



Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 04:20 PM EST

PDB ID : 9C6F
EMDB ID : EMD-45245
Title : cryoEM structure of CRISPR associated effector, CARF-Adenosine deaminase 1, Cad1, in apo form with ATP (Asymmetric sites).
Authors : Majumder, P.; Patel, D.J.
Deposited on : 2024-06-07
Resolution : 3.60 Å(reported)
Based on initial model : .

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

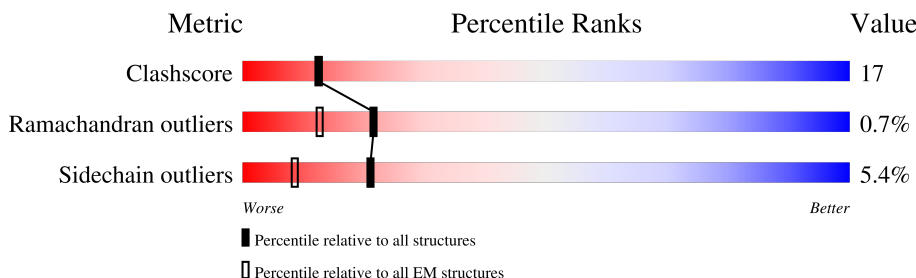
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	600	<div> <div>5%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>
1	B	600	<div> <div>.</div> <div>63%</div> <div>34%</div> <div>.</div> </div>
1	C	600	<div> <div>7%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	D	600	<div> <div>.</div> <div>62%</div> <div>33%</div> <div>.</div> </div>
1	E	600	<div> <div>16%</div> <div>63%</div> <div>35%</div> <div>.</div> </div>
1	F	600	<div> <div>12%</div> <div>66%</div> <div>32%</div> <div>.</div> </div>

2 Entry composition [i](#)

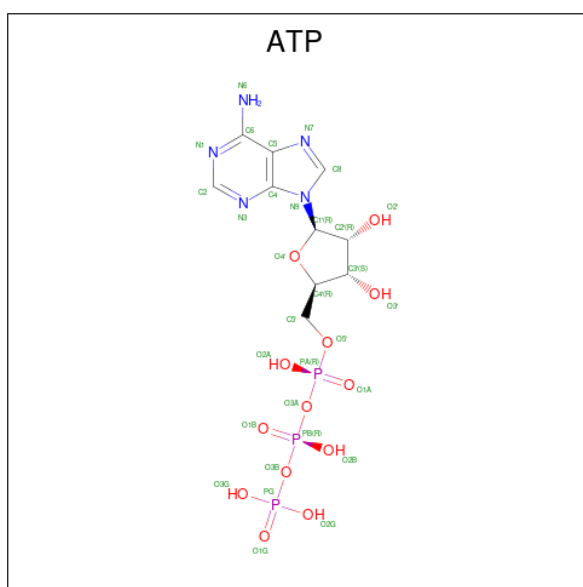
There are 3 unique types of molecules in this entry. The entry contains 28361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	598	Total	C	N	O	S	0	0
			4710	3002	810	871	27		
1	B	598	Total	C	N	O	S	0	0
			4710	3002	810	871	27		
1	C	598	Total	C	N	O	S	0	0
			4711	3002	811	871	27		
1	D	598	Total	C	N	O	S	0	0
			4711	3002	811	871	27		
1	E	598	Total	C	N	O	S	0	0
			4710	3002	810	871	27		
1	F	598	Total	C	N	O	S	0	0
			4710	3002	810	871	27		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	

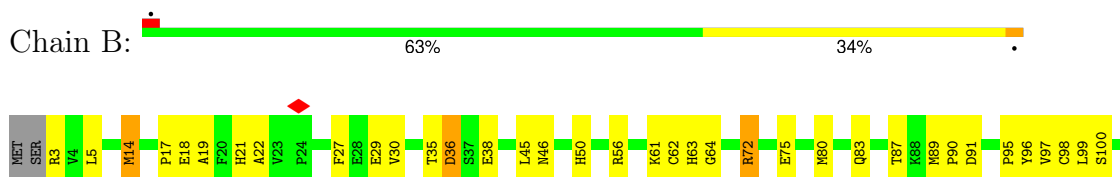
3 Residue-property plots

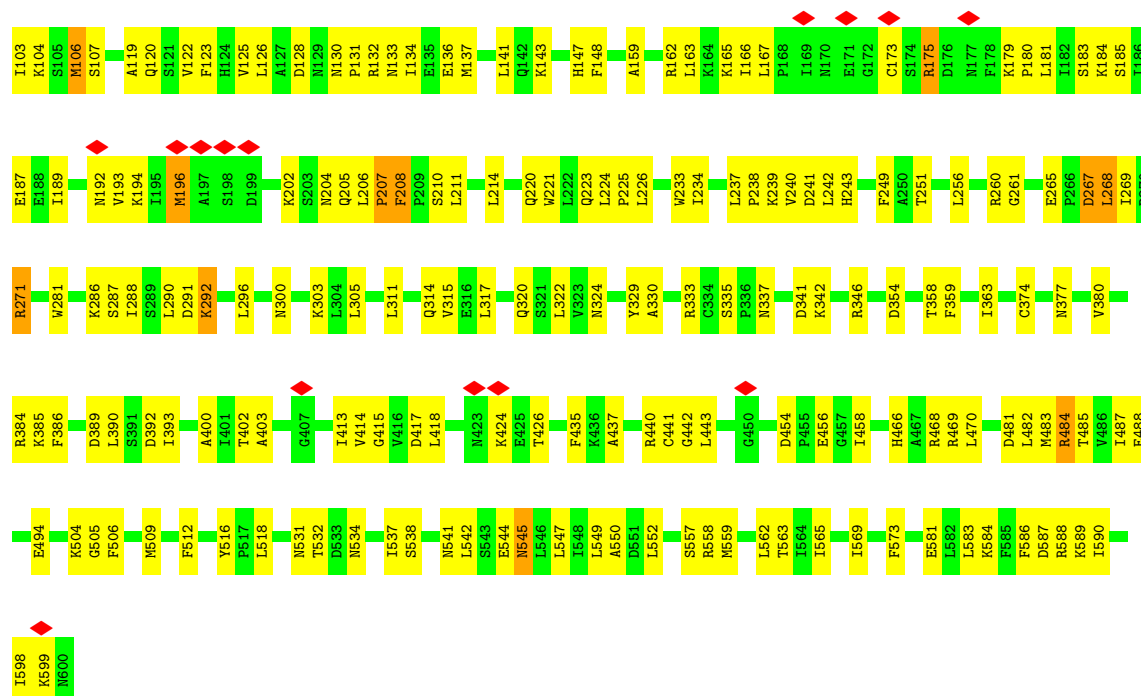
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Adenosine deaminase domain-containing protein

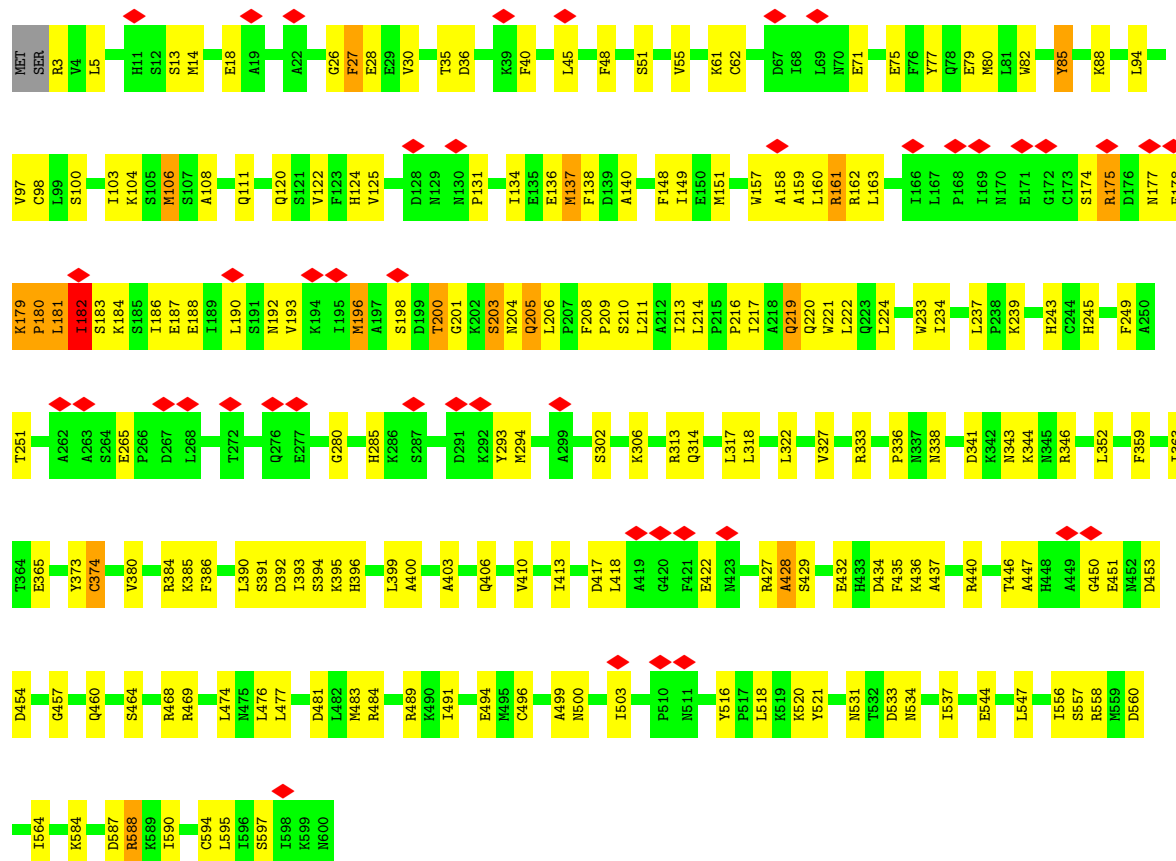


- Molecule 1: Adenosine deaminase domain-containing protein

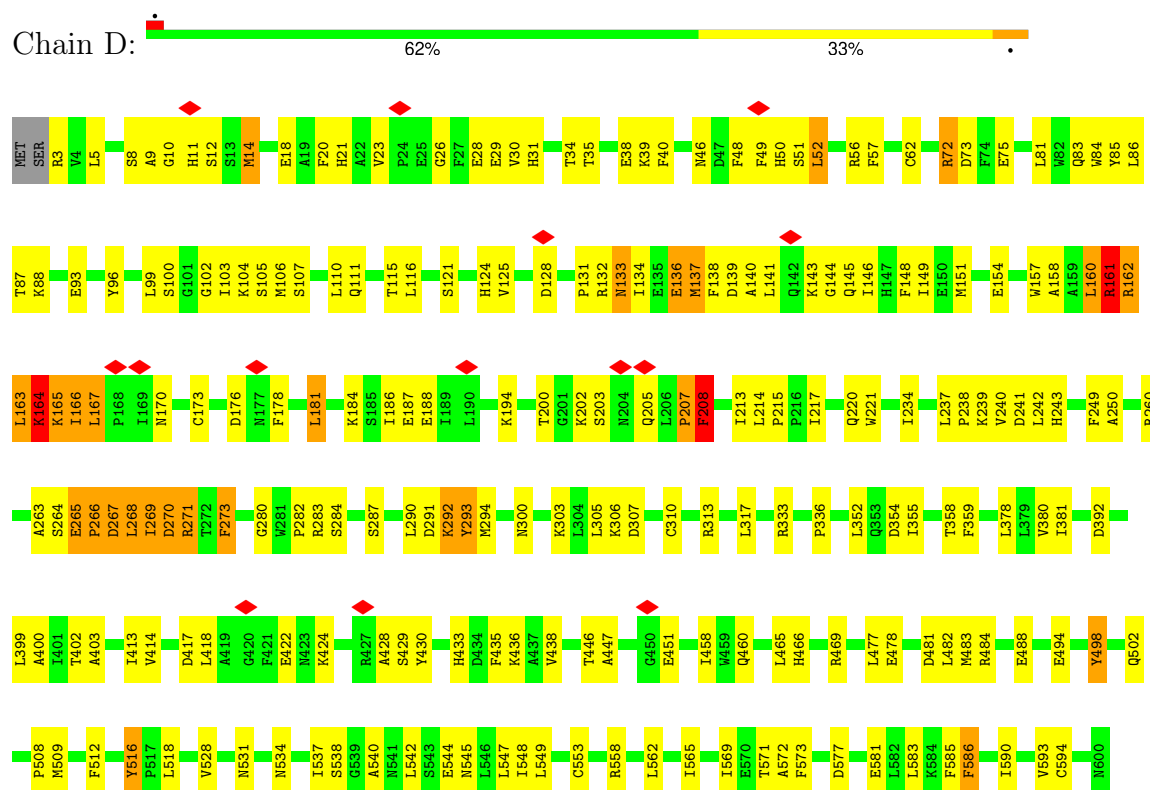




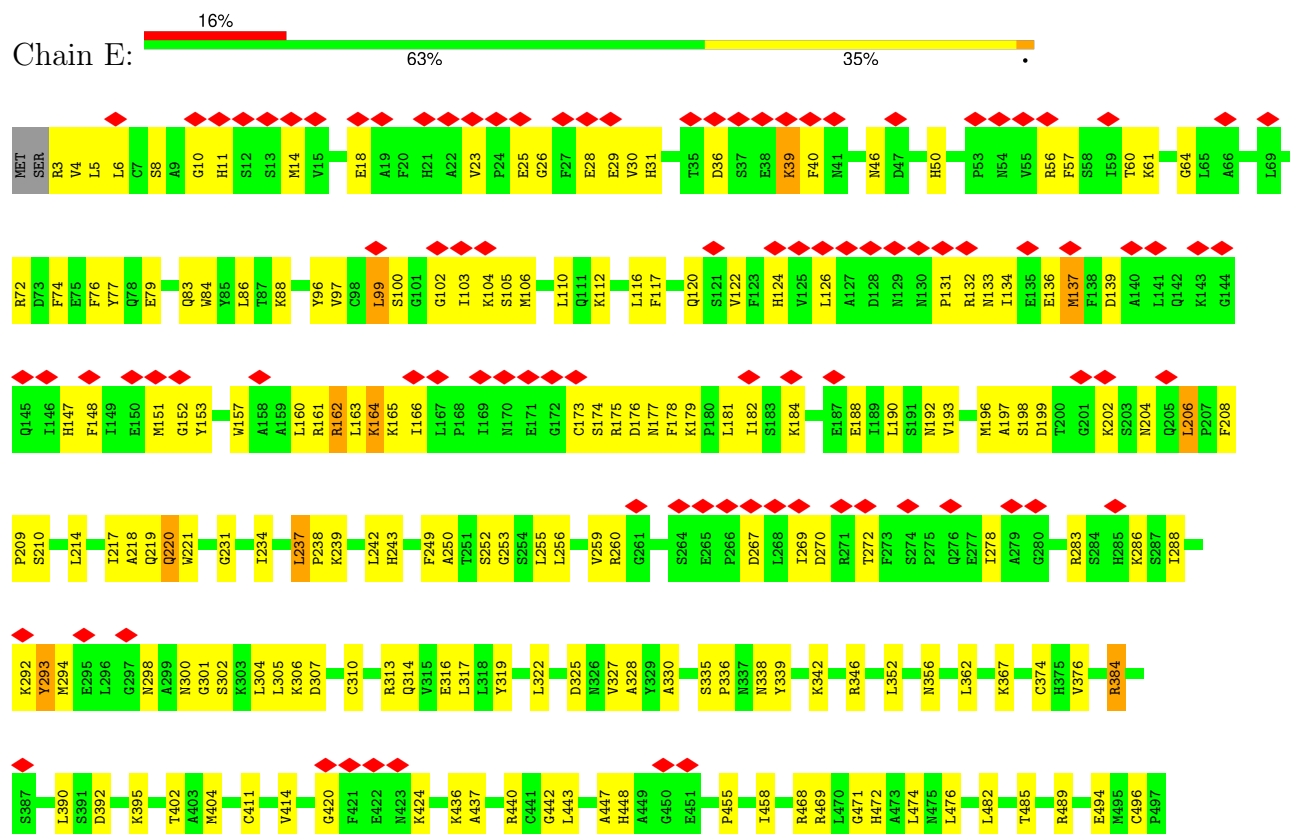
• Molecule 1: Adenosine deaminase domain-containing protein

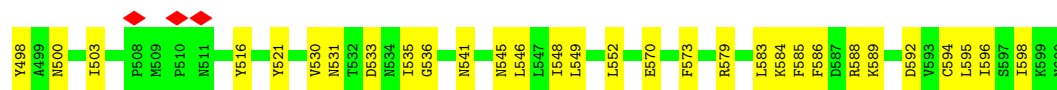


- Molecule 1: Adenosine deaminase domain-containing protein

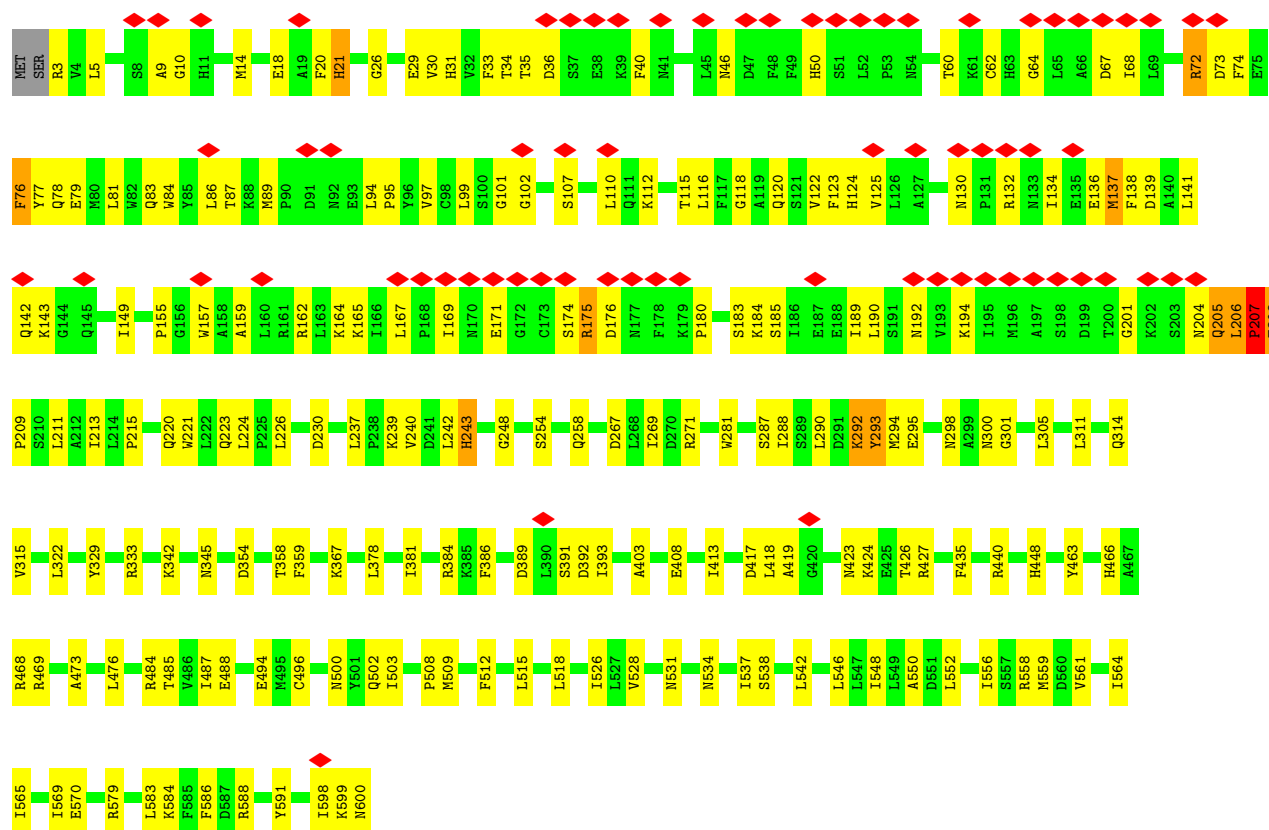


- Molecule 1: Adenosine deaminase domain-containing protein





• Molecule 1: Adenosine deaminase domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100094	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.939	Depositor
Minimum map value	-1.298	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.184	Depositor
Map size (\AA)	342.08002, 342.08002, 342.08002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.069, 1.069, 1.069	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/4815	0.52	1/6523 (0.0%)
1	B	0.27	0/4815	0.52	0/6523
1	C	0.27	0/4816	0.54	0/6525
1	D	0.27	0/4816	0.52	1/6525 (0.0%)
1	E	0.25	0/4815	0.52	2/6523 (0.0%)
1	F	0.26	0/4815	0.54	4/6523 (0.1%)
All	All	0.27	0/28892	0.53	8/39142 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	508	PRO	CA-N-CD	-10.35	97.00	111.50
1	A	199	ASP	C-N-CA	6.68	138.39	121.70
1	E	206	LEU	CA-CB-CG	6.60	130.49	115.30
1	F	207	PRO	N-CA-C	6.47	128.91	112.10
1	D	137	MET	CA-CB-CG	6.00	123.50	113.30
1	E	137	MET	CA-CB-CG	5.64	122.89	113.30
1	F	207	PRO	N-CA-CB	-5.48	96.57	102.60
1	F	508	PRO	N-CD-CG	-5.33	95.21	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	175	ARG	Sidechain
1	D	136	GLU	Peptide
1	D	161	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4710	0	4683	161	0
1	B	4710	0	4685	165	0
1	C	4711	0	4687	166	0
1	D	4711	0	4687	177	0
1	E	4710	0	4685	161	0
1	F	4710	0	4685	163	0
2	A	31	0	11	1	0
2	D	31	0	11	2	0
2	E	31	0	11	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	28361	0	28145	937	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 17.

