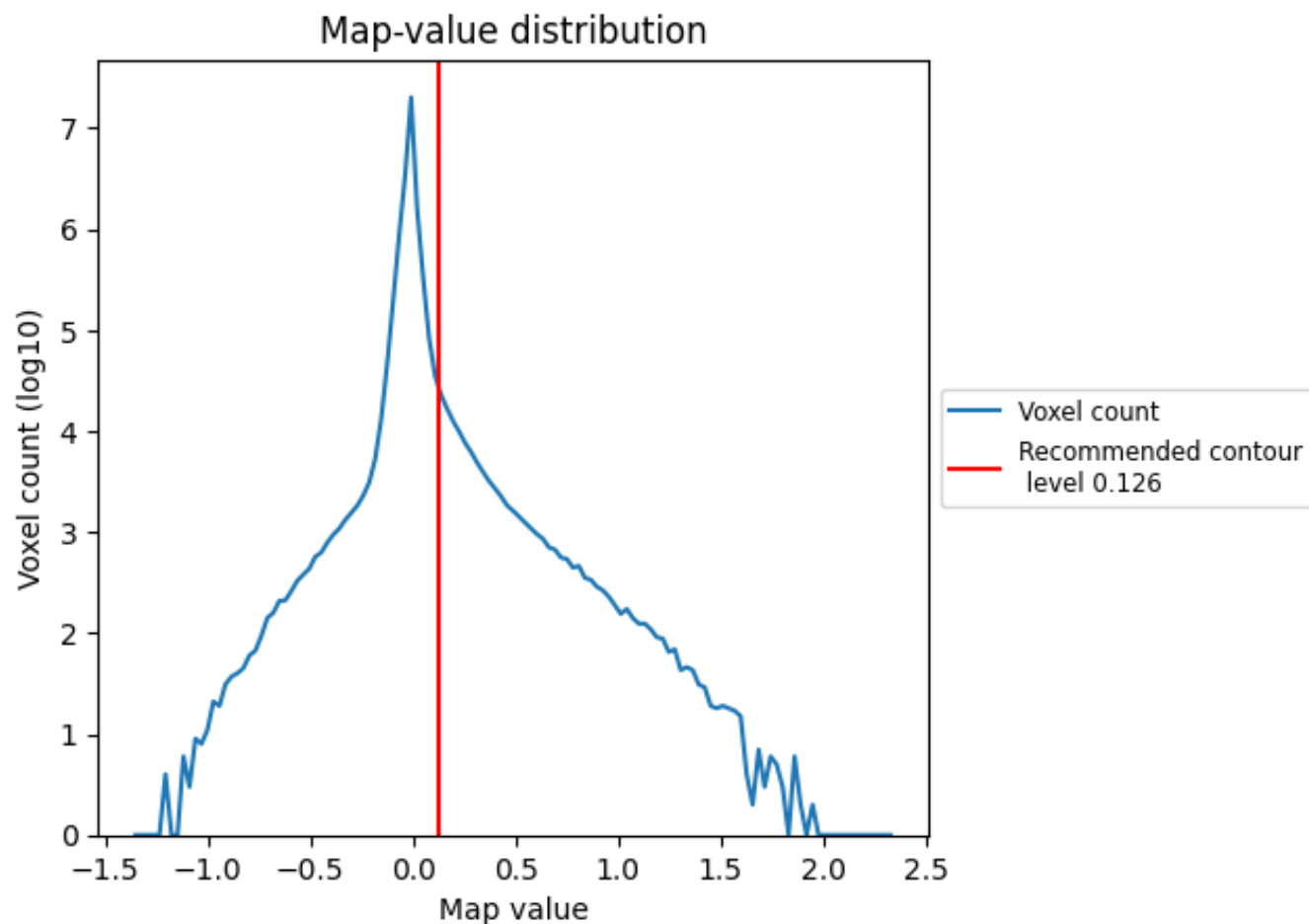
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