All (937) 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:181:LEU:HB3	1:C:184:LYS:HB2	1.22	1.12
1:A:87:THR:HB	1:A:169:ILE:HG21	1.33	1.10
1:A:83:GLN:NE2	1:A:169:ILE:HA	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:PRO:HG2	1:F:207:PRO:HD2	1.49	0.94
1:E:204:ASN:HD21	1:F:583:LEU:HB3	1.40	0.86
1:C:175:ARG:HG3	1:C:180:PRO:HB3	1.57	0.86
1:D:270:ASP:HB3	1:D:303:LYS:NZ	1.94	0.83
1:C:237:LEU:HD23	1:C:590:ILE:HD11	1.60	0.81
1:B:162:ARG:HG2	1:B:599:LYS:HD2	1.62	0.81
1:C:181:LEU:CB	1:C:184:LYS:HB2	2.10	0.81
1:F:35:THR:HA	1:F:62:CYS:HB3	1.65	0.79
1:E:163:LEU:HD11	1:E:182:ILE:HG21	1.63	0.78
1:E:173:CYS:SG	1:E:177:ASN:ND2	2.56	0.78
1:A:83:GLN:HE21	1:A:169:ILE:HG23	1.49	0.78
1:D:240:VAL:HG21	1:D:569:ILE:HG22	1.65	0.77
1:D:143:LYS:HB2	1:D:145:GLN:HE21	1.49	0.76
1:C:251:THR:HG21	1:C:537:ILE:HG12	1.66	0.76
1:C:160:LEU:HA	1:C:162:ARG:HH22	1.50	0.76
1:F:239:LYS:HD2	1:F:542:LEU:HD22	1.69	0.75
1:F:192:ASN:ND2	1:F:220:GLN:O	2.21	0.73
1:B:237:LEU:HD12	1:B:238:PRO:HD2	1.70	0.73
1:B:192:ASN:ND2	1:B:220:GLN:O	2.22	0.73
1:C:104:LYS:NZ	1:D:99:LEU:O	2.22	0.73
1:D:429:SER:HB3	1:D:460:GLN:HG2	1.70	0.73
1:A:163:LEU:HA	1:A:166:ILE:HG12	1.69	0.73
1:C:108:ALA:HA	1:C:111:GLN:HE21	1.54	0.73
1:B:207:PRO:HG3	1:B:562:LEU:HB3	1.72	0.71
1:B:484:ARG:HA	1:B:487:ILE:HD12	1.73	0.71
1:D:134:ILE:HA	1:D:137:MET:HG2	1.72	0.71
1:A:391:SER:HB3	1:F:440:ARG:HE	1.55	0.71
1:B:288:ILE:HB	1:B:292:LYS:HD3	1.73	0.71
1:C:363:ILE:HG21	1:C:410:VAL:HG11	1.74	0.70
1:F:226:LEU:HD23	1:F:550:ALA:HB2	1.72	0.70
1:D:509:MET:HB3	1:D:512:PHE:HB2	1.74	0.69
1:A:292:LYS:HA	1:A:295:GLU:HG2	1.74	0.69
1:E:384:ARG:O	1:E:424:LYS:NZ	2.24	0.69
1:A:510:PRO:O	1:A:511:ASN:ND2	2.25	0.69
1:F:208:PHE:HB2	1:F:211:LEU:HD13	1.74	0.69
1:B:179:LYS:HA	1:B:179:LYS:HE3	1.73	0.69
1:B:251:THR:HG21	1:B:537:ILE:HG13	1.74	0.69
1:D:234:ILE:O	1:D:239:LYS:NZ	2.25	0.69
1:A:234:ILE:O	1:A:239:LYS:NZ	2.26	0.69
1:D:10:GLY:HA3	1:D:102:GLY:HA2	1.73	0.69
1:B:125:VAL:HG12	1:B:148:PHE:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:MET:HE2	1:C:18:GLU:HG3	1.76	0.68
1:A:83:GLN:HE21	1:A:169:ILE:CG2	2.05	0.68
1:A:534:ASN:HD22	1:A:537:ILE:HD13	1.59	0.68
1:C:98:CYS:SG	1:C:100:SER:OG	2.52	0.68
1:D:270:ASP:HB3	1:D:303:LYS:HZ1	1.58	0.68
1:A:427:ARG:NH1	1:A:454:ASP:O	2.25	0.68
1:F:294:MET:SD	1:F:294:MET:N	2.67	0.67
1:C:179:LYS:HB3	1:C:182:ILE:HG12	1.74	0.67
1:D:35:THR:HA	1:D:62:CYS:HB3	1.75	0.67
1:D:46:ASN:O	1:D:50:HIS:ND1	2.27	0.67
1:E:209:PRO:HD2	1:F:206:LEU:HD13	1.76	0.67
1:A:403:ALA:HB1	1:A:413:ILE:HG13	1.77	0.67
1:B:163:LEU:HD13	1:B:166:ILE:HD11	1.76	0.67
1:D:18:GLU:HB3	1:D:125:VAL:HG21	1.77	0.67
1:D:188:GLU:HG3	1:D:215:PRO:HG3	1.77	0.67
1:F:3:ARG:NH1	1:F:26:GLY:O	2.28	0.67
1:D:280:GLY:O	1:D:284:SER:OG	2.12	0.66
1:B:89:MET:HE3	1:B:90:PRO:HD2	1.78	0.66
1:D:263:ALA:HB2	1:D:310:CYS:SG	2.36	0.66
1:D:562:LEU:HD11	1:D:590:ILE:HG12	1.78	0.66
1:A:560:ASP:O	1:A:564:ILE:HG13	1.95	0.66
1:B:14:MET:SD	1:B:14:MET:N	2.68	0.66
1:F:295:GLU:O	1:F:298:ASN:ND2	2.28	0.66
1:C:474:LEU:HD21	1:C:500:ASN:HB3	1.78	0.65
1:D:267:ASP:C	1:D:269:ILE:H	1.99	0.65
1:C:432:GLU:O	1:C:436:LYS:NZ	2.29	0.65
1:A:518:LEU:HD13	1:A:549:LEU:HD11	1.79	0.65
1:B:97:VAL:HB	1:B:122:VAL:HG12	1.78	0.65
1:A:3:ARG:NH2	1:A:26:GLY:O	2.30	0.65
1:A:204:ASN:HD22	1:B:583:LEU:HB3	1.62	0.65
1:A:306:LYS:O	1:A:344:LYS:NZ	2.30	0.65
1:D:3:ARG:NH1	1:D:26:GLY:O	2.30	0.65
1:E:157:TRP:O	1:E:161:ARG:NH1	2.30	0.65
1:A:187:GLU:O	1:A:191:SER:OG	2.15	0.65
1:B:237:LEU:O	1:B:239:LYS:NZ	2.28	0.65
1:F:162:ARG:HE	1:F:599:LYS:HB2	1.60	0.65
1:F:237:LEU:O	1:F:239:LYS:NZ	2.29	0.65
1:F:496:CYS:O	1:F:500:ASN:ND2	2.29	0.65
1:B:534:ASN:O	1:B:538:SER:OG	2.14	0.64
1:C:182:ILE:HG22	1:C:183:SER:N	2.12	0.64
1:D:132:ARG:N	1:D:136:GLU:OE2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:HE21	1:A:169:ILE:HA	1.59	0.64
1:F:99:LEU:HB2	1:F:124:HIS:CE1	2.32	0.64
1:A:234:ILE:HD11	1:A:546:LEU:HB3	1.79	0.64
1:B:225:PRO:HA	1:B:557:SER:HA	1.80	0.63
1:E:104:LYS:HZ2	1:F:107:SER:HB3	1.64	0.63
1:D:270:ASP:HB3	1:D:303:LYS:HZ2	1.62	0.63
1:C:220:GLN:N	1:C:220:GLN:OE1	2.31	0.63
1:B:290:LEU:O	1:B:292:LYS:N	2.32	0.63
1:E:530:VAL:O	1:E:531:ASN:ND2	2.31	0.63
1:A:46:ASN:O	1:A:50:HIS:ND1	2.29	0.63
1:A:302:SER:OG	1:A:338:ASN:O	2.17	0.63
1:D:93:GLU:N	1:D:93:GLU:OE2	2.32	0.63
1:D:478:GLU:OE2	1:D:478:GLU:N	2.31	0.63
1:C:427:ARG:NH2	1:C:454:ASP:O	2.31	0.63
1:A:168:PRO:O	1:A:170:ASN:N	2.32	0.63
1:F:134:ILE:HG22	1:F:138:PHE:CZ	2.34	0.63
1:C:190:LEU:HB3	1:C:224:LEU:HD21	1.80	0.63
1:E:469:ARG:NE	1:E:494:GLU:OE2	2.27	0.63
1:E:163:LEU:HA	1:E:166:ILE:HG12	1.80	0.62
1:F:97:VAL:HB	1:F:122:VAL:HG12	1.80	0.62
1:A:432:GLU:O	1:A:436:LYS:NZ	2.30	0.62
1:B:132:ARG:N	1:B:136:GLU:OE2	2.30	0.62
1:D:72:ARG:NH1	1:D:73:ASP:OD1	2.32	0.62
1:C:481:ASP:OD1	1:C:484:ARG:NH1	2.32	0.62
1:D:234:ILE:HA	1:D:237:LEU:HB3	1.80	0.62
1:D:283:ARG:HH22	1:D:548:ILE:HD12	1.65	0.62
1:E:173:CYS:SG	1:E:174:SER:N	2.72	0.62
1:F:68:ILE:HG21	1:F:74:PHE:HD1	1.64	0.62
1:F:5:LEU:HB3	1:F:30:VAL:HG12	1.81	0.62
1:F:112:LYS:HA	1:F:115:THR:HG22	1.79	0.62
1:A:157:TRP:HB2	1:A:160:LEU:HB2	1.81	0.62
1:B:80:MET:SD	1:B:80:MET:N	2.72	0.62
1:C:82:TRP:HE3	1:C:181:LEU:HD12	1.65	0.62
1:C:151:MET:SD	1:C:151:MET:N	2.73	0.62
1:B:296:LEU:HD22	1:B:537:ILE:HG23	1.82	0.61
1:D:249:PHE:HE2	1:D:317:LEU:HB3	1.65	0.61
1:B:249:PHE:HE2	1:B:317:LEU:HB3	1.64	0.61
1:D:237:LEU:HD12	1:D:238:PRO:HD2	1.82	0.61
1:D:269:ILE:O	1:D:271:ARG:HG2	1.99	0.61
1:D:534:ASN:HB3	1:D:537:ILE:HB	1.83	0.61
1:D:23:VAL:HG12	1:D:26:GLY:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HB2	1:A:216:PRO:HG2	1.80	0.61
1:C:217:ILE:HA	1:C:220:GLN:HE22	1.66	0.61
1:C:544:GLU:HA	1:C:547:LEU:HG	1.82	0.61
1:E:209:PRO:HB3	1:F:209:PRO:HA	1.82	0.61
1:B:482:LEU:HA	1:B:485:THR:HG22	1.83	0.61
1:F:192:ASN:HD21	1:F:223:GLN:HB2	1.66	0.61
1:A:79:GLU:OE2	1:A:181:LEU:N	2.34	0.60
1:F:137:MET:O	1:F:141:LEU:HG	2.00	0.60
1:D:18:GLU:HA	1:D:21:HIS:CE1	2.36	0.60
1:A:407:GLY:O	1:A:412:ARG:NH1	2.32	0.60
1:D:477:LEU:HD23	1:D:483:MET:HE1	1.83	0.60
1:E:99:LEU:HB3	1:E:110:LEU:HD11	1.83	0.60
1:D:217:ILE:HD12	1:D:220:GLN:NE2	2.17	0.60
1:E:570:GLU:O	1:E:579:ARG:NH2	2.34	0.60
1:A:167:LEU:O	1:A:169:ILE:N	2.35	0.60
1:B:342:LYS:NZ	1:C:406:GLN:O	2.30	0.60
1:C:333:ARG:NE	1:C:417:ASP:OD2	2.34	0.60
1:E:56:ARG:NH1	1:E:57:PHE:O	2.35	0.60
1:A:158:ALA:O	1:A:161:ARG:NH1	2.34	0.60
1:E:250:ALA:H	1:E:314:GLN:HE22	1.48	0.60
1:F:381:ILE:HD13	1:F:417:ASP:HB3	1.84	0.60
1:F:417:ASP:OD1	1:F:418:LEU:N	2.34	0.60
1:D:381:ILE:HA	1:D:417:ASP:HB3	1.83	0.60
1:E:356:ASN:ND2	1:E:411:CYS:O	2.35	0.60
1:B:221:TRP:CZ3	1:B:598:ILE:HD11	2.37	0.59
1:B:260:ARG:HD3	1:B:271:ARG:HH11	1.66	0.59
1:A:134:ILE:HA	1:A:137:MET:SD	2.43	0.59
1:A:530:VAL:HG23	1:A:564:ILE:HG21	1.84	0.59
1:D:137:MET:O	1:D:141:LEU:HG	2.01	0.59
1:F:46:ASN:O	1:F:50:HIS:ND1	2.36	0.59
1:F:248:GLY:HA3	1:F:534:ASN:HD21	1.68	0.59
1:B:468:ARG:HH21	1:B:573:PHE:HD1	1.51	0.59
1:C:302:SER:OG	1:C:338:ASN:O	2.20	0.59
1:D:29:GLU:OE1	1:D:31:HIS:NE2	2.35	0.59
1:B:234:ILE:O	1:B:239:LYS:NZ	2.31	0.59
1:E:112:LYS:NZ	1:E:112:LYS:O	2.35	0.59
1:C:5:LEU:HB3	1:C:30:VAL:HG22	1.84	0.59
1:E:133:ASN:O	1:E:136:GLU:HG2	2.03	0.59
1:F:130:ASN:O	1:F:132:ARG:NH1	2.35	0.59
1:F:221:TRP:HA	1:F:224:LEU:HD13	1.85	0.59
1:B:234:ILE:HA	1:B:237:LEU:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ALA:HB1	1:B:413:ILE:HD13	1.85	0.59
1:D:162:ARG:HB3	1:D:162:ARG:CZ	2.32	0.58
1:E:548:ILE:HG13	1:E:552:LEU:HD23	1.83	0.58
1:E:46:ASN:O	1:E:50:HIS:ND1	2.35	0.58
1:B:35:THR:HA	1:B:62:CYS:HB3	1.85	0.58
1:B:36:ASP:HA	1:B:61:LYS:HE3	1.85	0.58
1:B:125:VAL:HG12	1:B:148:PHE:HE1	1.68	0.58
1:E:126:LEU:HG	1:E:147:HIS:HB2	1.86	0.58
1:B:202:LYS:C	1:B:204:ASN:H	2.07	0.58
1:C:200:THR:O	1:C:204:ASN:N	2.37	0.58
1:D:234:ILE:HD11	1:D:547:LEU:HD23	1.85	0.58
1:E:293:TYR:HD2	1:E:503:ILE:HD11	1.67	0.58
1:F:162:ARG:H	1:F:599:LYS:HD2	1.68	0.58
1:B:240:VAL:HG21	1:B:569:ILE:HG22	1.85	0.58
1:D:428:ALA:HB1	1:D:465:LEU:HD11	1.85	0.58
1:A:204:ASN:HD21	1:B:584:LYS:HG2	1.68	0.58
1:B:537:ILE:HD12	1:B:537:ILE:H	1.68	0.58
1:F:72:ARG:NH1	1:F:73:ASP:OD1	2.37	0.58
1:B:162:ARG:HB2	1:B:165:LYS:HD3	1.84	0.58
1:B:267:ASP:C	1:B:269:ILE:H	2.08	0.57
1:E:153:TYR:HB3	1:F:190:LEU:HD22	1.86	0.57
1:C:392:ASP:O	1:C:395:LYS:HB2	2.03	0.57
1:A:87:THR:HB	1:A:169:ILE:CG2	2.21	0.57
1:C:77:TYR:HE2	1:C:106:MET:HB3	1.68	0.57
1:A:82:TRP:CZ3	1:A:182:ILE:HG12	2.39	0.57
1:B:243:HIS:N	1:B:531:ASN:OD1	2.37	0.57
1:C:134:ILE:HG12	1:C:138:PHE:CE2	2.38	0.57
1:C:201:GLY:O	1:C:205:GLN:NE2	2.36	0.57
1:D:336:PRO:HG3	1:D:352:LEU:HD13	1.86	0.57
1:E:117:PHE:HA	1:E:161:ARG:HH21	1.69	0.57
1:A:406:GLN:NE2	1:A:408:GLU:O	2.37	0.57
1:B:63:HIS:O	1:B:175:ARG:NH2	2.30	0.57
1:B:91:ASP:N	1:B:91:ASP:OD1	2.38	0.57
1:C:181:LEU:HA	1:C:184:LYS:HD2	1.87	0.57
1:E:132:ARG:O	1:E:132:ARG:NH1	2.34	0.57
1:C:233:TRP:CD1	1:C:597:SER:HB2	2.39	0.57
1:A:250:ALA:O	1:A:300:ASN:ND2	2.32	0.57
1:E:23:VAL:HG12	1:E:26:GLY:H	1.69	0.57
1:A:448:HIS:NE2	1:A:451:GLU:OE1	2.35	0.57
1:B:380:VAL:HG21	1:B:400:ALA:HB2	1.87	0.57
1:D:116:LEU:HD21	1:D:186:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:LEU:HD12	1:E:317:LEU:HD23	1.87	0.57
1:B:46:ASN:O	1:B:50:HIS:ND1	2.38	0.57
1:A:112:LYS:HA	1:A:115:THR:HG22	1.87	0.57
1:A:202:LYS:HA	1:A:205:GLN:HB2	1.86	0.57
1:A:221:TRP:O	1:A:558:ARG:NH1	2.38	0.57
1:C:336:PRO:HG3	1:C:352:LEU:HD13	1.86	0.57
1:A:17:PRO:O	1:A:21:HIS:ND1	2.38	0.56
1:D:565:ILE:O	1:D:569:ILE:HG23	2.05	0.56
1:E:256:LEU:O	1:E:260:ARG:HG2	2.05	0.56
1:D:417:ASP:OD1	1:D:418:LEU:N	2.38	0.56
1:A:204:ASN:OD1	1:A:205:GLN:N	2.38	0.56
1:B:238:PRO:HG3	1:B:589:LYS:HB3	1.88	0.56
1:C:429:SER:HA	1:C:432:GLU:HB2	1.87	0.56
1:E:36:ASP:HA	1:E:61:LYS:HE2	1.88	0.56
1:F:242:LEU:N	1:F:531:ASN:OD1	2.38	0.56
1:E:209:PRO:CG	1:F:207:PRO:HD2	2.28	0.56
1:E:294:MET:O	1:E:298:ASN:N	2.38	0.56
1:F:174:SER:OG	1:F:176:ASP:OD1	2.24	0.56
1:C:36:ASP:HA	1:C:61:LYS:HE2	1.88	0.56
1:C:124:HIS:HB3	1:C:149:ILE:HB	1.87	0.56
1:D:290:LEU:O	1:D:292:LYS:N	2.39	0.56
1:B:189:ILE:O	1:B:193:VAL:HG23	2.05	0.56
1:B:518:LEU:HD23	1:B:549:LEU:HD21	1.88	0.56
1:A:5:LEU:HD11	1:A:30:VAL:HG13	1.86	0.56
1:A:204:ASN:ND2	1:B:583:LEU:HB3	2.20	0.56
1:E:392:ASP:HA	1:E:395:LYS:HD2	1.87	0.56
1:F:243:HIS:N	1:F:531:ASN:OD1	2.37	0.56
1:C:203:SER:C	1:C:205:GLN:N	2.58	0.56
1:E:209:PRO:HG2	1:F:207:PRO:CD	2.32	0.56
1:A:199:ASP:N	1:A:199:ASP:OD1	2.39	0.56
1:A:316:GLU:OE2	1:A:361:ARG:NH2	2.38	0.56
1:B:260:ARG:HG3	1:B:261:GLY:N	2.21	0.56
1:C:203:SER:O	1:C:206:LEU:N	2.39	0.56
1:F:290:LEU:O	1:F:292:LYS:N	2.39	0.56
1:C:179:LYS:CB	1:C:182:ILE:HG12	2.36	0.55
1:D:8:SER:HB2	1:D:110:LEU:HD22	1.87	0.55
1:D:86:LEU:HD13	1:D:164:LYS:HA	1.87	0.55
1:F:185:SER:O	1:F:189:ILE:HG23	2.06	0.55
1:B:224:LEU:HD23	1:B:225:PRO:HD2	1.88	0.55
1:B:239:LYS:HD2	1:B:542:LEU:HD22	1.88	0.55
1:B:202:LYS:HE2	1:B:559:MET:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:TRP:O	1:F:87:THR:OG1	2.21	0.55
1:A:206:LEU:HD22	1:A:211:LEU:HB3	1.88	0.55
1:D:184:LYS:O	1:D:187:GLU:HG3	2.06	0.55
1:E:209:PRO:HA	1:F:209:PRO:HB3	1.88	0.55
1:A:249:PHE:HA	1:A:535:ILE:HG23	1.87	0.55
1:C:322:LEU:HD22	1:C:374:CYS:SG	2.46	0.55
1:D:103:ILE:HG12	1:D:106:MET:SD	2.47	0.55
1:D:133:ASN:O	1:D:136:GLU:HG3	2.06	0.55
1:D:217:ILE:HD12	1:D:220:GLN:HE22	1.70	0.55
1:A:242:LEU:O	1:A:333:ARG:NH2	2.39	0.55
1:A:249:PHE:HE2	1:A:317:LEU:HB3	1.70	0.55
1:B:532:THR:HG22	1:B:545:ASN:HD22	1.71	0.55
1:D:48:PHE:O	1:D:51:SER:OG	2.22	0.55
1:F:570:GLU:O	1:F:579:ARG:NH1	2.40	0.55
1:A:139:ASP:HA	1:A:142:GLN:HB2	1.89	0.55
1:E:196:MET:SD	1:F:588:ARG:NH1	2.80	0.54
1:E:202:LYS:NZ	1:E:219:GLN:O	2.40	0.54
1:D:207:PRO:HD2	1:D:208:PHE:CE1	2.42	0.54
1:F:159:ALA:HB2	1:F:598:ILE:HD12	1.89	0.54
1:D:3:ARG:N	1:D:28:GLU:OE2	2.39	0.54
1:A:234:ILE:HG13	1:A:237:LEU:HD12	1.89	0.54
1:C:180:PRO:C	1:C:181:LEU:HD13	2.27	0.54
1:D:103:ILE:HG13	1:D:105:SER:H	1.73	0.54
1:D:160:LEU:HD23	1:D:163:LEU:HD23	1.90	0.54
1:E:5:LEU:HB3	1:E:96:TYR:HB2	1.90	0.54
1:F:116:LEU:HD13	1:F:157:TRP:HD1	1.73	0.54
1:F:240:VAL:HG21	1:F:569:ILE:HG22	1.89	0.54
1:B:237:LEU:HD11	1:B:590:ILE:HG12	1.88	0.54
1:C:192:ASN:O	1:C:196:MET:HG2	2.08	0.54
1:A:83:GLN:HE22	1:A:169:ILE:HA	1.67	0.54
1:C:71:GLU:HG2	1:D:149:ILE:HG22	1.89	0.54
1:C:200:THR:O	1:C:203:SER:N	2.30	0.54
1:B:202:LYS:C	1:B:204:ASN:N	2.61	0.54
1:C:489:ARG:HH22	1:D:466:HIS:HB3	1.73	0.54
2:D:701:ATP:O3'	2:D:701:ATP:O3G	2.26	0.54
1:B:17:PRO:O	1:B:21:HIS:ND1	2.41	0.53
1:B:126:LEU:HG	1:B:147:HIS:HB2	1.90	0.53
1:A:204:ASN:ND2	1:B:584:LYS:HG2	2.24	0.53
1:B:509:MET:SD	1:B:509:MET:N	2.74	0.53
1:C:427:ARG:HB3	1:C:457:GLY:HA3	1.89	0.53
1:F:565:ILE:O	1:F:569:ILE:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:O	1:A:56:ARG:NH2	2.41	0.53
1:C:213:ILE:HG12	1:D:213:ILE:HG22	1.90	0.53
1:D:9:ALA:HB3	1:D:34:THR:HB	1.88	0.53
1:D:84:TRP:O	1:D:88:LYS:HG2	2.08	0.53
1:B:441:CYS:SG	1:C:395:LYS:NZ	2.68	0.53
1:B:481:ASP:OD1	1:B:481:ASP:N	2.41	0.53
1:D:221:TRP:O	1:D:558:ARG:NH1	2.41	0.53
1:E:455:PRO:HA	1:E:458:ILE:HD12	1.89	0.53
1:A:421:PHE:HE2	1:A:424:LYS:HB2	1.72	0.53
1:E:300:ASN:OD1	1:E:301:GLY:N	2.39	0.53
1:F:124:HIS:HB2	1:F:149:ILE:HG13	1.89	0.53
1:A:129:ASN:ND2	1:A:145:GLN:OE1	2.39	0.53
1:C:48:PHE:O	1:C:51:SER:OG	2.25	0.53
1:C:468:ARG:NH1	1:D:488:GLU:OE1	2.42	0.53
1:A:103:ILE:HG22	1:A:106:MET:SD	2.48	0.53
1:C:343:ASN:HB2	1:C:344:LYS:HZ3	1.72	0.53
1:F:83:GLN:O	1:F:87:THR:HG23	2.08	0.53
1:B:288:ILE:HD12	1:B:292:LYS:HB2	1.91	0.53
1:E:404:MET:HB2	1:E:443:LEU:HD21	1.91	0.53
1:A:251:THR:HG21	1:A:537:ILE:HG13	1.91	0.53
1:E:546:LEU:HD12	1:E:549:LEU:HD11	1.90	0.53
1:F:267:ASP:OD1	1:F:267:ASP:N	2.42	0.53
1:D:333:ARG:NH2	1:D:494:GLU:OE1	2.42	0.53
1:E:293:TYR:CD2	1:E:503:ILE:HD11	2.43	0.53
1:A:163:LEU:HA	1:A:166:ILE:CG1	2.38	0.52