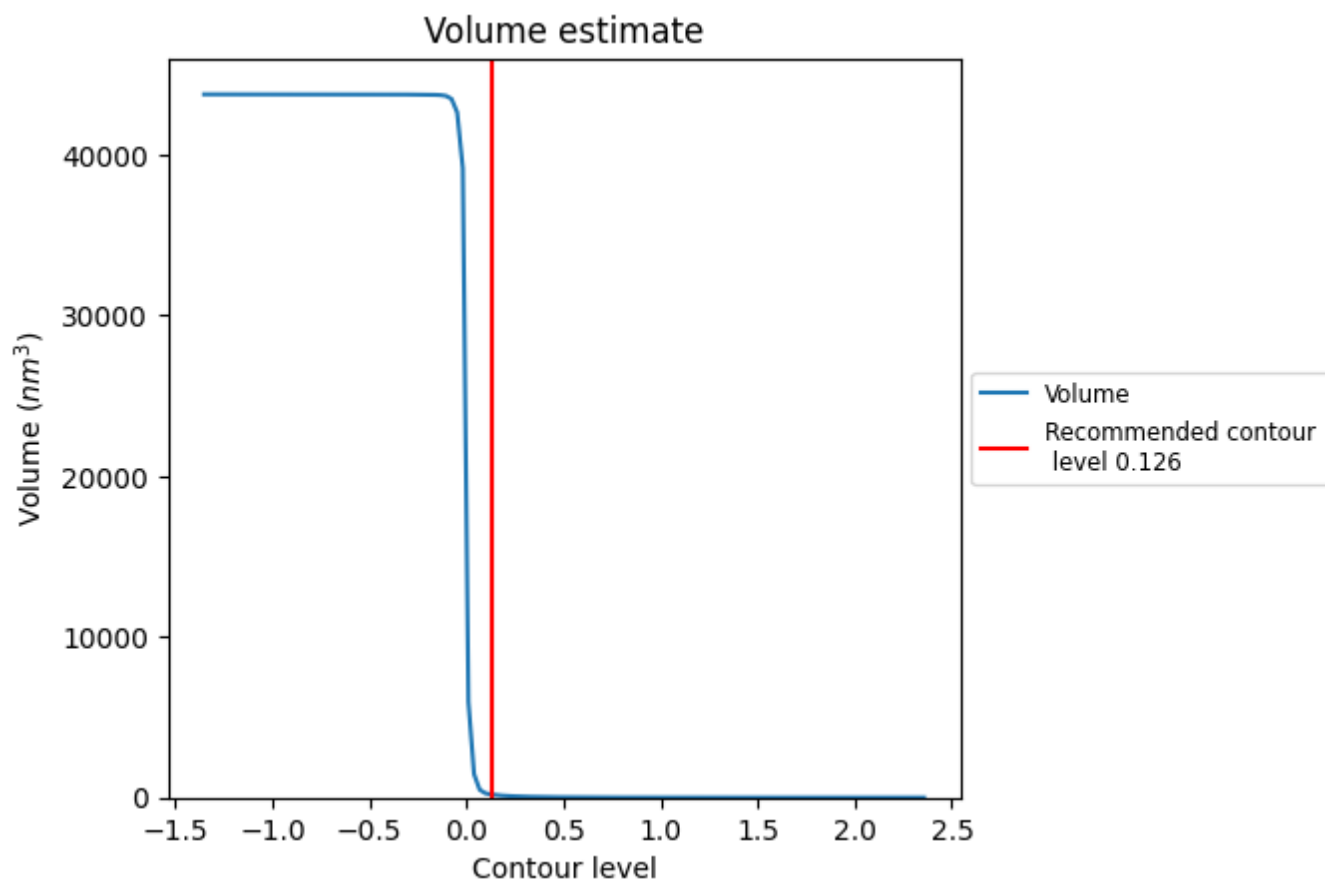
This section contains the results of statistical analysis of the map.

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.