1:E:131:PRO:CB	1:E:136:GLU:HG3	2.39	0.52
1:E:448:HIS:HA	1:E:471:GLY:HA3	1.90	0.52
1:A:440:ARG:HH21	1:F:391:SER:H	1.56	0.52
1:F:509:MET:HB2	1:F:512:PHE:HD2	1.73	0.52
1:B:17:PRO:HG2	1:B:137:MET:HE1	1.92	0.52
1:B:36:ASP:OD2	1:B:64:GLY:N	2.38	0.52
1:B:315:VAL:HG11	1:B:358:THR:HG21	1.92	0.52
1:B:565:ILE:O	1:B:569:ILE:HG23	2.09	0.52
1:D:12:SER:OG	1:D:14:MET:SD	2.68	0.52
1:D:237:LEU:HD13	1:D:590:ILE:HD13	1.91	0.52
1:F:408:GLU:OE1	1:F:408:GLU:N	2.39	0.52
1:A:29:GLU:HG3	1:A:56:ARG:HB2	1.91	0.52
1:A:195:ILE:HD12	1:A:200:THR:HG22	1.92	0.52
1:A:86:LEU:HD21	1:A:164:LYS:HA	1.92	0.52
1:A:390:LEU:O	1:A:393:ILE:HG22	2.10	0.52
1:C:97:VAL:HG23	1:C:122:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ARG:NH1	1:D:203:SER:OG	2.38	0.52
1:D:158:ALA:HA	1:D:161:ARG:CZ	2.40	0.52
1:E:218:ALA:HB2	1:E:598:ILE:HG21	1.91	0.52
1:F:60:THR:OG1	1:F:84:TRP:NE1	2.38	0.52
1:F:287:SER:OG	1:F:503:ILE:O	2.27	0.52
1:A:266:PRO:HB3	1:A:271:ARG:HH21	1.74	0.52
1:B:202:LYS:HZ3	1:B:223:GLN:HA	1.74	0.52
1:E:134:ILE:HA	1:E:137:MET:HG2	1.91	0.52
1:A:484:ARG:HH11	1:B:442:GLY:HA3	1.74	0.52
1:C:5:LEU:HB2	1:C:27:PHE:CZ	2.45	0.52
1:D:294:MET:SD	1:D:294:MET:N	2.83	0.52
1:B:29:GLU:HB3	1:B:56:ARG:HH21	1.75	0.52
1:D:243:HIS:N	1:D:531:ASN:OD1	2.43	0.52
1:E:190:LEU:HD23	1:F:155:PRO:HG2	1.92	0.52
1:E:242:LEU:H	1:E:531:ASN:ND2	2.08	0.52
1:A:427:ARG:O	1:A:429:SER:N	2.42	0.51
1:B:5:LEU:HD21	1:B:27:PHE:CG	2.44	0.51
1:C:200:THR:O	1:C:201:GLY:C	2.47	0.51
1:E:267:ASP:OD1	1:E:267:ASP:N	2.42	0.51
1:A:497:PRO:O	1:A:501:TYR:HB3	2.09	0.51
1:C:557:SER:N	1:C:560:ASP:OD2	2.36	0.51
1:F:116:LEU:HA	1:F:157:TRP:CD1	2.46	0.51
1:D:139:ASP:O	1:D:143:LYS:HG3	2.09	0.51
1:D:313:ARG:HD3	1:D:317:LEU:HD23	1.92	0.51
1:E:313:ARG:O	1:E:317:LEU:HD13	2.10	0.51
1:A:139:ASP:O	1:A:143:LYS:N	2.40	0.51
1:D:380:VAL:HG21	1:D:400:ALA:HB2	1.91	0.51
1:E:319:TYR:CE2	1:E:362:LEU:HB3	2.45	0.51
1:A:336:PRO:HG3	1:A:352:LEU:HD13	1.91	0.51
1:C:243:HIS:HD2	1:C:533:ASP:HA	1.76	0.51
1:D:165:LYS:O	1:D:166:ILE:C	2.49	0.51
1:F:305:LEU:HD12	1:F:311:LEU:HD12	1.91	0.51
1:C:175:ARG:CG	1:C:180:PRO:HB3	2.37	0.51
1:C:496:CYS:O	1:C:500:ASN:ND2	2.43	0.51
1:D:136:GLU:HA	1:D:139:ASP:HB3	1.91	0.51
1:D:237:LEU:O	1:D:239:LYS:NZ	2.35	0.51
1:A:137:MET:HA	1:A:140:ALA:HB3	1.92	0.51
1:B:541:ASN:N	1:B:544:GLU:OE1	2.41	0.51
1:D:21:HIS:CE1	1:D:141:LEU:HD21	2.45	0.51
1:E:176:ASP:O	1:E:177:ASN:ND2	2.43	0.51
1:A:86:LEU:HD21	1:A:169:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:HIS:N	1:C:531:ASN:OD1	2.41	0.51
1:C:403:ALA:HB1	1:C:413:ILE:HG13	1.93	0.51
1:C:434:ASP:OD1	1:C:434:ASP:N	2.44	0.51
1:D:234:ILE:HG22	1:D:237:LEU:HD23	1.93	0.51
1:A:489:ARG:HH12	1:B:466:HIS:HB3	1.76	0.51
1:D:14:MET:SD	1:D:14:MET:N	2.81	0.51
1:E:237:LEU:O	1:E:239:LYS:NZ	2.41	0.51
1:E:242:LEU:H	1:E:531:ASN:HD21	1.59	0.51
1:E:584:LYS:HD2	1:F:204:ASN:HA	1.93	0.51
1:F:333:ARG:NH1	1:F:417:ASP:OD2	2.43	0.51
1:B:208:PHE:HE2	1:B:590:ILE:HD12	1.76	0.50
1:C:182:ILE:HG22	1:C:183:SER:H	1.76	0.50
1:D:115:THR:HA	1:D:154:GLU:HG3	1.93	0.50
1:B:559:MET:O	1:B:563:THR:HG23	2.11	0.50
1:C:103:ILE:HG13	1:C:106:MET:SD	2.51	0.50
1:D:143:LYS:HB2	1:D:145:GLN:NE2	2.23	0.50
1:C:417:ASP:OD1	1:C:418:LEU:N	2.44	0.50
1:D:484:ARG:O	1:D:488:GLU:HG2	2.12	0.50
1:E:11:HIS:HA	1:E:39:LYS:HD3	1.93	0.50
1:F:240:VAL:HG22	1:F:329:TYR:HB3	1.92	0.50
1:D:260:ARG:HB3	1:D:271:ARG:HH11	1.77	0.50
1:F:288:ILE:HB	1:F:292:LYS:HD3	1.93	0.50
1:A:499:ALA:O	1:A:503:ILE:HG12	2.12	0.50
1:B:159:ALA:HA	1:B:599:LYS:HD3	1.94	0.50
1:E:103:ILE:HG13	1:E:105:SER:H	1.76	0.50
1:E:234:ILE:O	1:E:239:LYS:NZ	2.44	0.50
1:B:192:ASN:HD21	1:B:224:LEU:N	2.09	0.50
1:C:208:PHE:O	1:C:211:LEU:HD12	2.10	0.50
1:E:6:LEU:HB3	1:E:84:TRP:CH2	2.47	0.50
1:F:509:MET:SD	1:F:509:MET:N	2.85	0.50
1:B:100:SER:HB2	1:B:125:VAL:HG22	1.93	0.50
1:C:322:LEU:HD23	1:C:327:VAL:HB	1.94	0.50
1:D:181:LEU:HA	1:D:184:LYS:HG2	1.93	0.50
1:D:242:LEU:HD21	1:D:572:ALA:HB2	1.93	0.50
1:B:505:GLY:HA3	1:B:512:PHE:HD2	1.77	0.50
1:E:328:ALA:O	1:E:374:CYS:HA	2.12	0.50
1:D:202:LYS:O	1:D:205:GLN:HG3	2.12	0.50
1:E:164:LYS:HG3	1:E:165:LYS:HG2	1.92	0.50
1:C:158:ALA:O	1:C:161:ARG:NH2	2.40	0.49
1:D:124:HIS:HB2	1:D:149:ILE:HD11	1.94	0.49
1:E:3:ARG:NH2	1:E:28:GLU:OE2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:MET:O	1:F:18:GLU:HG2	2.12	0.49
1:A:48:PHE:O	1:A:51:SER:OG	2.26	0.49
1:C:3:ARG:NH2	1:C:26:GLY:O	2.44	0.49
1:C:280:GLY:HA3	1:C:285:HIS:CE1	2.47	0.49
1:F:36:ASP:OD2	1:F:64:GLY:N	2.42	0.49
1:C:469:ARG:NE	1:C:494:GLU:OE2	2.33	0.49
1:D:265:GLU:OE2	1:D:269:ILE:HG12	2.12	0.49
1:E:288:ILE:HG13	1:E:292:LYS:HD2	1.94	0.49
1:F:116:LEU:HD13	1:F:157:TRP:CD1	2.48	0.49
1:B:300:ASN:ND2	1:B:314:GLN:OE1	2.44	0.49
1:D:267:ASP:C	1:D:269:ILE:N	2.65	0.49
1:E:313:ARG:NH2	1:E:316:GLU:OE1	2.45	0.49
1:B:335:SER:O	1:B:335:SER:OG	2.28	0.49
1:C:137:MET:HA	1:C:140:ALA:HB3	1.94	0.49
1:E:74:PHE:CD2	1:F:149:ILE:HD12	2.47	0.49
1:F:99:LEU:HB2	1:F:124:HIS:HE1	1.74	0.49
1:F:201:GLY:HA2	1:F:204:ASN:ND2	2.28	0.49
1:F:473:ALA:HB1	1:F:476:LEU:HD21	1.95	0.49
1:A:468:ARG:NH2	1:B:488:GLU:O	2.46	0.49
1:A:7:CYS:SG	1:A:8:SER:N	2.86	0.49
1:A:311:LEU:HD11	1:A:355:ILE:HD11	1.94	0.49
1:A:342:LYS:NZ	1:A:345:ASN:OD1	2.45	0.49
1:C:179:LYS:HA	1:C:182:ILE:HG12	1.93	0.49
1:C:204:ASN:C	1:C:206:LEU:H	2.16	0.49
1:E:196:MET:CE	1:E:197:ALA:H	2.25	0.49
1:A:167:LEU:HB3	1:A:179:LYS:HZ1	1.77	0.49
1:A:384:ARG:HB2	1:A:420:GLY:HA3	1.94	0.49
1:D:354:ASP:O	1:D:358:THR:HG22	2.13	0.49
1:E:188:GLU:OE2	1:E:192:ASN:ND2	2.46	0.49
1:E:198:SER:OG	1:E:199:ASP:N	2.46	0.49
1:E:270:ASP:OD1	1:E:272:THR:OG1	2.27	0.49
1:A:589:LYS:O	1:A:593:VAL:HG12	2.12	0.49
1:C:390:LEU:O	1:C:393:ILE:HB	2.13	0.49
1:C:518:LEU:HD21	1:C:564:ILE:HD11	1.95	0.49
1:C:161:ARG:H	1:C:162:ARG:HH12	1.61	0.48
1:D:140:ALA:O	1:D:144:GLY:N	2.45	0.48
1:F:389:ASP:OD1	1:F:391:SER:OG	2.31	0.48
1:A:593:VAL:HA	1:A:596:ILE:HG22	1.94	0.48
1:C:208:PHE:O	1:C:210:SER:N	2.46	0.48
1:D:241:ASP:HB2	1:D:542:LEU:HD11	1.96	0.48
1:D:516:TYR:HB3	1:D:553:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLN:NE2	1:B:324:ASN:OD1	2.46	0.48
1:C:446:THR:OG1	1:C:447:ALA:N	2.46	0.48
1:A:234:ILE:HA	1:A:237:LEU:HG	1.95	0.48
1:A:369:LYS:HB2	1:A:371:GLN:OE1	2.13	0.48
1:A:405:GLN:O	1:F:342:LYS:NZ	2.42	0.48
1:A:541:ASN:N	1:A:544:GLU:OE1	2.46	0.48
1:F:132:ARG:N	1:F:136:GLU:OE2	2.45	0.48
1:F:192:ASN:ND2	1:F:224:LEU:HD12	2.28	0.48
1:F:134:ILE:HA	1:F:137:MET:SD	2.53	0.48
1:A:250:ALA:H	1:A:314:GLN:HE22	1.62	0.48
1:D:531:ASN:O	1:D:545:ASN:ND2	2.46	0.48
1:E:72:ARG:HH12	1:E:175:ARG:HH21	1.62	0.48
1:A:173:CYS:SG	1:A:177:ASN:O	2.72	0.48
1:B:5:LEU:HB2	1:B:30:VAL:HG22	1.95	0.48
1:B:83:GLN:O	1:B:87:THR:HG22	2.13	0.48
1:C:131:PRO:HB3	1:C:136:GLU:HB2	1.95	0.48
1:D:590:ILE:HA	1:D:593:VAL:HG12	1.95	0.48
1:E:79:GLU:OE2	1:E:179:LYS:N	2.43	0.48
1:A:243:HIS:HA	1:A:333:ARG:HH21	1.79	0.48
1:C:122:VAL:HG13	1:C:151:MET:SD	2.53	0.48
1:C:179:LYS:CA	1:C:182:ILE:HG12	2.44	0.48
1:A:342:LYS:HD2	1:A:342:LYS:HA	1.70	0.47
1:C:204:ASN:OD1	1:C:205:GLN:N	2.46	0.47
1:D:96:TYR:CD2	1:D:121:SER:HB2	2.49	0.47
1:E:489:ARG:HA	1:F:468:ARG:NH1	2.29	0.47
1:F:208:PHE:HD1	1:F:211:LEU:HB2	1.78	0.47
1:B:202:LYS:O	1:B:204:ASN:N	2.47	0.47
1:C:182:ILE:O	1:C:186:ILE:N	2.36	0.47
1:D:5:LEU:HD12	1:D:30:VAL:HG12	1.96	0.47
1:D:163:LEU:O	1:D:164:LYS:C	2.53	0.47
1:F:204:ASN:O	1:F:206:LEU:HD23	2.14	0.47
1:A:126:LEU:HG	1:A:147:HIS:HB2	1.97	0.47
1:B:534:ASN:OD1	1:B:538:SER:N	2.41	0.47
1:C:211:LEU:O	1:C:219:GLN:NE2	2.48	0.47
1:E:64:GLY:O	1:E:175:ARG:NH1	2.46	0.47
1:E:104:LYS:NZ	1:F:101:GLY:O	2.46	0.47
1:B:210:SER:OG	1:B:587:ASP:OD1	2.30	0.47
1:B:267:ASP:O	1:B:269:ILE:N	2.46	0.47
1:B:281:TRP:NE1	1:B:537:ILE:O	2.47	0.47
1:C:233:TRP:CZ3	1:C:558:ARG:HG2	2.49	0.47
1:B:402:THR:HG21	1:C:399:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:HE2	1:D:165:LYS:HB3	1.56	0.47
1:D:498:TYR:CZ	1:D:548:ILE:HG13	2.49	0.47
1:D:577:ASP:O	1:D:581:GLU:HG2	2.14	0.47
1:E:474:LEU:HD21	1:E:500:ASN:HB3	1.95	0.47
1:A:99:LEU:HB2	1:A:124:HIS:NE2	2.30	0.47
1:E:319:TYR:HD2	1:E:362:LEU:HD13	1.80	0.47
1:A:587:ASP:O	1:A:590:ILE:HG22	2.15	0.47
1:B:95:PRO:O	1:B:120:GLN:N	2.40	0.47
1:B:241:ASP:OD1	1:B:242:LEU:N	2.47	0.47
1:B:440:ARG:HE	1:C:391:SER:HB3	1.80	0.47
1:C:237:LEU:HD12	1:C:237:LEU:H	1.80	0.47
1:C:280:GLY:HA3	1:C:285:HIS:HE1	1.80	0.47
1:C:380:VAL:HG21	1:C:400:ALA:HB2	1.97	0.47
1:E:166:ILE:HA	1:E:596:ILE:HD11	1.96	0.47
1:E:181:LEU:HD13	1:E:184:LYS:HD2	1.96	0.47
1:E:530:VAL:HG11	1:E:546:LEU:HD13	1.97	0.47
1:F:300:ASN:OD1	1:F:301:GLY:N	2.47	0.47
1:A:295:GLU:HA	1:A:298:ASN:HB2	1.97	0.47
1:B:241:ASP:O	1:B:330:ALA:HA	2.14	0.47
1:C:234:ILE:HD11	1:C:547:LEU:HB3	1.96	0.47
1:C:243:HIS:CD2	1:C:533:ASP:HA	2.50	0.47
1:D:14:MET:H	1:D:14:MET:CE	2.26	0.47
1:D:125:VAL:HG23	1:D:148:PHE:HD1	1.80	0.47
1:E:166:ILE:HB	1:E:595:LEU:HD22	1.97	0.47
1:F:204:ASN:O	1:F:206:LEU:N	2.48	0.47
1:F:537:ILE:HG13	1:F:538:SER:N	2.30	0.47
1:A:417:ASP:OD1	1:A:418:LEU:N	2.48	0.47
1:C:134:ILE:HA	1:C:137:MET:SD	2.55	0.47
1:E:208:PHE:O	1:E:210:SER:N	2.48	0.47
1:F:419:ALA:HA	1:F:448:HIS:HB3	1.97	0.47
1:A:488:GLU:O	1:B:468:ARG:NH1	2.47	0.47
1:B:180:PRO:O	1:B:184:LYS:HG2	2.15	0.47
1:B:506:PHE:HB2	1:B:552:LEU:HD11	1.97	0.47
1:C:237:LEU:O	1:C:239:LYS:NZ	2.45	0.47
1:E:86:LEU:HD22	1:E:163:LEU:HB3	1.97	0.47
1:E:122:VAL:HG13	1:E:151:MET:SD	2.55	0.47
1:E:131:PRO:HB2	1:E:137:MET:SD	2.55	0.47
1:E:302:SER:OG	1:E:338:ASN:O	2.23	0.47
1:F:518:LEU:HD11	1:F:528:VAL:HG11	1.97	0.47
1:B:211:LEU:HD12	1:B:214:LEU:HD13	1.96	0.46
1:E:496:CYS:SG	1:E:533:ASP:HB2	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:ILE:HG13	1:F:190:LEU:HD23	1.98	0.46
1:F:194:LYS:HD2	1:F:194:LYS:HA	1.61	0.46
1:A:72:ARG:HH21	1:A:175:ARG:HG2	1.80	0.46
1:A:166:ILE:HG21	1:A:595:LEU:HB3	1.96	0.46
1:B:184:LYS:O	1:B:187:GLU:HG3	2.14	0.46
1:C:422:GLU:OE2	1:C:451:GLU:N	2.42	0.46
1:F:89:MET:SD	1:F:89:MET:N	2.88	0.46
1:F:487:ILE:HD11	1:F:526:ILE:HG12	1.97	0.46
1:A:202:LYS:NZ	1:A:223:GLN:HG2	2.30	0.46
1:C:594:CYS:HA	1:C:597:SER:HB3	1.98	0.46
1:A:3:ARG:HH12	1:A:23:VAL:HG21	1.80	0.46
1:C:161:ARG:H	1:C:162:ARG:NH1	2.13	0.46
1:C:234:ILE:HA	1:C:237:LEU:CD1	2.45	0.46
1:E:60:THR:HG21	1:E:84:TRP:HE1	1.80	0.46
1:E:489:ARG:HD2	1:F:468:ARG:HH11	1.79	0.46
1:F:469:ARG:NE	1:F:494:GLU:OE2	2.31	0.46
1:C:392:ASP:O	1:C:396:HIS:ND1	2.49	0.46
1:D:293:TYR:HB3	1:D:294:MET:SD	2.56	0.46
1:F:162:ARG:HB3	1:F:599:LYS:HB3	1.96	0.46
1:A:489:ARG:HH22	1:B:466:HIS:HB3	1.79	0.46
1:C:245:HIS:CE1	1:C:333:ARG:HD3	2.51	0.46
1:F:384:ARG:NH2	1:F:418:LEU:O	2.49	0.46
1:D:56:ARG:NH1	1:D:57:PHE:O	2.49	0.46
1:D:481:ASP:OD1	1:D:481:ASP:N	2.47	0.46
1:F:354:ASP:O	1:F:358:THR:HG22	2.16	0.46
1:C:77:TYR:CE2	1:C:106:MET:HB3	2.50	0.46
1:D:586:PHE:O	1:D:590:ILE:HG22	2.16	0.46
2:E:701:ATP:O3G	2:E:701:ATP:O3'	2.33	0.46
1:F:9:ALA:HB3	1:F:34:THR:HB	1.97	0.46
1:D:270:ASP:OD2	1:D:273:PHE:HB3	2.16	0.46
1:D:498:TYR:HB3	1:D:538:SER:OG	2.16	0.46
1:E:162:ARG:HH22	1:E:588:ARG:HG3	1.81	0.46
1:A:519:LYS:O	1:A:523:GLU:HG2	2.15	0.46
1:C:157:TRP:HD1	1:C:159:ALA:H	1.64	0.46
1:D:141:LEU:HD23	1:D:146:ILE:HD12	1.98	0.46
1:D:446:THR:OG1	1:D:447:ALA:N	2.49	0.46
1:E:152:GLY:HA2	1:F:190:LEU:HD11	1.98	0.46
1:E:330:ALA:HB3	1:E:376:VAL:HG22	1.98	0.46
1:A:36:ASP:OD2	1:A:64:GLY:N	2.48	0.45
1:A:210:SER:HB2	1:A:587:ASP:OD1	2.16	0.45
1:C:584:LYS:HG3	1:D:205:GLN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:GLU:OE1	1:E:83:GLN:NE2	2.49	0.45
1:B:22:ALA:HA	1:B:148:PHE:CE2	2.52	0.45
1:B:99:LEU:HD23	1:B:99:LEU:HA	1.74	0.45
1:E:250:ALA:HA	1:E:255:LEU:HD23	1.99	0.45
1:A:240:VAL:HG22	1:A:329:TYR:HB3	1.97	0.45
1:C:163:LEU:HD12	1:C:163:LEU:H	1.81	0.45
1:F:60:THR:HG1	1:F:84:TRP:HE1	1.55	0.45
1:F:83:GLN:O	1:F:86:LEU:HG	2.16	0.45
1:F:558:ARG:O	1:F:561:VAL:HG12	2.17	0.45
1:B:226:LEU:HD23	1:B:550:ALA:HB2	1.99	0.45
1:D:518:LEU:HD11	1:D:528:VAL:HG11	1.99	0.45
1:B:131:PRO:HB3	1:B:137:MET:HB3	1.98	0.45
1:B:569:ILE:HD12	1:B:583:LEU:HD22	1.97	0.45
1:D:414:VAL:HG21	1:D:573:PHE:O	2.16	0.45
1:E:325:ASP:OD2	1:E:541:ASN:HB2	2.17	0.45
1:E:447:ALA:O	1:E:471:GLY:N	2.49	0.45
1:E:585:PHE:CE1	2:E:701:ATP:H2'	2.52	0.45
1:E:10:GLY:HA3	1:E:102:GLY:HA2	1.99	0.45
1:F:29:GLU:OE1	1:F:31:HIS:NE2	2.49	0.45
1:B:45:LEU:HD12	1:B:45:LEU:H	1.81	0.45
1:C:427:ARG:O	1:C:429:SER:N	2.49	0.45
1:D:164:LYS:O	1:D:165:LYS:C	2.53	0.45
1:F:518:LEU:O	1:F:518:LEU:HD12	2.16	0.45
1:C:476:LEU:HG	1:C:483:MET:SD	2.57	0.45
1:D:72:ARG:O	1:D:75:GLU:HG3	2.17	0.45
1:E:151:MET:HG3	1:F:112:LYS:HE3	1.99	0.45
1:F:94:LEU:HD22	1:F:118:GLY:HA3	1.98	0.45
1:B:504:LYS:HB2	1:B:506:PHE:CE2	2.51	0.45
1:E:160:LEU:HB3	1:E:161:ARG:NH2	2.32	0.45
1:F:10:GLY:HA3	1:F:102:GLY:HA2	1.99	0.45
1:F:207:PRO:O	1:F:208:PHE:C	2.55	0.45
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.81	0.45
1:A:584:LYS:HE3	1:B:204:ASN:OD1	2.17	0.45
1:D:100:SER:HG	1:D:125:VAL:H	1.59	0.45
1:D:162:ARG:O	1:D:163:LEU:C	2.56	0.45
1:E:214:LEU:HD23	1:E:219:GLN:HA	1.99	0.45
1:E:231:GLY:O	1:E:234:ILE:HB	2.15	0.45
1:F:423:ASN:HB3	1:F:426:THR:HG23	1.98	0.45
1:A:131:PRO:HG3	1:A:137:MET:HB3	2.00	0.44
1:B:103:ILE:HG12	1:B:106:MET:CE	2.47	0.44
1:B:265:GLU:OE1	1:B:268:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:N	1:D:531:ASN:OD1	2.50	0.44
1:A:469:ARG:NE	1:A:494:GLU:OE2	2.28	0.44
1:B:167:LEU:HG	1:B:181:LEU:HD11	1.98	0.44
1:C:175:ARG:CZ	1:C:175:ARG:HB3	2.44	0.44
1:C:313:ARG:HD3	1:C:317:LEU:HD23	1.99	0.44
1:C:476:LEU:HG	1:C:483:MET:HE1	1.99	0.44
1:A:184:LYS:O	1:A:187:GLU:HG3	2.18	0.44
1:A:498:TYR:CD2	1:A:545:ASN:HA	2.52	0.44
1:C:80:MET:SD	1:C:80:MET:N	2.91	0.44
1:C:595:LEU:HD12	1:C:595:LEU:HA	1.85	0.44
1:D:11:HIS:O	1:D:39:LYS:NZ	2.50	0.44
1:E:97:VAL:HG23	1:E:122:VAL:HA	2.00	0.44
1:B:95:PRO:HD2	1:B:119:ALA:HA	1.98	0.44
1:B:133:ASN:N	1:B:136:GLU:OE2	2.46	0.44
1:B:469:ARG:NE	1:B:494:GLU:OE2	2.29	0.44
1:F:288:ILE:HG13	1:F:293:TYR:OH	2.17	0.44
1:A:381:ILE:HD13	1:A:417:ASP:HB3	1.98	0.44
1:B:159:ALA:HB1	1:B:599:LYS:HA	1.98	0.44
1:B:418:LEU:HD21	1:B:435:PHE:CZ	2.52	0.44
1:C:124:HIS:CE1	1:D:104:LYS:HD2	2.52	0.44
1:C:556:ILE:HG23	1:C:560:ASP:HB2	2.00	0.44
1:D:263:ALA:HB3	1:D:265:GLU:O	2.16	0.44
1:D:266:PRO:C	1:D:271:ARG:HH21	2.20	0.44
1:E:442:GLY:HA3	1:F:484:ARG:HH21	1.82	0.44
1:F:134:ILE:HD13	1:F:134:ILE:N	2.32	0.44
1:A:233:TRP:CZ3	1:A:558:ARG:HG2	2.53	0.44
1:C:94:LEU:HB2	1:C:120:GLN:HB2	2.00	0.44
1:D:161:ARG:HE	1:D:161:ARG:HB2	1.44	0.44
1:D:355:ILE:HG22	1:D:378:LEU:HD21	1.99	0.44
1:E:243:HIS:CD2	1:E:533:ASP:HA	2.52	0.44
1:A:384:ARG:HD3	1:A:420:GLY:HA3	1.98	0.44
1:A:422:GLU:OE1	1:A:452:ASN:N	2.47	0.44
1:B:143:LYS:HA	1:B:143:LYS:HD3	1.71	0.44
1:C:85:TYR:O	1:C:88:LYS:N	2.42	0.44
1:D:165:LYS:H	1:D:165:LYS:HD2	1.83	0.44
1:D:433:HIS:HA	1:D:436:LYS:HE2	1.99	0.44
1:E:31:HIS:ND1	1:E:88:LYS:HD2	2.33	0.44
1:F:9:ALA:HB1	1:F:40:PHE:CE2	2.53	0.44
1:A:241:ASP:O	1:A:330:ALA:HA	2.18	0.44
1:B:385:LYS:HA	1:B:385:LYS:HD2	1.62	0.44
1:D:162:ARG:H	1:D:162:ARG:HG2	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ARG:HD3	1:E:304:LEU:HD11	1.99	0.44
1:E:327:VAL:O	1:E:374:CYS:HB3	2.18	0.44
1:A:534:ASN:ND2	1:A:537:ILE:HD13	2.31	0.44
1:B:134:ILE:HA	1:B:137:MET:CE	2.48	0.44
1:B:192:ASN:O	1:B:196:MET:HG3	2.18	0.44
1:D:81:LEU:HD11	1:D:110:LEU:HD13	1.99	0.44
1:D:307:ASP:OD1	1:D:307:ASP:N	2.51	0.44
1:E:14:MET:SD	1:E:14:MET:N	2.91	0.44
1:E:197:ALA:N	1:E:198:SER:HA	2.33	0.44
1:F:184:LYS:HD3	1:F:184:LYS:HA	1.76	0.44
1:F:418:LEU:HD21	1:F:435:PHE:CZ	2.52	0.44
1:A:243:HIS:CD2	1:A:533:ASP:HA	2.52	0.43
1:A:251:THR:HG21	1:A:537:ILE:HA	2.00	0.43
1:A:530:VAL:HG11	1:A:546:LEU:HD13	2.00	0.43
2:A:701:ATP:O3G	2:A:701:ATP:O3'	2.36	0.43
1:B:104:LYS:HB3	1:B:104:LYS:HE3	1.72	0.43
1:C:28:GLU:O	1:C:55:VAL:HA	2.18	0.43
1:C:82:TRP:CE3	1:C:181:LEU:HD12	2.48	0.43
1:C:249:PHE:HB2	1:C:318:LEU:HD12	2.00	0.43
1:D:18:GLU:HG2	1:D:146:ILE:HG21	2.00	0.43
1:E:100:SER:HA	1:E:124:HIS:NE2	2.33	0.43
1:B:233:TRP:CZ3	1:B:558:ARG:HB3	2.53	0.43
1:D:134:ILE:HG23	1:D:138:PHE:HE1	1.83	0.43
1:E:278:ILE:HD12	1:E:286:LYS:HZ1	1.83	0.43
1:E:384:ARG:HB2	1:E:420:GLY:HA3	2.00	0.43
1:A:214:LEU:HD21	1:A:218:ALA:HB3	2.00	0.43
1:A:497:PRO:HD2	1:A:545:ASN:OD1	2.17	0.43
1:D:131:PRO:HB2	1:D:137:MET:CE	2.48	0.43
1:E:249:PHE:O	1:E:536:GLY:HA3	2.19	0.43
1:F:67:ASP:OD1	1:F:68:ILE:N	2.50	0.43
1:A:153:TYR:CD1	1:B:193:VAL:HG21	2.52	0.43
1:C:196:MET:HG2	1:C:196:MET:H	1.52	0.43
1:D:436:LYS:H	1:D:436:LYS:HG2	1.59	0.43
1:D:585:PHE:CE1	2:D:701:ATP:H2'	2.53	0.43
1:F:86:LEU:HA	1:F:89:MET:SD	2.58	0.43
1:F:167:LEU:O	1:F:167:LEU:HD23	2.19	0.43
1:A:169:ILE:H	1:A:169:ILE:HG13	1.56	0.43
1:B:265:GLU:HG2	1:B:267:ASP:OD1	2.18	0.43
1:B:265:GLU:O	1:B:267:ASP:N	2.51	0.43
1:C:496:CYS:HB2	1:C:499:ALA:HB3	1.99	0.43
1:D:125:VAL:HG23	1:D:148:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ALA:O	1:D:300:ASN:ND2	2.35	0.43
1:A:307:ASP:OD2	1:A:310:CYS:N	2.40	0.43
1:B:14:MET:HG2	1:B:132:ARG:HA	1.99	0.43
1:B:256:LEU:H	1:B:256:LEU:HD23	1.84	0.43
1:D:164:LYS:HB3	1:D:164:LYS:HE2	1.78	0.43
1:E:77:TYR:OH	1:E:106:MET:HB2	2.18	0.43
1:E:336:PRO:HG3	1:E:352:LEU:HD13	2.01	0.43
1:E:384:ARG:HD3	1:E:420:GLY:HA3	1.99	0.43
1:D:167:LEU:HD21	1:D:170:ASN:HB2	2.00	0.43
1:D:269:ILE:HD13	1:D:269:ILE:HA	1.76	0.43
1:D:458:ILE:HG22	1:D:482:LEU:HD11	2.00	0.43
1:E:30:VAL:O	1:E:57:PHE:HA	2.17	0.43
1:F:95:PRO:O	1:F:120:GLN:N	2.47	0.43
1:F:205:GLN:OE1	1:F:205:GLN:N	2.50	0.43
1:F:254:SER:OG	1:F:258:GLN:NE2	2.51	0.43
1:F:556:ILE:HD12	1:F:556:ILE:HA	1.87	0.43
1:A:150:GLU:HG3	1:A:152:GLY:H	1.84	0.43
1:A:276:GLN:HE22	1:A:295:GLU:HG3	1.84	0.43
1:A:300:ASN:OD1	1:A:301:GLY:N	2.39	0.43
1:A:426:THR:OG1	1:A:431:TYR:OH	2.34	0.43
1:B:377:ASN:HD22	1:B:414:VAL:HG11	1.84	0.43
1:C:75:GLU:HG2	1:C:175:ARG:CD	2.49	0.43
1:C:79:GLU:OE2	1:C:180:PRO:HA	2.19	0.43
1:E:252:SER:OG	1:E:253:GLY:N	2.52	0.43
1:E:260:ARG:HH21	1:E:269:ILE:HG23	1.83	0.43
1:A:427:ARG:NH1	1:A:454:ASP:OD1	2.52	0.43
1:B:363:ILE:HD11	1:B:374:CYS:O	2.19	0.43
1:C:174:SER:HB2	1:C:177:ASN:CG	2.39	0.43
1:C:214:LEU:HD11	1:C:594:CYS:HB3	2.00	0.43
1:D:103:ILE:N	1:D:106:MET:SD	2.92	0.43
1:D:403:ALA:HB1	1:D:413:ILE:HG13	2.01	0.43
1:D:549:LEU:HD23	1:D:549:LEU:HA	1.77	0.43
1:E:193:VAL:HG12	1:F:591:TYR:CZ	2.54	0.43
1:E:367:LYS:HB2	1:E:367:LYS:HE3	1.79	0.43
1:E:535:ILE:HG23	1:E:536:GLY:H	1.84	0.43
1:F:546:LEU:HD23	1:F:546:LEU:HA	1.86	0.43
1:A:220:GLN:OE1	1:A:221:TRP:N	2.52	0.43
1:A:426:THR:HG22	1:A:430:TYR:CD2	2.54	0.43
1:B:180:PRO:HB2	1:B:183:SER:HB3	2.00	0.43
1:C:175:ARG:HB3	1:C:175:ARG:NH2	2.34	0.43
1:C:184:LYS:HA	1:C:187:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:GLU:O	1:E:148:PHE:HZ	2.01	0.43
1:F:463:TYR:HH	1:F:485:THR:HG1	1.66	0.43
1:B:130:ASN:O	1:B:132:ARG:NH1	2.51	0.42
1:B:267:ASP:C	1:B:269:ILE:N	2.73	0.42
1:B:341:ASP:N	1:B:346:ARG:O	2.49	0.42
1:B:437:ALA:HB1	1:C:394:SER:HB3	2.01	0.42
1:C:103:ILE:N	1:C:106:MET:SD	2.92	0.42
1:C:203:SER:O	1:C:204:ASN:C	2.57	0.42
1:E:531:ASN:HD22	1:E:531:ASN:HA	1.62	0.42
1:C:293:TYR:CE1	1:C:537:ILE:HG21	2.54	0.42
1:E:76:PHE:HD2	1:E:178:PHE:HE1	1.66	0.42
1:E:204:ASN:HD22	1:F:584:LYS:HA	1.83	0.42
1:E:546:LEU:HD12	1:E:546:LEU:HA	1.88	0.42
1:F:157:TRP:CE3	1:F:215:PRO:HB3	2.55	0.42
1:F:403:ALA:HB1	1:F:413:ILE:HG13	2.00	0.42
1:F:561:VAL:HA	1:F:564:ILE:HG12	2.00	0.42
1:B:415:GLY:HA2	1:B:443:LEU:HD22	2.01	0.42
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.77	0.42
1:C:477:LEU:HA	1:C:483:MET:HE2	2.02	0.42
1:D:418:LEU:HD21	1:D:435:PHE:CE2	2.54	0.42
1:E:342:LYS:O	1:E:342:LYS:NZ	2.33	0.42
1:F:68:ILE:HG23	1:F:73:ASP:HB2	2.01	0.42
1:F:230:ASP:OD2	1:F:558:ARG:NH2	2.52	0.42
1:B:137:MET:O	1:B:141:LEU:HG	2.19	0.42
1:C:209:PRO:HG2	1:D:207:PRO:O	2.19	0.42
1:E:250:ALA:HB3	1:E:300:ASN:ND2	2.34	0.42
1:E:414:VAL:HG21	1:E:573:PHE:O	2.19	0.42
1:E:489:ARG:HH22	1:F:466:HIS:HB3	1.83	0.42
1:A:115:THR:HA	1:A:154:GLU:CD	2.39	0.42
1:A:237:LEU:O	1:A:239:LYS:NZ	2.28	0.42
1:C:428:ALA:O	1:C:432:GLU:N	2.52	0.42
1:D:20:PHE:HE2	1:D:52:LEU:HD13	1.83	0.42
1:D:133:ASN:C	1:D:137:MET:HE3	2.39	0.42
1:D:435:PHE:O	1:D:438:VAL:HG12	2.19	0.42
1:D:469:ARG:NE	1:D:494:GLU:OE2	2.35	0.42
1:F:87:THR:HA	1:F:164:LYS:HE3	2.01	0.42
1:F:548:ILE:HG13	1:F:552:LEU:HD23	2.01	0.42
1:A:291:ASP:HA	1:A:294:MET:SD	2.60	0.42
1:B:175:ARG:H	1:B:175:ARG:HD2	1.85	0.42
1:C:104:LYS:HZ3	1:D:107:SER:HB2	1.85	0.42
1:D:194:LYS:HA	1:D:194:LYS:HD2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:GLU:OE2	1:D:451:GLU:HB3	2.19	0.42
1:E:4:VAL:HG13	1:E:29:GLU:HB2	2.02	0.42
1:F:180:PRO:HB2	1:F:183:SER:OG	2.19	0.42
1:F:281:TRP:CH2	1:F:502:GLN:HG3	2.55	0.42
1:D:217:ILE:HA	1:D:220:GLN:HE21	1.85	0.42
1:D:402:THR:HG21	1:E:402:THR:HG21	2.02	0.42
1:D:569:ILE:HD11	1:D:583:LEU:HD12	2.02	0.42
1:E:305:LEU:HD23	1:E:305:LEU:HA	1.85	0.42
1:F:208:PHE:CD1	1:F:211:LEU:HD22	2.53	0.42
1:F:300:ASN:HD21	1:F:314:GLN:HE22	1.67	0.42
1:A:61:LYS:HE2	1:A:61:LYS:HB3	1.82	0.42
1:A:86:LEU:CD2	1:A:169:ILE:HG12	2.50	0.42
1:C:35:THR:HA	1:C:62:CYS:HB3	2.02	0.42
1:C:108:ALA:HA	1:C:111:GLN:HG2	2.01	0.42
1:C:160:LEU:HA	1:C:160:LEU:HD12	1.84	0.42
1:D:83:GLN:O	1:D:86:LEU:HG	2.20	0.42
1:D:163:LEU:HD13	1:D:163:LEU:HA	1.86	0.42
1:E:583:LEU:HG	1:F:206:LEU:CD1	2.50	0.42
1:F:342:LYS:HD2	1:F:342:LYS:HA	1.83	0.42
1:F:345:ASN:O	1:F:345:ASN:ND2	2.53	0.42
1:B:3:ARG:HG2	1:B:96:TYR:HE1	1.84	0.42
1:B:286:LYS:HD2	1:B:286:LYS:HA	1.73	0.42
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.86	0.42
1:B:458:ILE:HG23	1:B:470:LEU:HD21	2.01	0.42
1:D:540:ALA:HB1	1:D:544:GLU:HB2	2.02	0.42
1:D:544:GLU:HA	1:D:547:LEU:HG	2.02	0.42
1:C:174:SER:H	1:C:177:ASN:HB2	1.84	0.42
1:C:188:GLU:O	1:C:192:ASN:ND2	2.52	0.42
1:E:132:ARG:H	1:E:136:GLU:CD	2.23	0.42
1:E:243:HIS:HD2	1:E:533:ASP:HA	1.85	0.42
1:E:482:LEU:HA	1:E:485:THR:HG22	2.01	0.42
1:E:585:PHE:HE1	2:E:701:ATP:H2'	1.85	0.42
1:A:168:PRO:O	1:A:169:ILE:C	2.56	0.41
1:A:265:GLU:HG3	1:A:265:GLU:O	2.20	0.41
1:B:240:VAL:HG22	1:B:329:TYR:HB3	2.02	0.41
1:B:384:ARG:HD2	1:B:426:THR:HB	2.01	0.41
1:C:181:LEU:HD13	1:C:181:LEU:N	2.35	0.41
1:D:282:PRO:HB2	1:D:498:TYR:CE1	2.55	0.41
1:E:198:SER:O	1:F:588:ARG:NE	2.53	0.41
1:A:96:TYR:CD2	1:A:121:SER:HB3	2.55	0.41
1:A:344:LYS:HE3	1:A:346:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:CE2	1:A:424:LYS:HB2	2.53	0.41
1:C:422:GLU:OE2	1:C:450:GLY:N	2.53	0.41
1:C:460:GLN:O	1:C:464:SER:N	2.52	0.41
1:D:267:ASP:HA	1:D:271:ARG:HH21	1.85	0.41
1:E:103:ILE:HG12	1:E:106:MET:SD	2.60	0.41
1:B:19:ALA:HB1	1:B:98:CYS:SG	2.61	0.41
1:B:134:ILE:HA	1:B:137:MET:HE2	2.03	0.41
1:B:333:ARG:NH1	1:B:417:ASP:OD2	2.53	0.41
1:D:469:ARG:NH1	1:D:571:THR:O	2.49	0.41
1:E:250:ALA:HB3	1:E:300:ASN:HD22	1.85	0.41
1:F:21:HIS:CD2	1:F:141:LEU:HD22	2.55	0.41
1:F:139:ASP:O	1:F:143:LYS:HG2	2.19	0.41
1:C:125:VAL:HG22	1:C:148:PHE:CD1	2.55	0.41
1:C:306:LYS:NZ	1:C:341:ASP:HB2	2.35	0.41
1:C:520:LYS:H	1:C:520:LYS:HG2	1.71	0.41
1:D:498:TYR:O	1:D:502:GLN:HG2	2.20	0.41
1:E:217:ILE:HA	1:E:220:GLN:HE22	1.85	0.41
1:E:238:PRO:HG3	1:E:589:LYS:HB3	2.02	0.41
1:E:256:LEU:HA	1:E:259:VAL:HG22	2.02	0.41
1:F:192:ASN:ND2	1:F:223:GLN:HB2	2.33	0.41
1:A:84:TRP:NE1	1:A:88:LYS:HD2	2.36	0.41
1:A:167:LEU:HD13	1:A:179:LYS:NZ	2.35	0.41
1:A:418:LEU:HD13	1:A:418:LEU:HA	1.96	0.41
1:A:489:ARG:HA	1:A:489:ARG:HD2	1.87	0.41
1:C:249:PHE:HB3	1:C:314:GLN:NE2	2.35	0.41
1:C:476:LEU:HB3	1:C:521:TYR:OH	2.20	0.41
1:C:500:ASN:HA	1:C:503:ILE:HG12	2.02	0.41
1:D:3:ARG:HG2	1:D:96:TYR:HE1	1.86	0.41
1:D:5:LEU:HB2	1:D:30:VAL:HA	2.03	0.41
1:D:83:GLN:O	1:D:87:THR:HG23	2.20	0.41
1:D:399:LEU:O	1:D:402:THR:HG22	2.21	0.41
1:E:220:GLN:OE1	1:E:221:TRP:N	2.53	0.41
1:E:260:ARG:HE	1:E:269:ILE:HG23	1.86	0.41
1:A:238:PRO:HG3	1:A:589:LYS:HB3	2.01	0.41
1:B:483:MET:O	1:B:487:ILE:HG13	2.21	0.41
1:C:437:ALA:HA	1:C:440:ARG:HD3	2.02	0.41
1:D:99:LEU:HD21	1:D:111:GLN:HB2	2.02	0.41
1:D:242:LEU:HD12	1:D:469:ARG:NH2	2.35	0.41
1:E:3:ARG:HH22	1:E:25:GLU:HG3	1.86	0.41
1:E:162:ARG:NH2	1:E:592:ASP:OD2	2.37	0.41
1:C:193:VAL:HA	1:C:196:MET:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ASP:O	1:C:590:ILE:HG22	2.20	0.41
1:E:112:LYS:NZ	1:E:116:LEU:HB2	2.35	0.41
1:F:76:PHE:O	1:F:79:GLU:N	2.54	0.41
1:F:175:ARG:H	1:F:175:ARG:HD2	1.86	0.41
1:F:378:LEU:HD23	1:F:378:LEU:HA	1.85	0.41
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.86	0.41
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.89	0.41
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.83	0.41
1:C:384:ARG:HD3	1:C:384:ARG:N	2.36	0.41
1:E:39:LYS:HE2	1:E:39:LYS:HB2	1.92	0.41
1:E:83:GLN:O	1:E:86:LEU:HG	2.20	0.41
1:E:436:LYS:HB3	1:E:440:ARG:NH2	2.35	0.41
1:E:472:HIS:CD2	1:E:500:ASN:HD21	2.38	0.41
1:E:476:LEU:HB3	1:E:521:TYR:OH	2.21	0.41
1:A:58:SER:O	1:A:59:ILE:HD13	2.21	0.41
1:A:104:LYS:HE2	1:B:107:SER:HB3	2.03	0.41
1:A:304:LEU:HG	1:A:305:LEU:HD12	2.02	0.41
1:A:440:ARG:HE	1:F:391:SER:HB3	1.86	0.41
1:B:99:LEU:HD22	1:B:107:SER:HA	2.03	0.41
1:C:13:SER:O	1:C:45:LEU:HD21	2.20	0.41
1:C:216:PRO:HD3	1:D:157:TRP:CZ2	2.56	0.41
1:C:221:TRP:HA	1:C:224:LEU:HD13	2.03	0.41
1:C:222:LEU:HB3	1:C:558:ARG:HB2	2.02	0.41
1:D:214:LEU:HD11	1:D:594:CYS:SG	2.61	0.41
1:F:18:GLU:HA	1:F:21:HIS:ND1	2.35	0.41
1:F:110:LEU:HD12	1:F:110:LEU:HA	1.93	0.41
1:F:112:LYS:O	1:F:116:LEU:HD23	2.21	0.41
1:F:515:LEU:H	1:F:515:LEU:HD23	1.86	0.41
1:B:185:SER:O	1:B:189:ILE:HG23	2.21	0.41
1:D:263:ALA:CB	1:D:310:CYS:SG	3.07	0.41
1:E:468:ARG:NH1	1:F:488:GLU:HB3	2.35	0.41
1:F:269:ILE:O	1:F:271:ARG:NH1	2.54	0.41
1:A:3:ARG:NH1	1:A:25:GLU:OE1	2.54	0.40
1:A:369:LYS:HB2	1:A:369:LYS:HE3	1.87	0.40
1:B:581:GLU:OE1	1:B:581:GLU:HA	2.21	0.40
1:C:588:ARG:NH1	1:D:200:THR:HA	2.36	0.40
1:D:14:MET:H	1:D:14:MET:HE3	1.86	0.40
1:E:307:ASP:HB3	1:E:310:CYS:SG	2.61	0.40
1:E:322:LEU:HG	1:E:374:CYS:SG	2.61	0.40
1:E:437:ALA:HA	1:E:440:ARG:HD2	2.02	0.40
1:F:315:VAL:HG22	1:F:359:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:LEU:HD23	1:F:322:LEU:HA	1.89	0.40
1:A:72:ARG:O	1:A:75:GLU:HG3	2.21	0.40
1:A:504:LYS:HD2	1:A:504:LYS:HA	1.90	0.40
1:B:72:ARG:O	1:B:75:GLU:HG3	2.22	0.40
1:B:292:LYS:H	1:B:292:LYS:HD2	1.86	0.40
1:B:305:LEU:HD13	1:B:311:LEU:HD12	2.03	0.40
1:B:549:LEU:HD23	1:B:549:LEU:HA	1.80	0.40
1:C:590:ILE:HD12	1:C:590:ILE:HA	1.94	0.40
1:F:138:PHE:O	1:F:142:GLN:HG2	2.21	0.40
1:B:18:GLU:O	1:B:148:PHE:HZ	2.04	0.40
1:B:204:ASN:N	1:B:204:ASN:HD22	2.18	0.40
1:B:207:PRO:HD2	1:B:211:LEU:HD23	2.04	0.40
1:C:179:LYS:H	1:C:179:LYS:HG3	1.64	0.40
1:C:534:ASN:HB2	1:C:537:ILE:HB	2.02	0.40
1:D:498:TYR:CE2	1:D:548:ILE:HG13	2.56	0.40
1:F:18:GLU:HB3	1:F:125:VAL:HG11	2.02	0.40
1:F:33:PHE:CZ	1:F:62:CYS:HB2	2.55	0.40
1:F:169:ILE:HG22	1:F:171:GLU:H	1.86	0.40
1:A:90:PRO:HD3	1:A:95:PRO:HB3	2.02	0.40
1:A:231:GLY:HA2	1:A:234:ILE:HG22	2.04	0.40
1:C:385:LYS:HB3	1:C:385:LYS:HE3	2.00	0.40
1:F:78:GLN:O	1:F:81:LEU:HG	2.21	0.40
1:F:79:GLU:O	1:F:83:GLN:HG3	2.21	0.40
1:F:392:ASP:OD1	1:F:393:ILE:N	2.54	0.40
1:B:354:ASP:O	1:B:358:THR:HG22	2.22	0.40
1:B:392:ASP:OD1	1:B:393:ILE:N	2.54	0.40
1:B:454:ASP:OD1	1:B:456:GLU:HG3	2.21	0.40
1:B:483:MET:HG3	1:B:487:ILE:HD11	2.03	0.40
1:C:179:LYS:HB2	1:C:179:LYS:HE3	1.63	0.40
1:C:491:ILE:HD13	1:C:491:ILE:HA	1.90	0.40
1:D:283:ARG:NH2	1:D:548:ILE:HD12	2.35	0.40
1:F:99:LEU:HD22	1:F:110:LEU:HB3	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	A	596/600 (99%)	566 (95%)	28 (5%)	2 (0%)	37	67
1	B	596/600 (99%)	557 (94%)	34 (6%)	5 (1%)	16	51
1	C	596/600 (99%)	557 (94%)	34 (6%)	5 (1%)	16	51
1	D	596/600 (99%)	545 (91%)	41 (7%)	10 (2%)	7	37
1	E	596/600 (99%)	560 (94%)	36 (6%)	0	100	100
1	F	596/600 (99%)	555 (93%)	38 (6%)	3 (0%)	25	59
All	All	3576/3600 (99%)	3340 (93%)	211 (6%)	25 (1%)	21	53