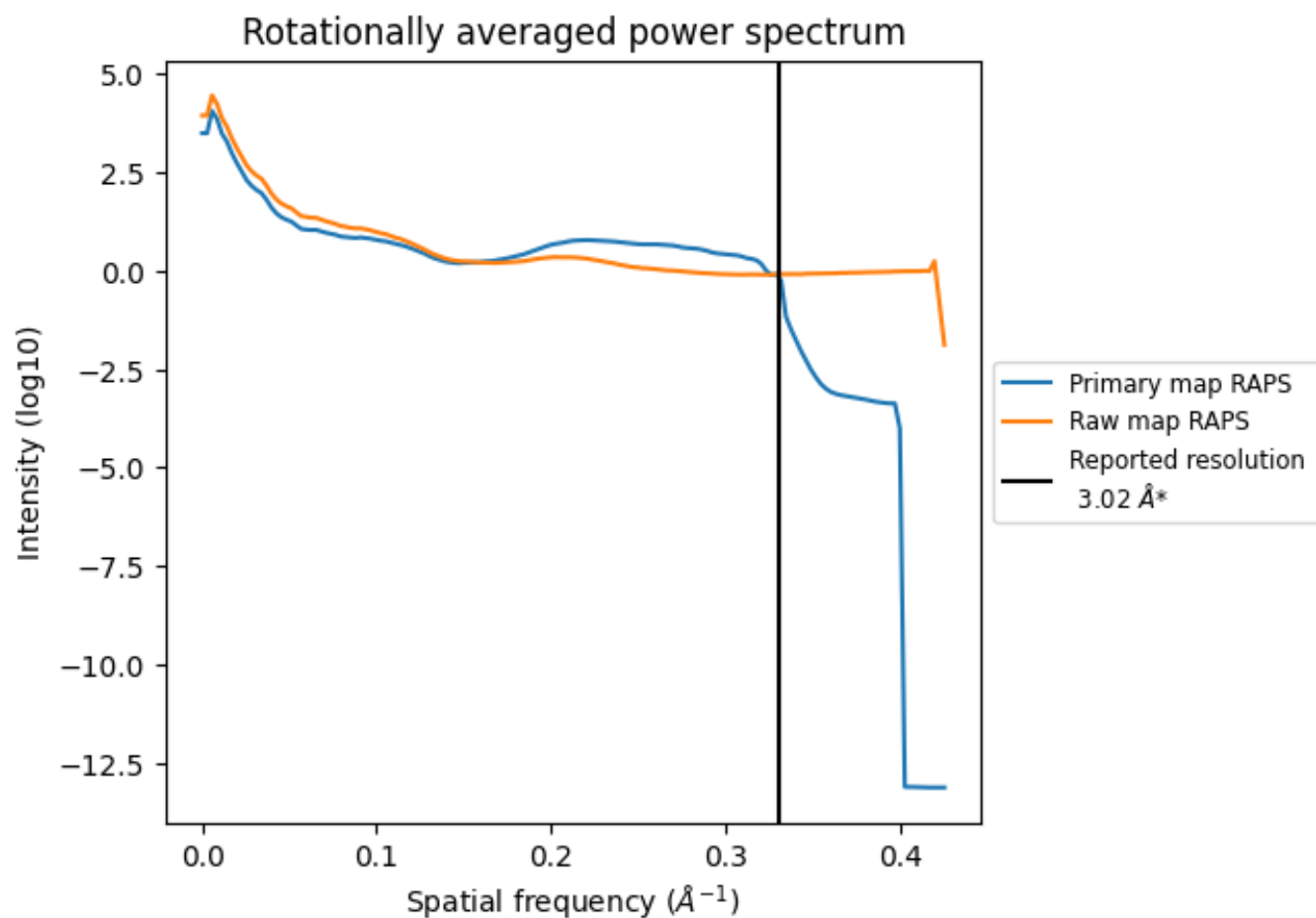
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 ⓘ

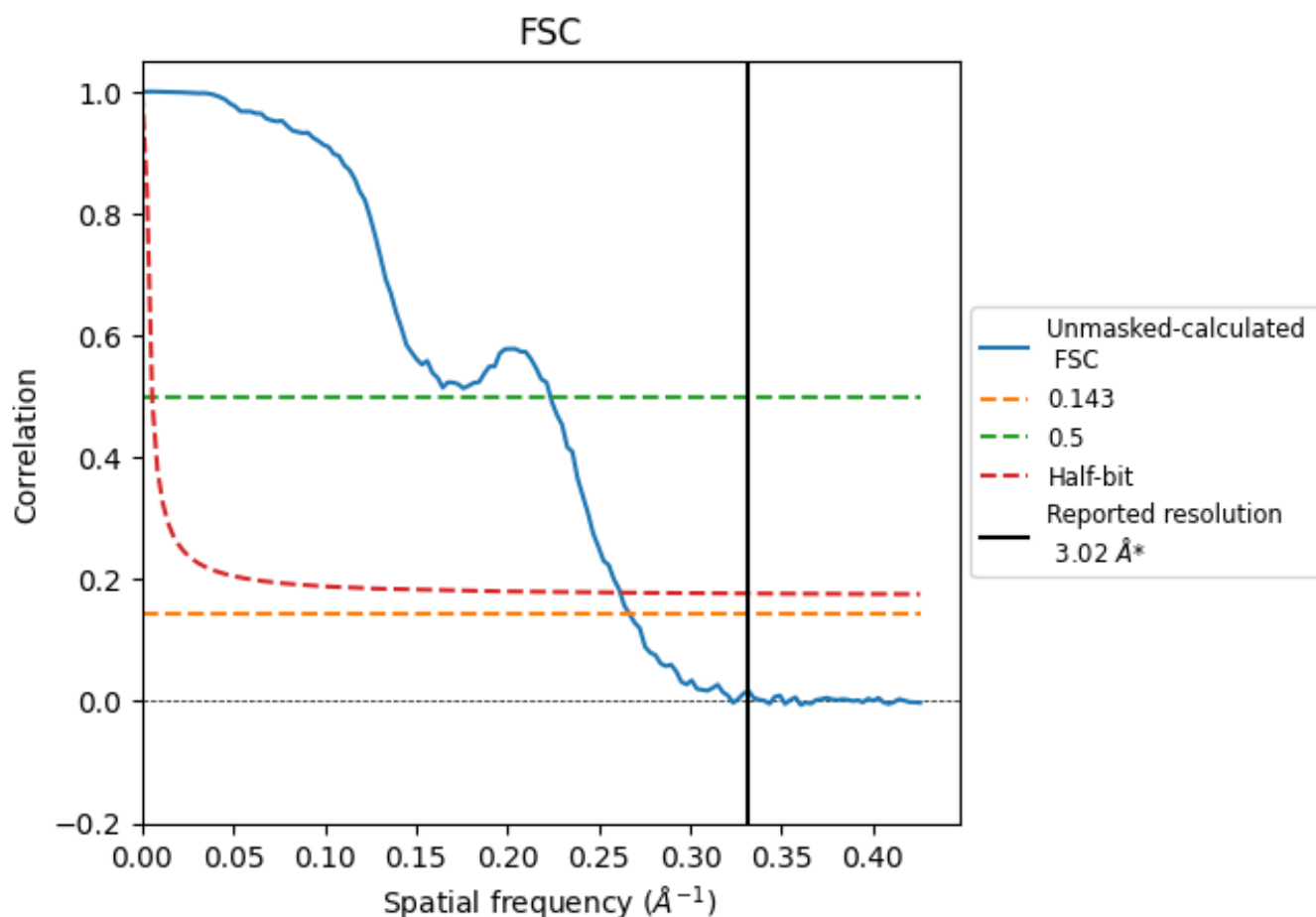


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

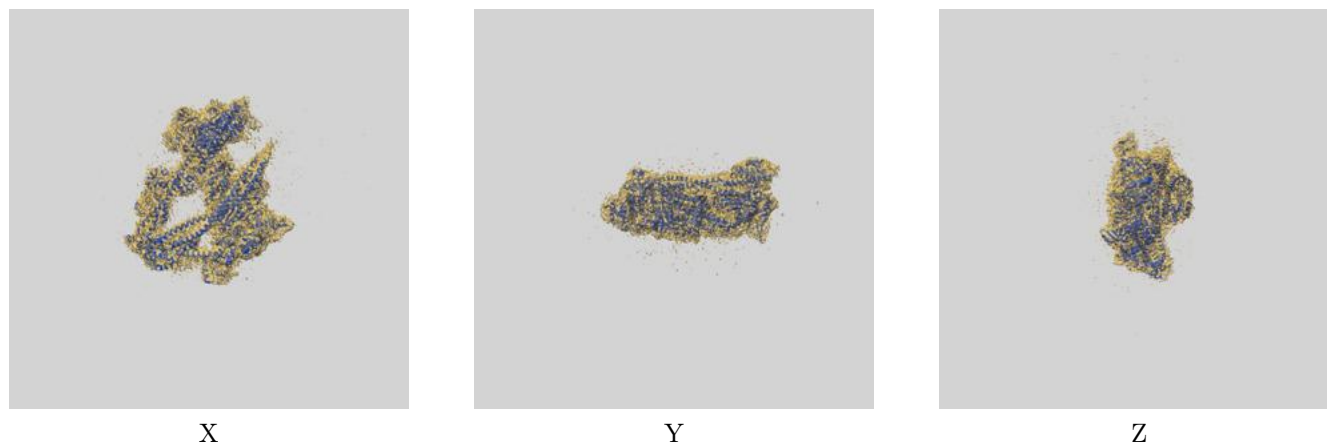
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	4.48	3.82