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	B	207	PRO
1	B	268	LEU
1	D	207	PRO
1	D	508	PRO
1	F	205	GLN
1	B	291	ASP
1	C	180	PRO
1	C	182	ILE
1	D	291	ASP
1	F	207	PRO
1	B	205	GLN
1	D	268	LEU
1	A	168	PRO
1	C	178	PHE
1	C	205	GLN
1	D	266	PRO
1	D	267	ASP
1	D	164	LYS
1	D	270	ASP
1	B	386	PHE
1	C	428	ALA
1	D	167	LEU
1	F	213	ILE
1	D	208	PHE

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	515/517 (100%)	485 (94%)	30 (6%)	17	46
1	B	515/517 (100%)	488 (95%)	27 (5%)	19	49
1	C	515/517 (100%)	489 (95%)	26 (5%)	20	49
1	D	515/517 (100%)	475 (92%)	40 (8%)	10	36
1	E	515/517 (100%)	491 (95%)	24 (5%)	22	51
1	F	515/517 (100%)	494 (96%)	21 (4%)	26	55
All	All	3090/3102 (100%)	2922 (95%)	168 (5%)	21	48

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	33	PHE
1	A	40	PHE
1	A	67	ASP
1	A	72	ARG
1	A	75	GLU
1	A	88	LYS
1	A	92	ASN
1	A	98	CYS
1	A	126	LEU
1	A	137	MET
1	A	138	PHE
1	A	164	LYS
1	A	170	ASN
1	A	171	GLU
1	A	178	PHE
1	A	196	MET
1	A	220	GLN
1	A	303	LYS
1	A	306	LYS
1	A	325	ASP
1	A	346	ARG