*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 3.75 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

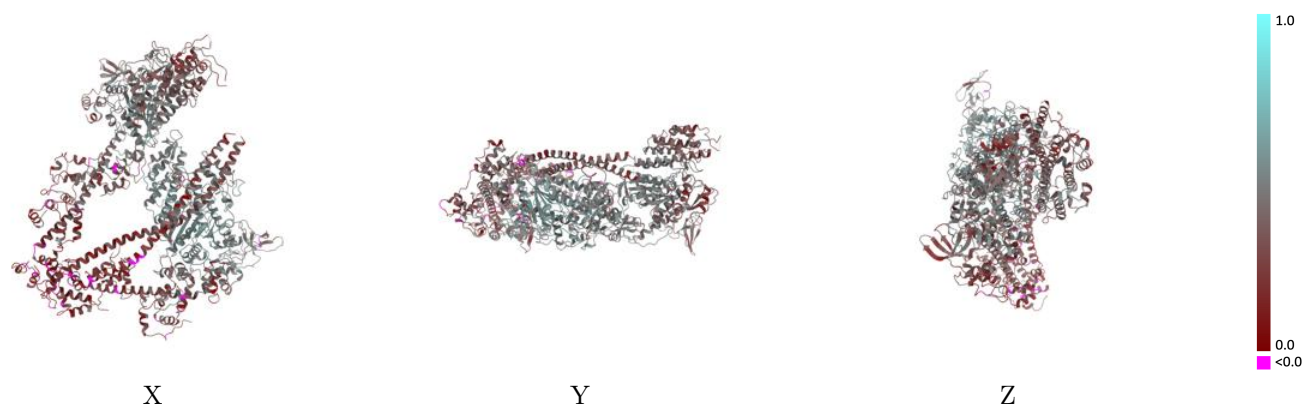
This section contains information regarding the fit between EMDB map EMD-56106 and PDB model 9TPJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



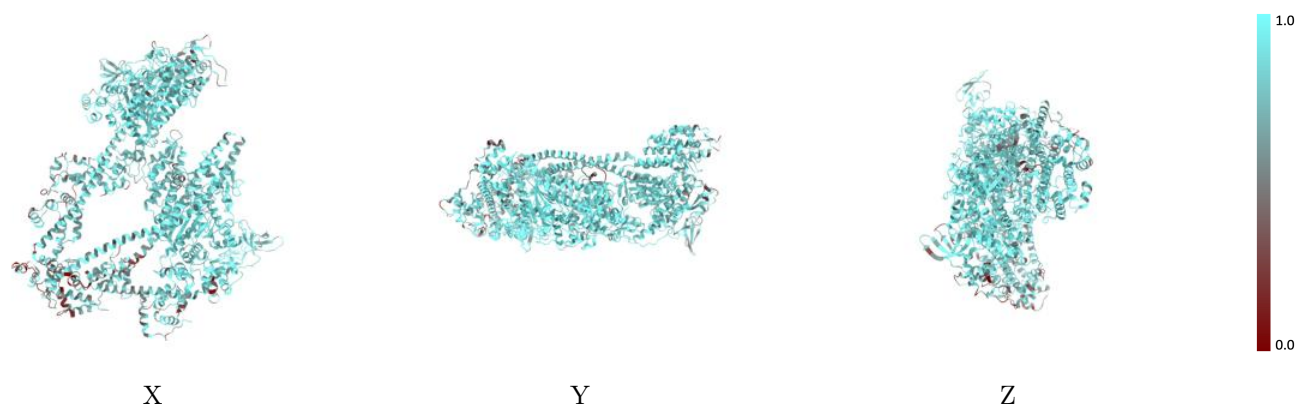
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