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Mol	Chain	Res	Type
1	A	354	ASP
1	A	359	PHE
1	A	384	ARG
1	A	386	PHE
1	A	411	CYS
1	A	459	TRP
1	A	542	LEU
1	A	586	PHE
1	B	14	MET
1	B	36	ASP
1	B	38	GLU
1	B	72	ARG
1	B	106	MET
1	B	123	PHE
1	B	128	ASP
1	B	173	CYS
1	B	175	ARG
1	B	194	LYS
1	B	196	MET
1	B	206	LEU
1	B	208	PHE
1	B	267	ASP
1	B	271	ARG
1	B	287	SER
1	B	292	LYS
1	B	303	LYS
1	B	337	ASN
1	B	359	PHE
1	B	389	ASP
1	B	424	LYS
1	B	484	ARG
1	B	516	TYR
1	B	545	ASN
1	B	586	PHE
1	B	588	ARG
1	C	27	PHE
1	C	40	PHE
1	C	85	TYR
1	C	106	MET
1	C	137	MET
1	C	161	ARG
1	C	179	LYS

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Mol	Chain	Res	Type
1	C	181	LEU
1	C	182	ILE
1	C	196	MET
1	C	198	SER
1	C	200	THR
1	C	203	SER
1	C	219	GLN
1	C	265	GLU
1	C	294	MET
1	C	346	ARG
1	C	359	PHE
1	C	365	GLU
1	C	373	TYR
1	C	374	CYS
1	C	386	PHE
1	C	435	PHE
1	C	453	ASP
1	C	516	TYR
1	C	588	ARG
1	D	14	MET
1	D	38	GLU
1	D	40	PHE
1	D	49	PHE
1	D	52	LEU
1	D	72	ARG
1	D	85	TYR
1	D	128	ASP
1	D	133	ASN
1	D	151	MET
1	D	160	LEU
1	D	161	ARG
1	D	162	ARG
1	D	163	LEU
1	D	164	LYS
1	D	165	LYS
1	D	166	ILE
1	D	173	CYS
1	D	176	ASP
1	D	178	PHE
1	D	181	LEU
1	D	208	PHE
1	D	264	SER

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Mol	Chain	Res	Type
1	D	265	GLU
1	D	268	LEU
1	D	269	ILE
1	D	271	ARG
1	D	273	PHE
1	D	287	SER
1	D	292	LYS
1	D	293	TYR
1	D	305	LEU
1	D	306	LYS
1	D	359	PHE
1	D	392	ASP
1	D	424	LYS
1	D	430	TYR
1	D	498	TYR
1	D	516	TYR
1	D	586	PHE
1	E	8	SER
1	E	39	LYS
1	E	40	PHE
1	E	99	LEU
1	E	120	GLN
1	E	139	ASP
1	E	162	ARG
1	E	164	LYS
1	E	206	LEU
1	E	220	GLN
1	E	237	LEU
1	E	283	ARG
1	E	293	TYR
1	E	306	LYS
1	E	335	SER
1	E	339	TYR
1	E	346	ARG
1	E	384	ARG
1	E	390	LEU
1	E	498	TYR
1	E	516	TYR
1	E	545	ASN
1	E	586	PHE
1	E	594	CYS
1	F	20	PHE

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Mol	Chain	Res	Type
1	F	21	HIS
1	F	72	ARG
1	F	76	PHE
1	F	77	TYR
1	F	123	PHE
1	F	137	MET
1	F	165	LYS
1	F	175	ARG
1	F	206	LEU
1	F	208	PHE
1	F	243	HIS
1	F	292	LYS
1	F	293	TYR
1	F	367	LYS
1	F	386	PHE
1	F	424	LYS
1	F	427	ARG
1	F	559	MET
1	F	586	PHE
1	F	600	ASN

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

Mol	Chain	Res	Type
1	A	83	GLN
1	A	170	ASN
1	B	204	ASN
1	B	320	GLN
1	C	111	GLN
1	C	285	HIS
1	C	576	HIS
1	D	21	HIS
1	D	145	GLN
1	D	220	GLN
1	E	177	ASN
1	E	204	ASN
1	E	500	ASN
1	F	124	HIS
1	F	192	ASN
1	F	258	GLN
1	F	314	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
2	ATP	D	701	-	28,33,33	4.07	9 (32%)	34,52,52	1.57	2 (5%)
2	ATP	A	701	-	28,33,33	4.06	9 (32%)	34,52,52	1.48	2 (5%)
2	ATP	E	701	-	28,33,33	4.07	9 (32%)	34,52,52	1.44	2 (5%)

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
2	ATP	D	701	-	-	6/18/38/38	0/3/3/3
2	ATP	A	701	-	-	4/18/38/38	0/3/3/3
2	ATP	E	701	-	-	4/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	ATP	O4'-C1'	16.45	1.62	1.40
2	D	701	ATP	O4'-C1'	16.43	1.62	1.40
2	A	701	ATP	O4'-C1'	16.37	1.62	1.40
2	D	701	ATP	O4'-C4'	-7.76	1.27	1.45
2	A	701	ATP	O4'-C4'	-7.75	1.27	1.45
2	E	701	ATP	O4'-C4'	-7.70	1.27	1.45
2	A	701	ATP	PB-O3A	5.34	1.65	1.59
2	E	701	ATP	PA-O3A	5.33	1.65	1.59
2	D	701	ATP	PB-O3A	5.30	1.65	1.59
2	D	701	ATP	PB-O3B	5.26	1.65	1.59
2	A	701	ATP	PA-O3A	5.25	1.65	1.59
2	E	701	ATP	PB-O3A	5.23	1.65	1.59
2	D	701	ATP	PA-O3A	5.20	1.65	1.59
2	E	701	ATP	PB-O3B	5.20	1.65	1.59
2	A	701	ATP	PB-O3B	5.17	1.65	1.59
2	E	701	ATP	O2'-C2'	3.35	1.51	1.43
2	D	701	ATP	O2'-C2'	3.34	1.51	1.43
2	A	701	ATP	O2'-C2'	3.29	1.51	1.43
2	A	701	ATP	C6-N6	3.23	1.45	1.34
2	D	701	ATP	C6-N6	3.21	1.45	1.34
2	E	701	ATP	C6-N6	3.20	1.45	1.34
2	E	701	ATP	O3'-C3'	-2.62	1.36	1.43
2	D	701	ATP	O3'-C3'	-2.61	1.36	1.43
2	A	701	ATP	O3'-C3'	-2.61	1.36	1.43
2	D	701	ATP	C1'-N9	-2.22	1.44	1.49
2	A	701	ATP	C1'-N9	-2.22	1.44	1.49
2	E	701	ATP	C1'-N9	-2.13	1.44	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	ATP	C4'-O4'-C1'	-5.81	104.60	109.92
2	D	701	ATP	N3-C2-N1	-5.59	121.09	128.67
2	A	701	ATP	N3-C2-N1	-5.55	121.14	128.67
2	E	701	ATP	N3-C2-N1	-5.51	121.19	128.67
2	A	701	ATP	C4'-O4'-C1'	-5.07	105.28	109.92
2	E	701	ATP	C4'-O4'-C1'	-4.72	105.60	109.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O3A

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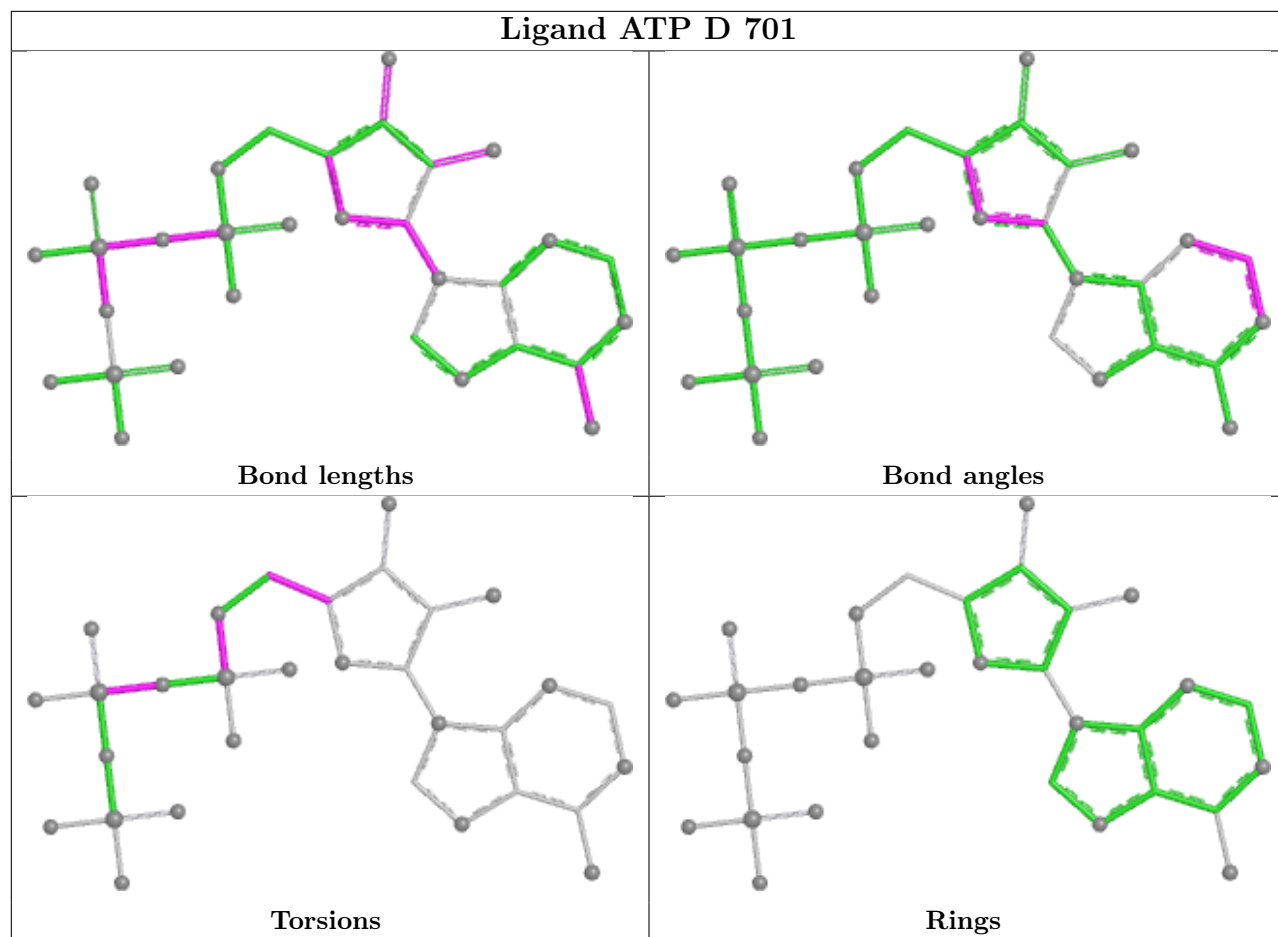
Mol	Chain	Res	Type	Atoms
2	D	701	ATP	C5'-O5'-PA-O2A
2	D	701	ATP	C5'-O5'-PA-O3A
2	E	701	ATP	C5'-O5'-PA-O3A
2	D	701	ATP	PA-O3A-PB-O1B
2	A	701	ATP	C5'-O5'-PA-O1A
2	D	701	ATP	C5'-O5'-PA-O1A
2	E	701	ATP	C5'-O5'-PA-O1A
2	A	701	ATP	O4'-C4'-C5'-O5'
2	A	701	ATP	PA-O3A-PB-O1B
2	E	701	ATP	PA-O3A-PB-O1B
2	D	701	ATP	O4'-C4'-C5'-O5'
2	E	701	ATP	O4'-C4'-C5'-O5'
2	D	701	ATP	PA-O3A-PB-O2B

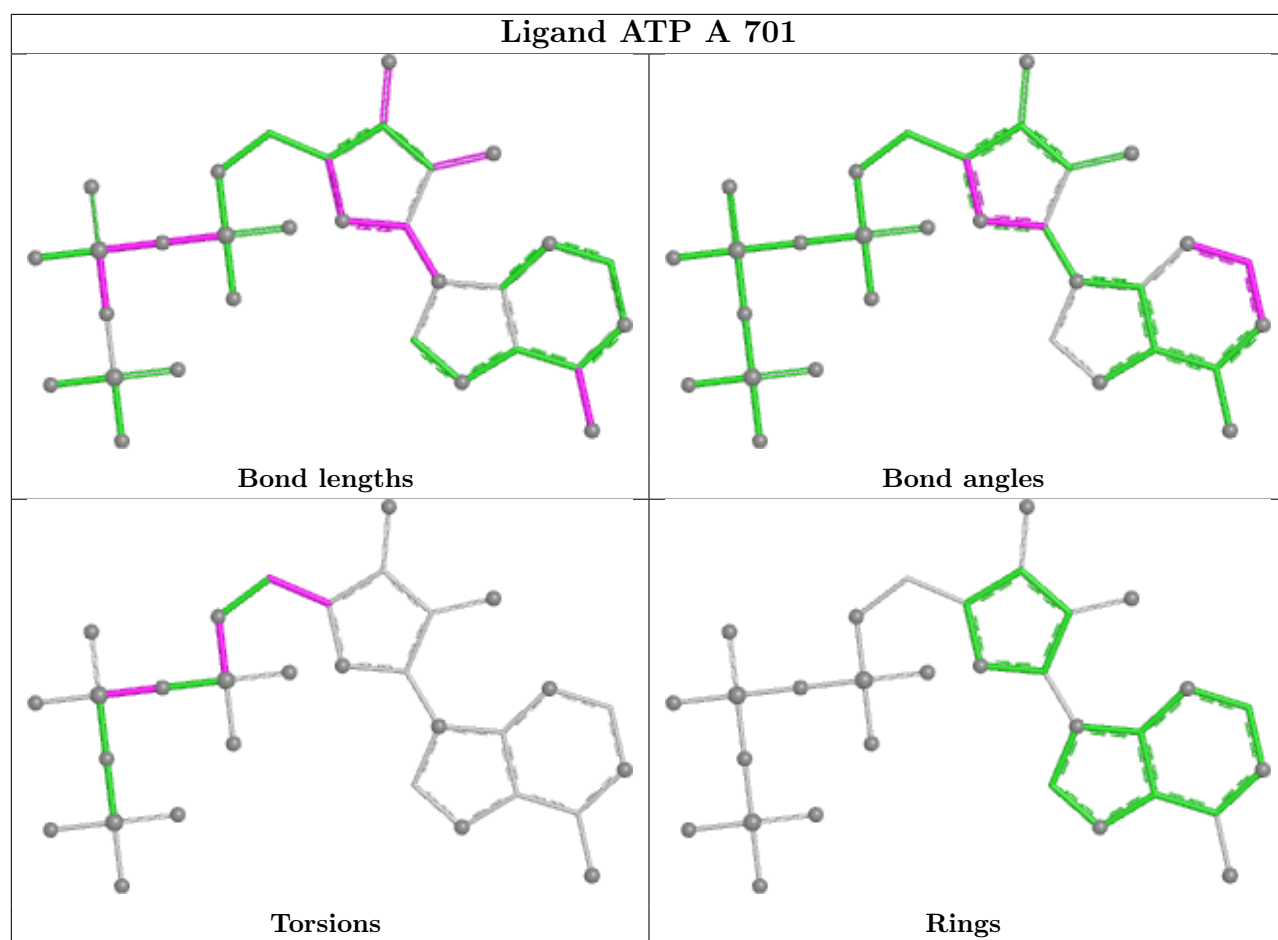
There are no ring outliers.

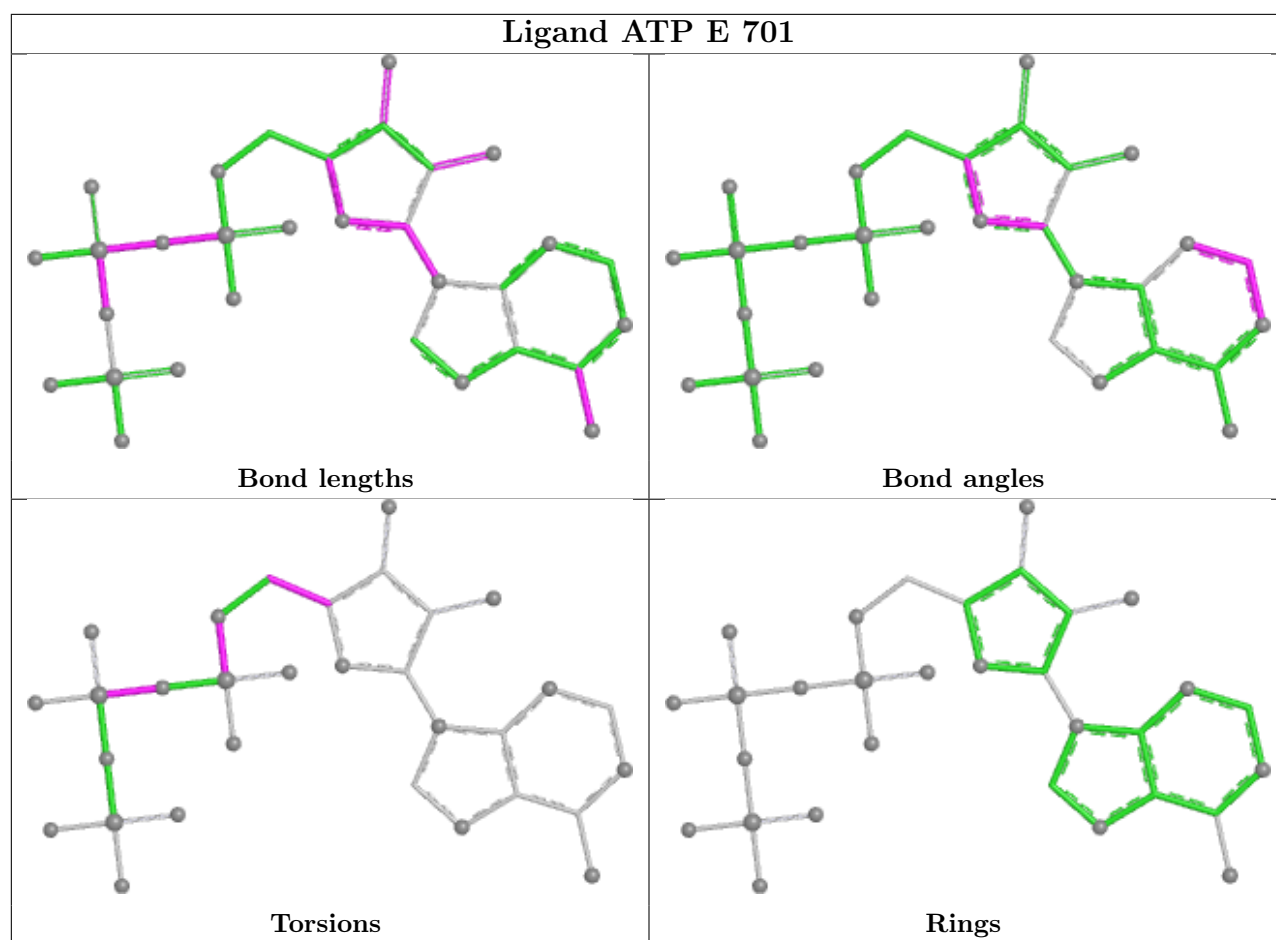
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ATP	2	0
2	A	701	ATP	1	0
2	E	701	ATP	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.

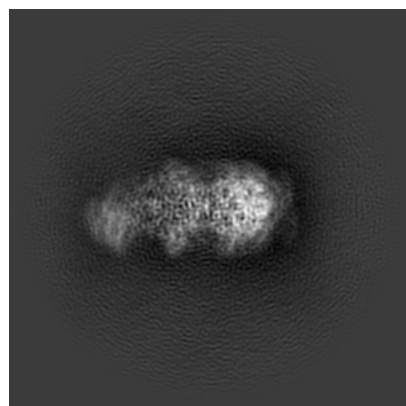
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45245. These allow visual inspection of the internal detail of the map and identification of artifacts.

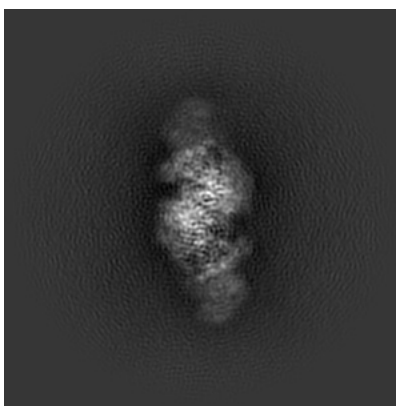
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

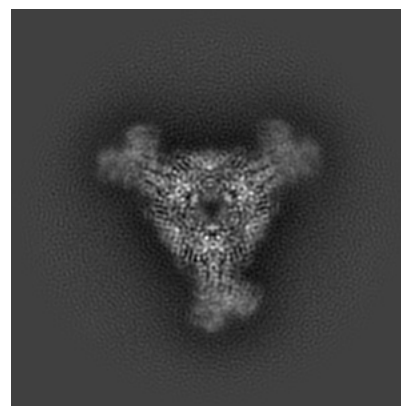
6.1.1 Primary map



X

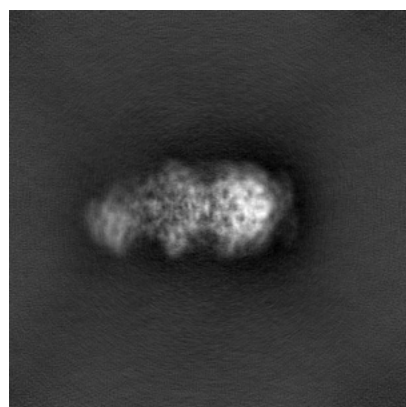


Y

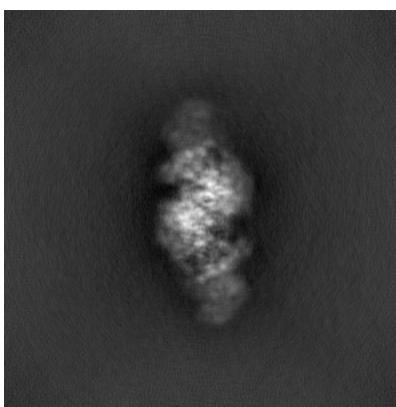


Z

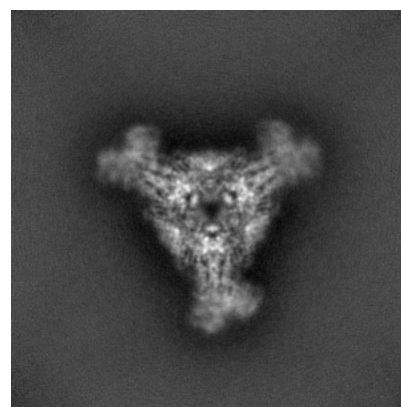
6.1.2 Raw map



X



Y

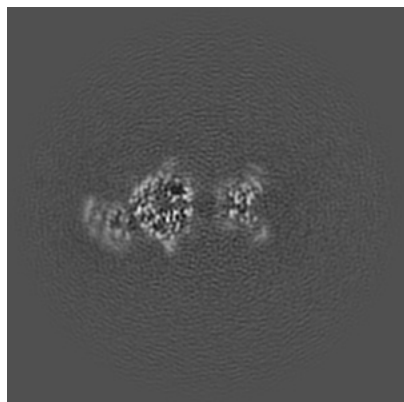


Z

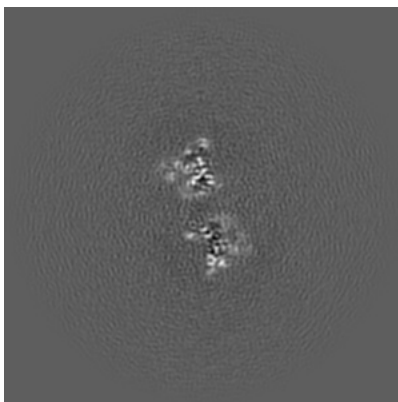
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

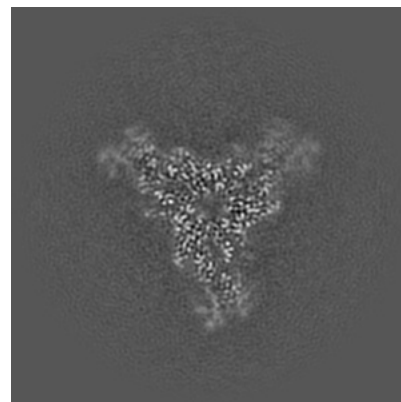
6.2.1 Primary map



X Index: 160

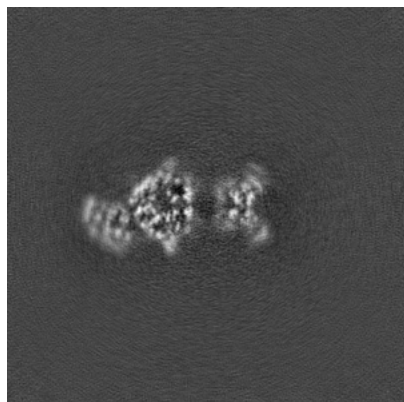


Y Index: 160

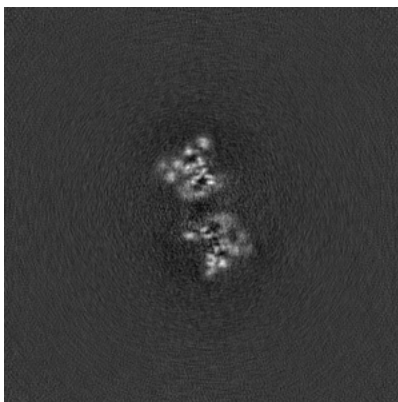


Z Index: 160

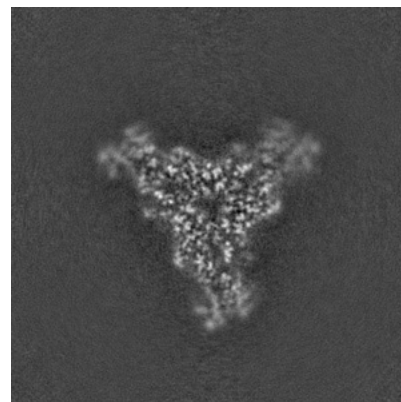
6.2.2 Raw map



X Index: 160



Y Index: 160

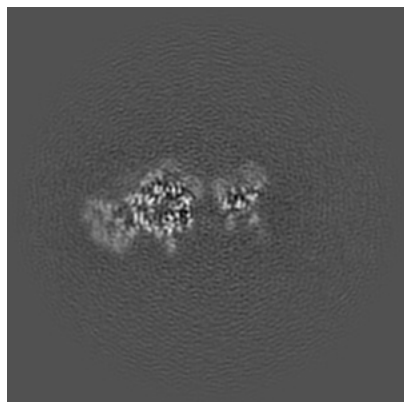


Z Index: 160

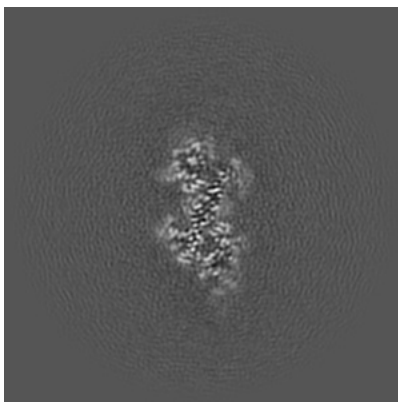
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

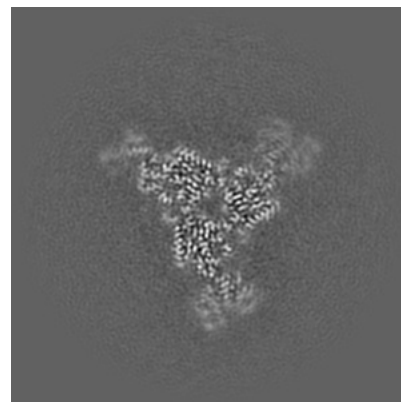
6.3.1 Primary map



X Index: 164

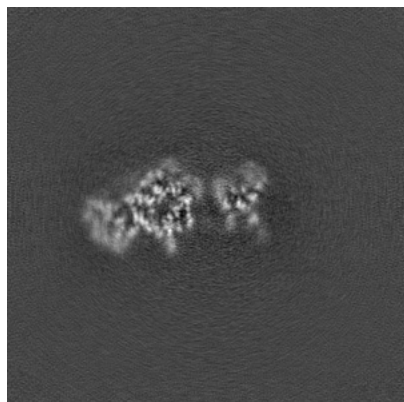


Y Index: 179

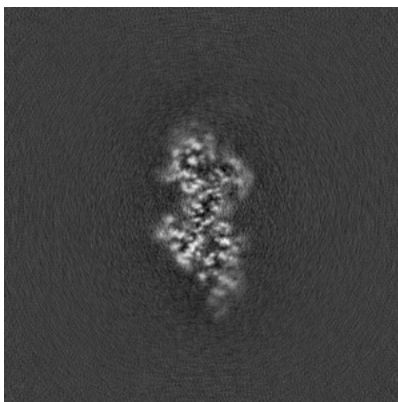


Z Index: 157

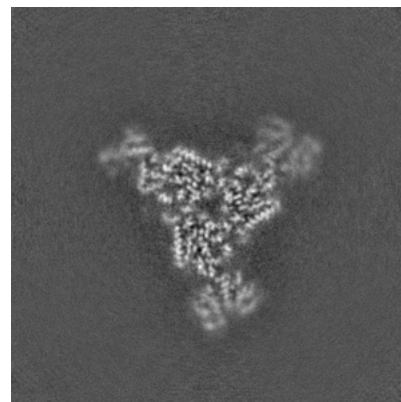
6.3.2 Raw map



X Index: 164



Y Index: 180

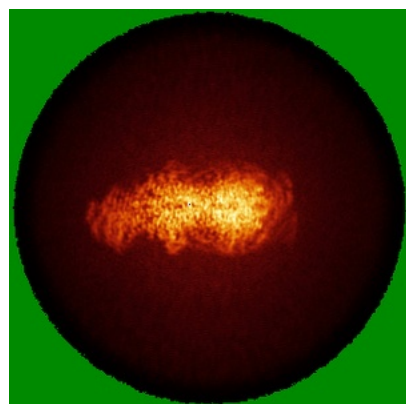


Z Index: 157

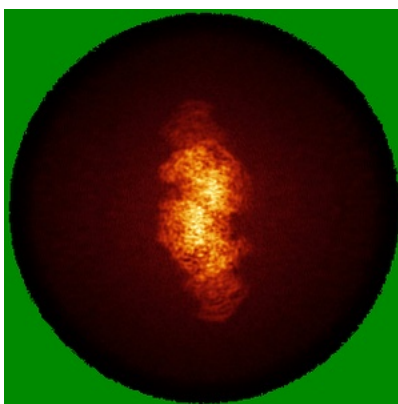
The images above show the largest variance slices of the map in three orthogonal directions.

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

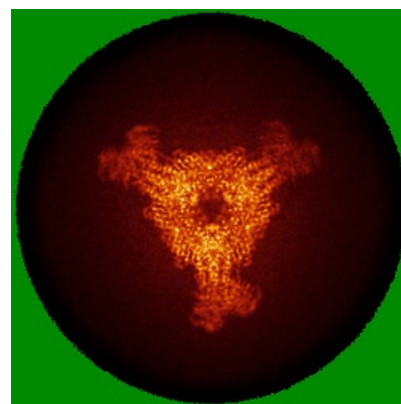
6.4.1 Primary map



X

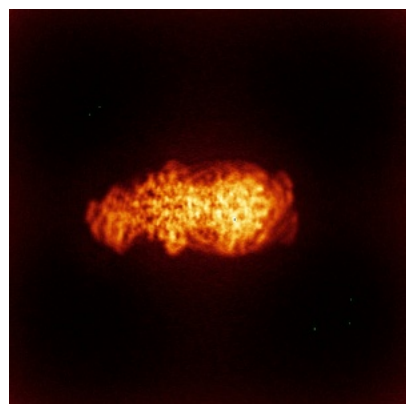


Y

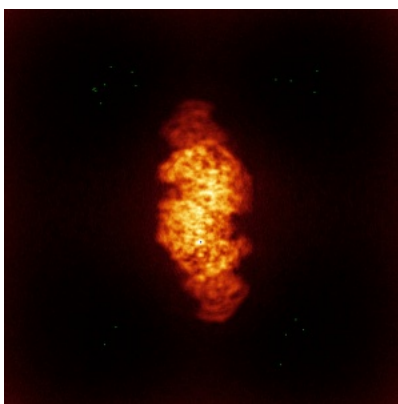


Z

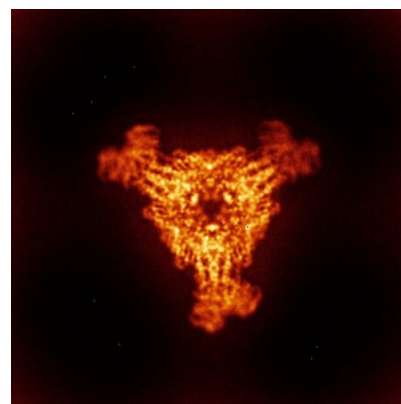
6.4.2 Raw map



X



Y

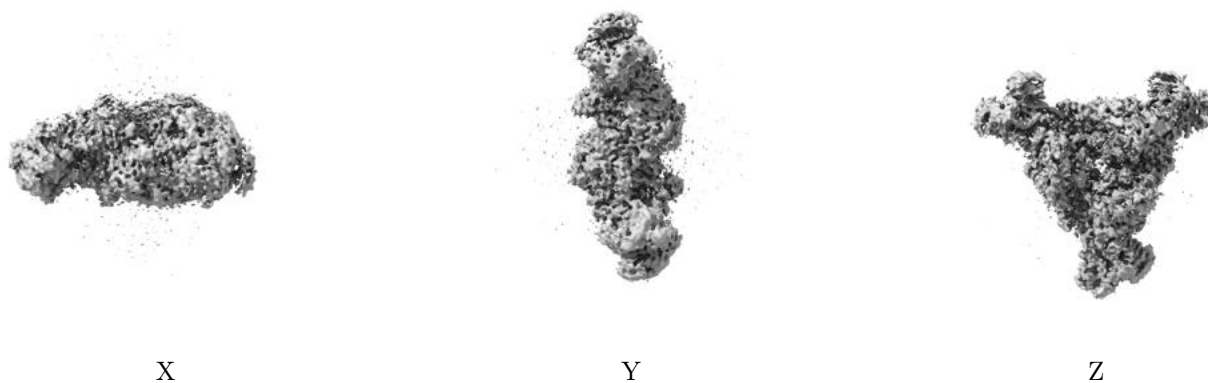


Z

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.

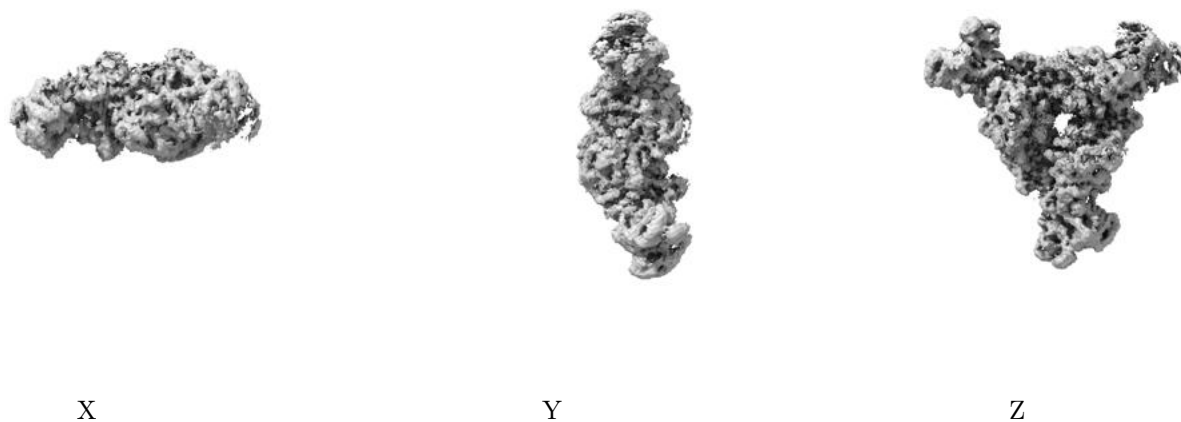
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.184. 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.

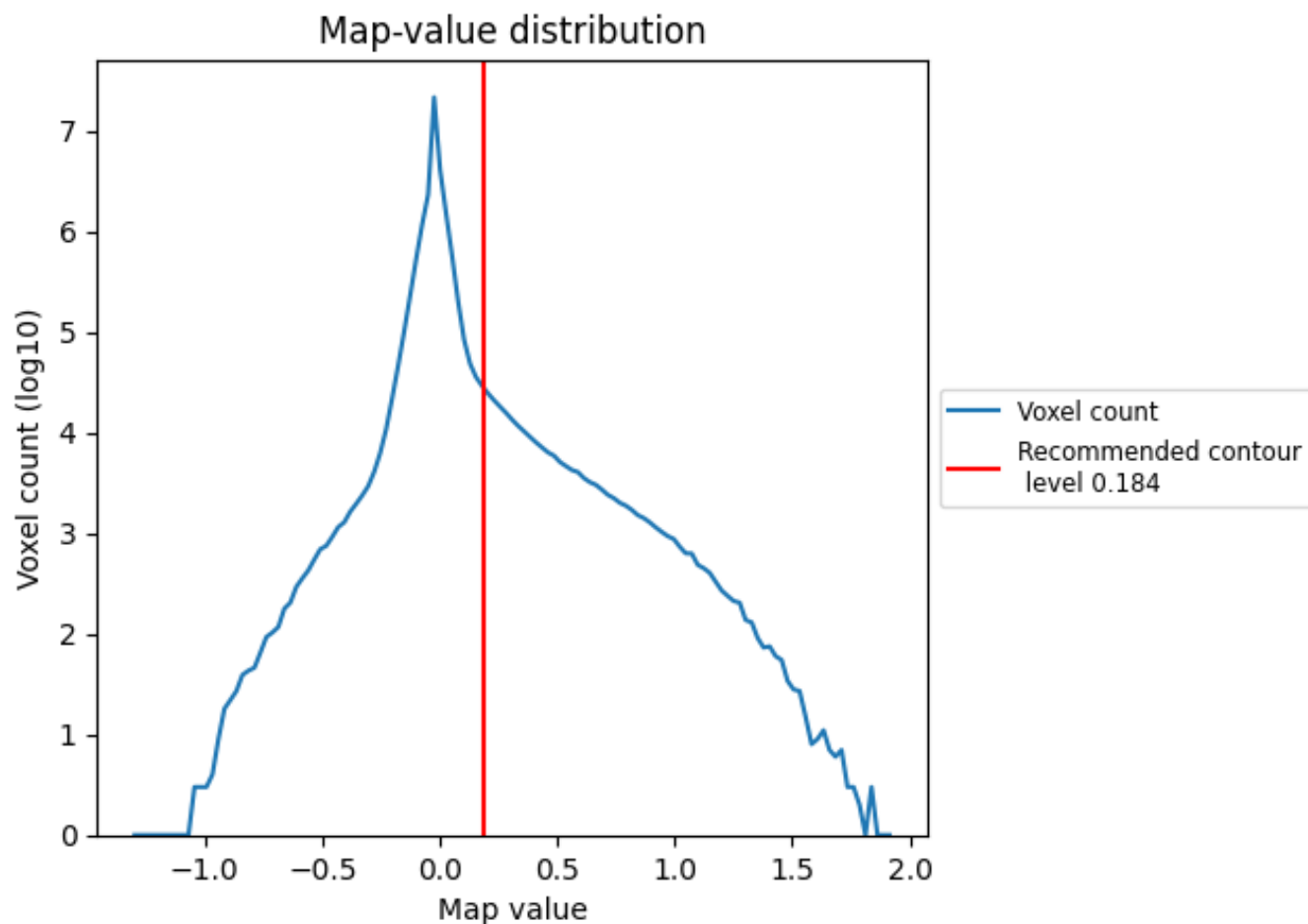
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

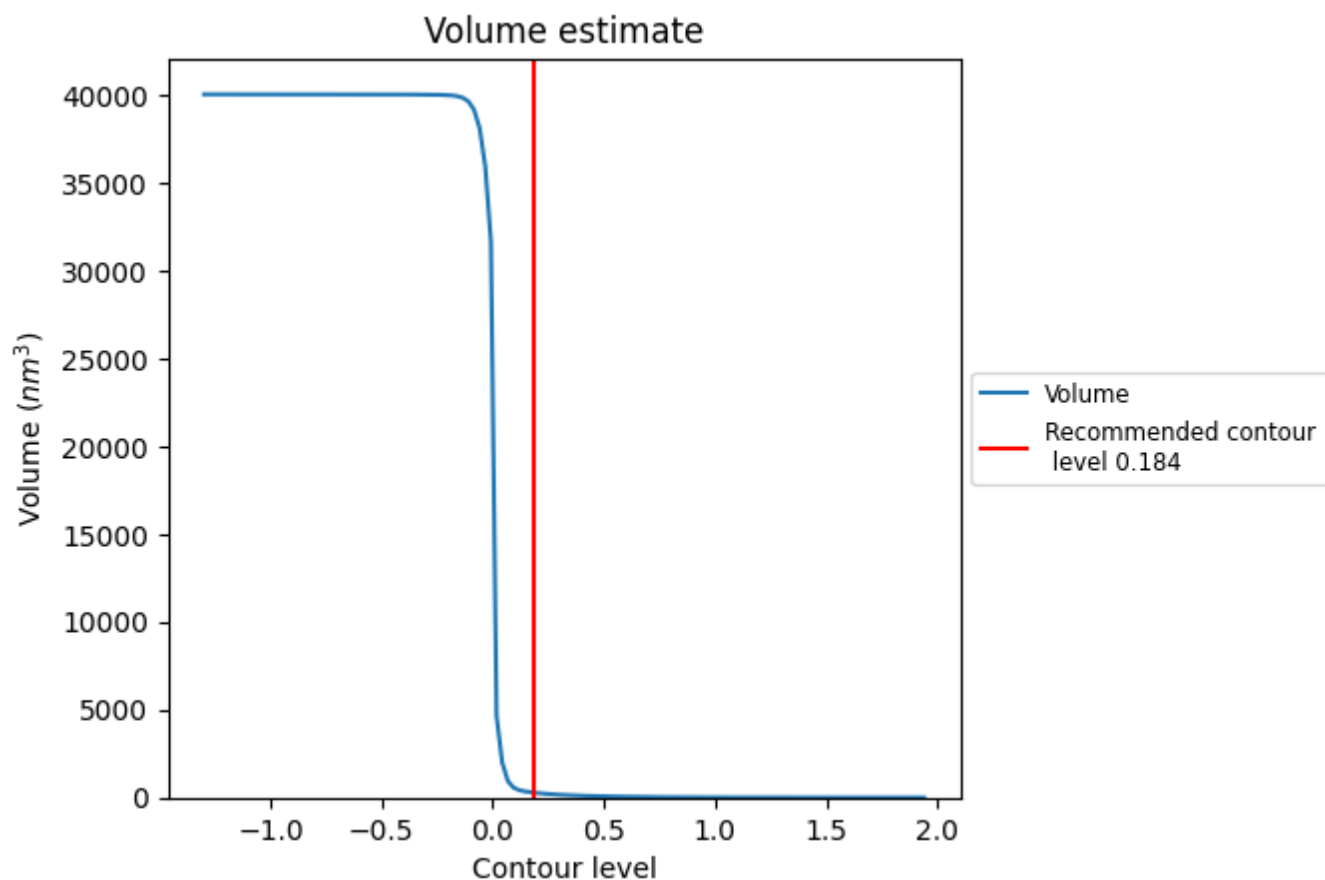
This section contains the results of statistical analysis of the map.