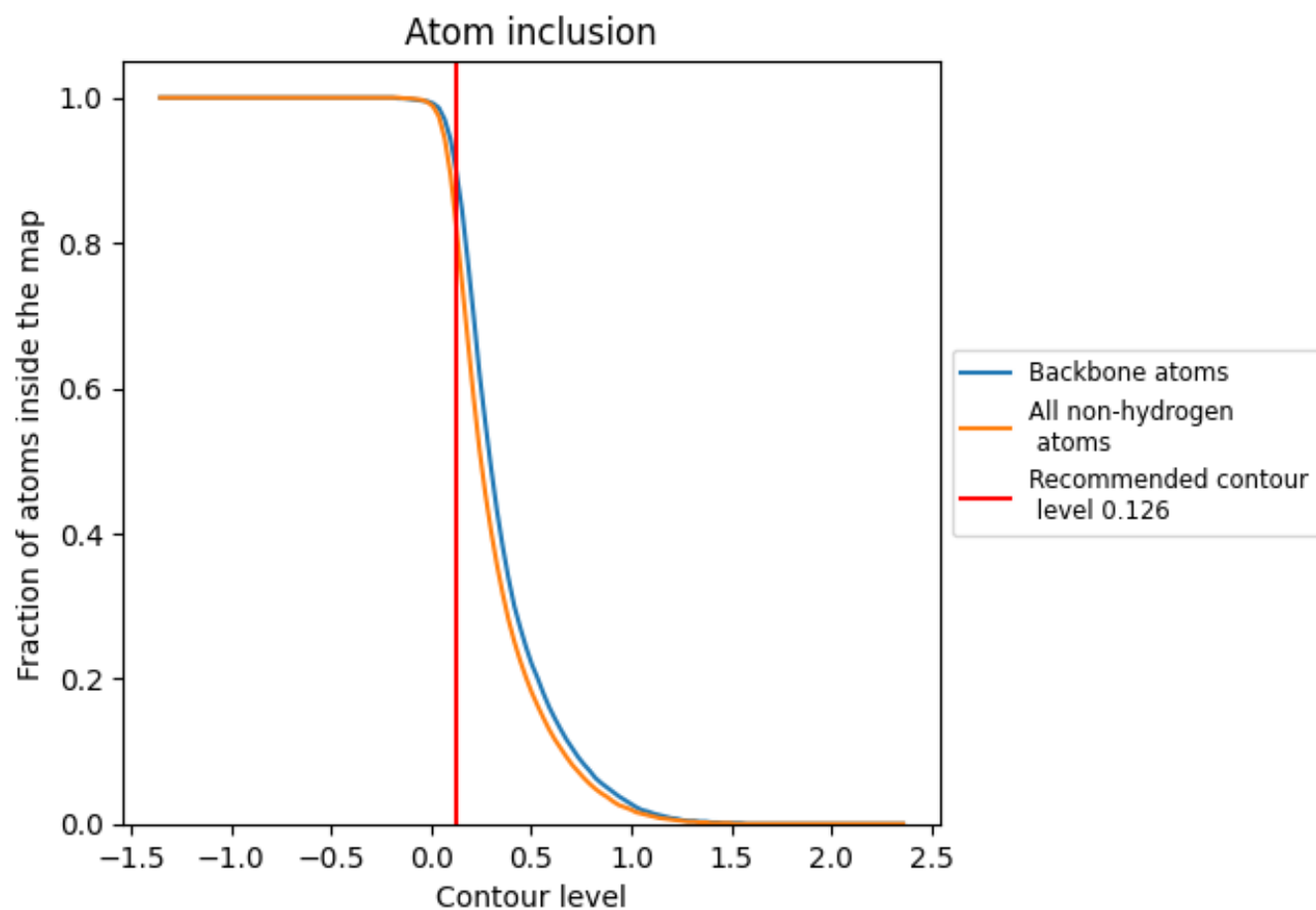
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.3850
A	0.8800	0.4600
B	0.8420	0.3940
C	0.7370	0.2890
D	0.7760	0.3150
E	0.6660	0.1930
F	0.6040	0.1990

1.0

0.0

<0.0