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.

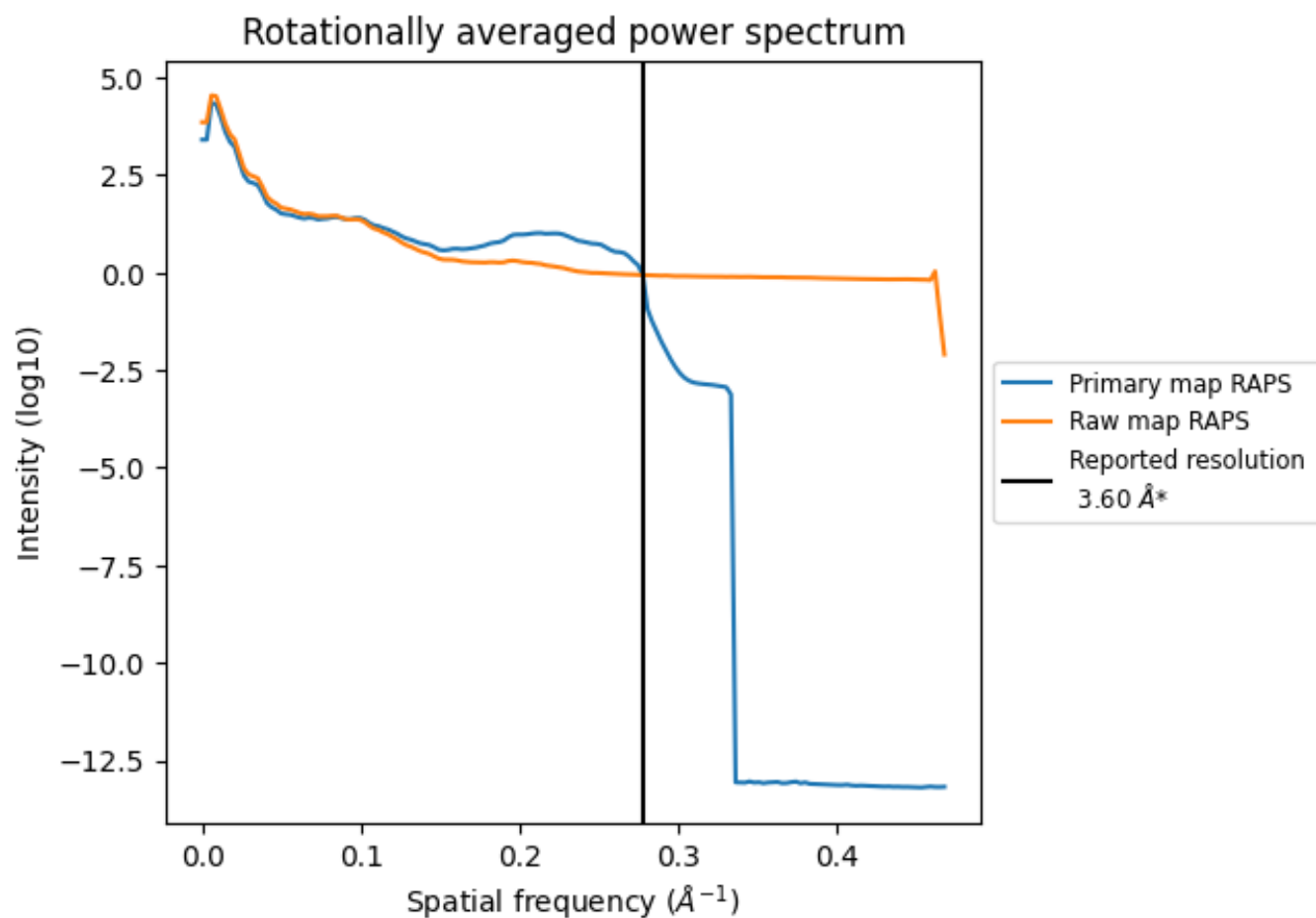
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 255 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 ⓘ

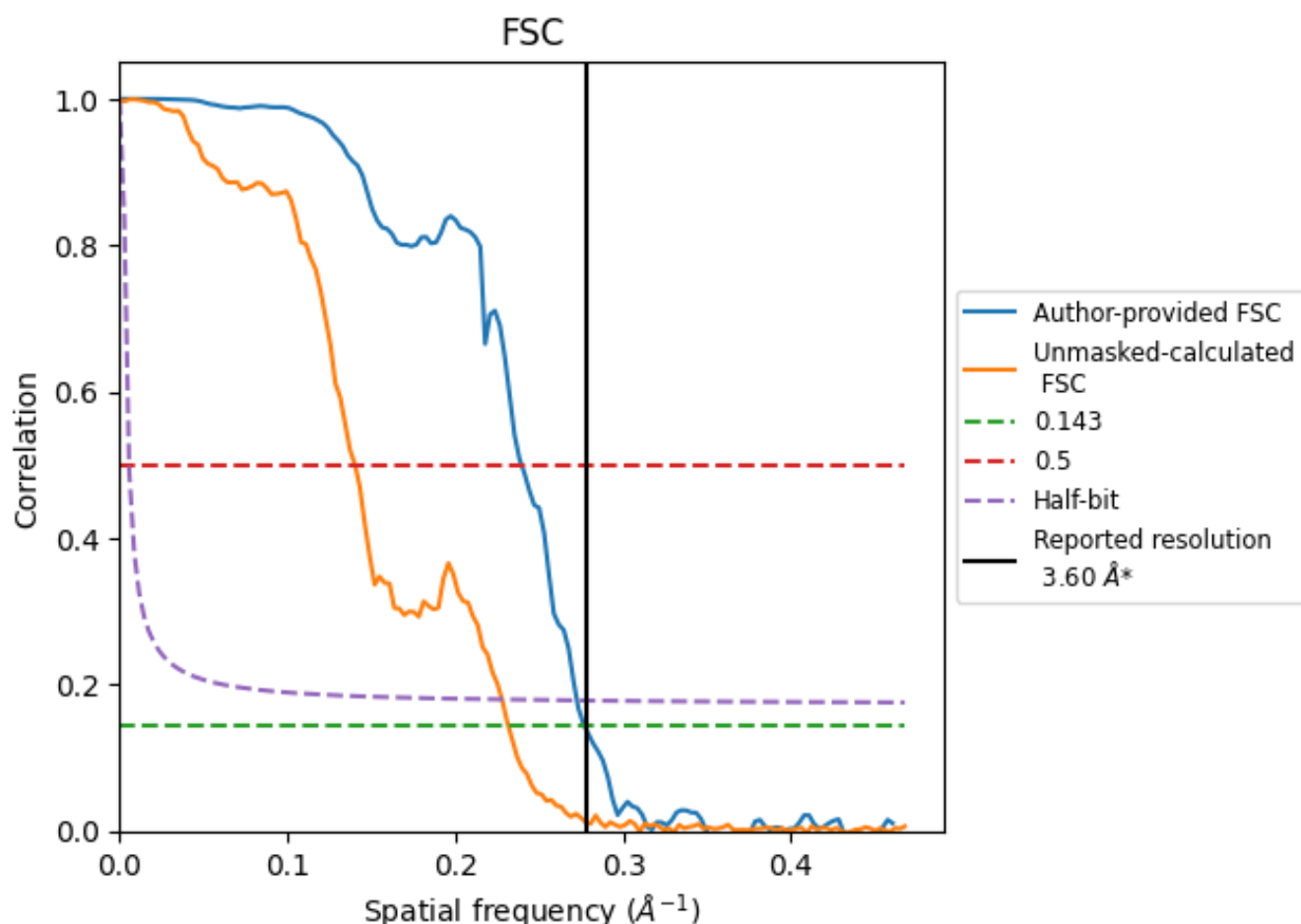


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

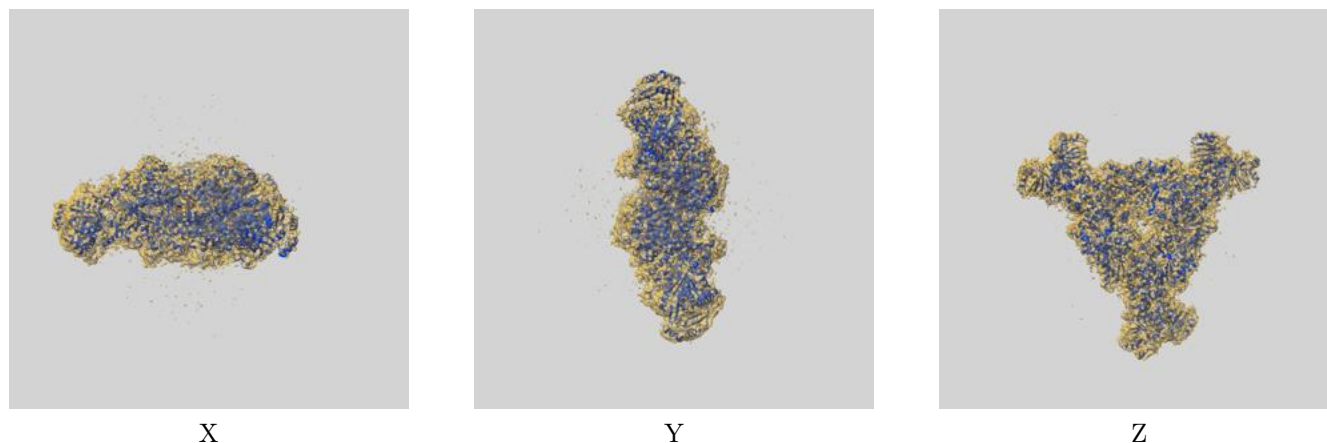
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.18	3.67
Unmasked-calculated*	4.32	7.13	4.39

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

9 Map-model fit [i](#)

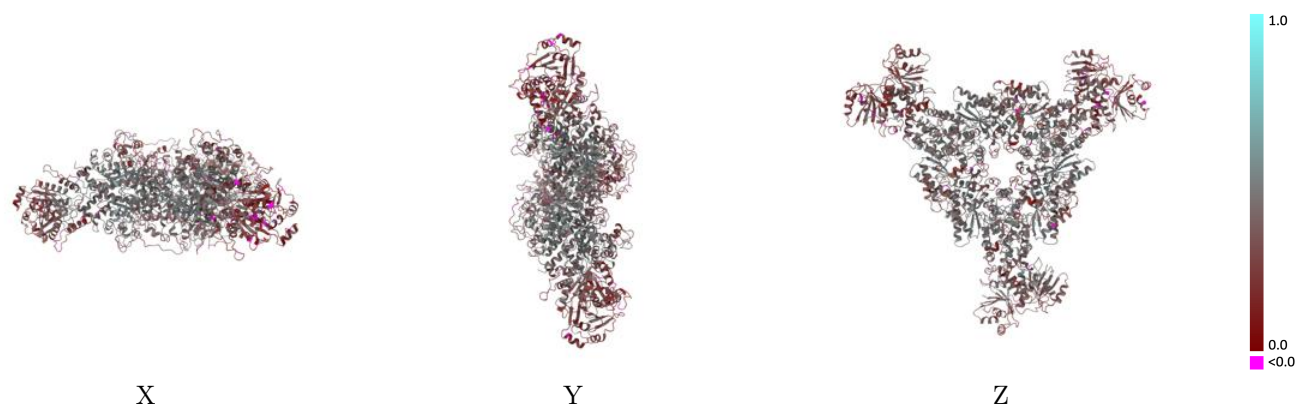
This section contains information regarding the fit between EMDB map EMD-45245 and PDB model 9C6F. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



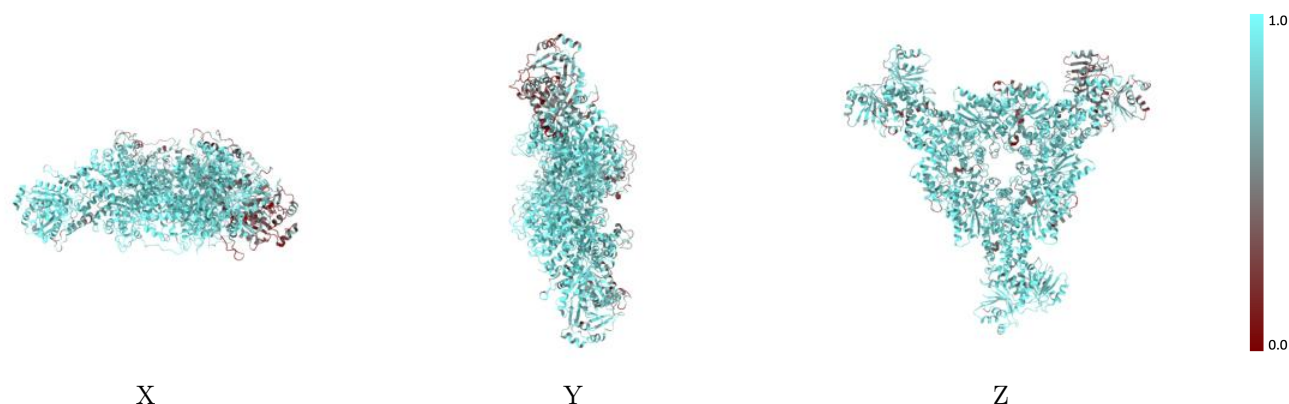
The images above show the 3D surface view of the map at the recommended contour level 0.184 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



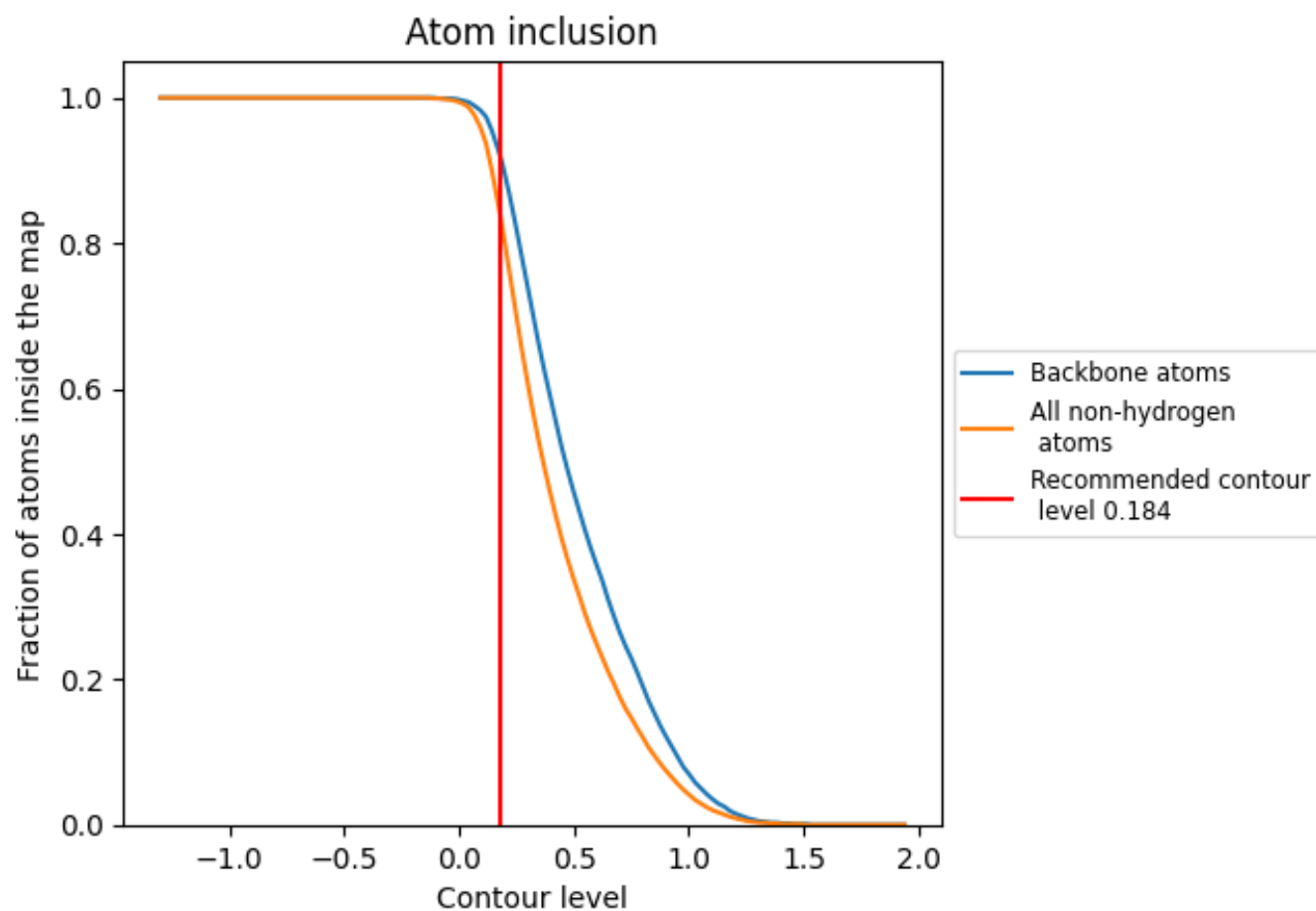
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.184).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8320</div>	<div><div></div>0.3730</div>
A	<div><div></div>0.8630</div>	<div><div></div>0.3850</div>
B	<div><div></div>0.8980</div>	<div><div></div>0.3940</div>
C	<div><div></div>0.8130</div>	<div><div></div>0.3650</div>
D	<div><div></div>0.8800</div>	<div><div></div>0.3910</div>
E	<div><div></div>0.7440</div>	<div><div></div>0.3510</div>
F	<div><div></div>0.7910</div>	<div><div></div>0.3540</div>

1.0

0.0

<0.0