Full wwPDB EM Validation Report

Aug 27, 2026 – 10:31 am BST

PDB ID	:	8ASW / pdb_00008asw
EMDB ID	:	EMD-15623
Title	:	Cryo-EM structure of yeast Elp123 in complex with alanine tRNA
Authors	:	Jaciuk, M.; Scherf, D.; Kaszuba, K.; Gaik, M.; Koscielniak, A.; Krutyholowa, R.; Rawski, M.; Indyka, P.; Biela, A.; Dobosz, D.; Lin, T.-Y.; Abbassi, N.; Hammermeister, A.; Chramiec-Glabik, A.; Kosinski, J.; Schaffrath, R.; Glatt, S.
Deposited on	:	2022-08-21
Resolution	:	3.96 Å(reported)
Based on initial models	:	6QK7, 1EHZ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

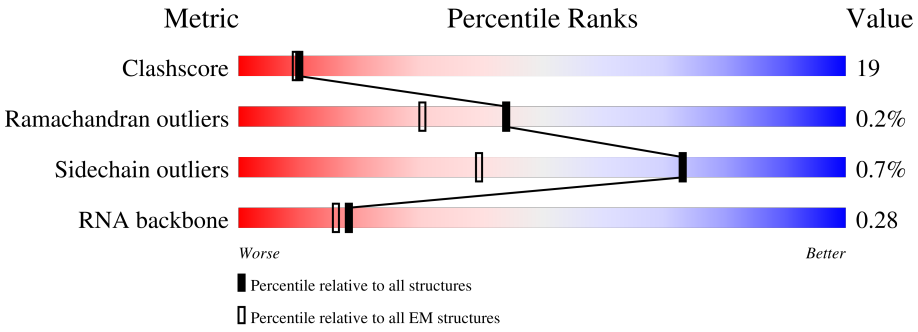
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)

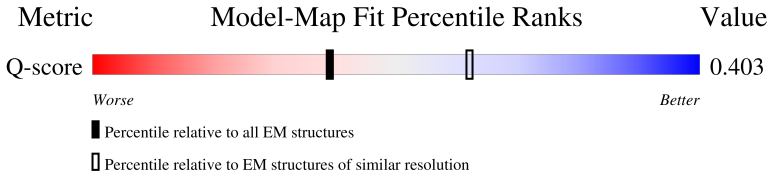
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.96 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	7646 (3.46 - 4.46)

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

Mol	Chain	Length	Quality of chain
1	A	1349	10% 57% 35% • 7%

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Mol	Chain	Length	Quality of chain
1	D	1349	13% 15% 10% 75%
2	B	788	5% 55% 43%
3	C	557	5% 57% 37% 5%
4	X	73	22% 16% 48% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SF4	C	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24781 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 Elongator complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1255	Total	C	N	O	S	0	0
			10014	6345	1663	1968	38		
1	D	343	Total	C	N	O	S	0	0
			2769	1738	487	536	8		

- Molecule 2 is a protein called Elongator complex protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	772	Total	C	N	O	S	0	0
			6177	3939	1047	1164	27		

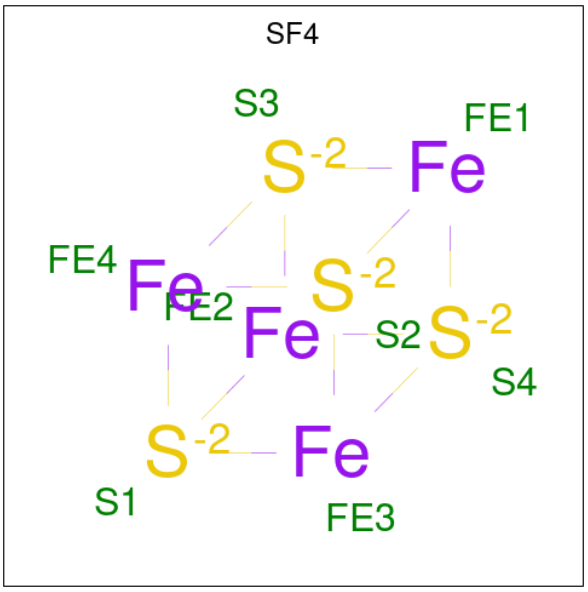
- Molecule 3 is a protein called Elongator complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	527	Total	C	N	O	S	0	0
			4236	2677	741	795	23		

- Molecule 4 is a RNA chain called Alanine tRNA.

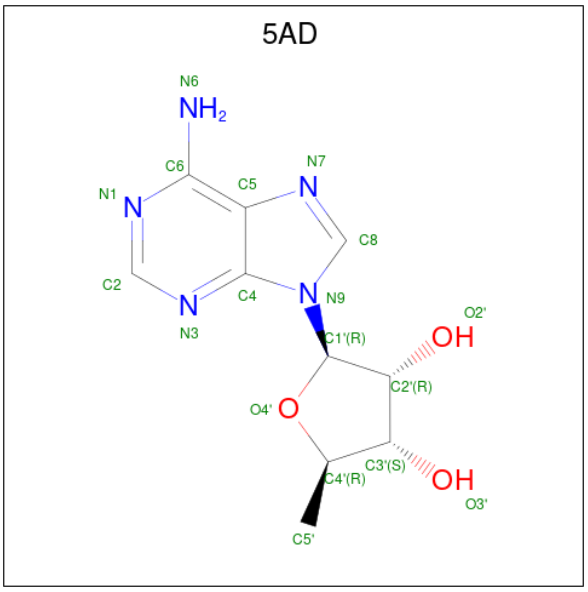
Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	73	Total	C	N	O	P	0	0
			1559	694	276	516	73		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	C	1	8	4	4	0

- Molecule 6 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



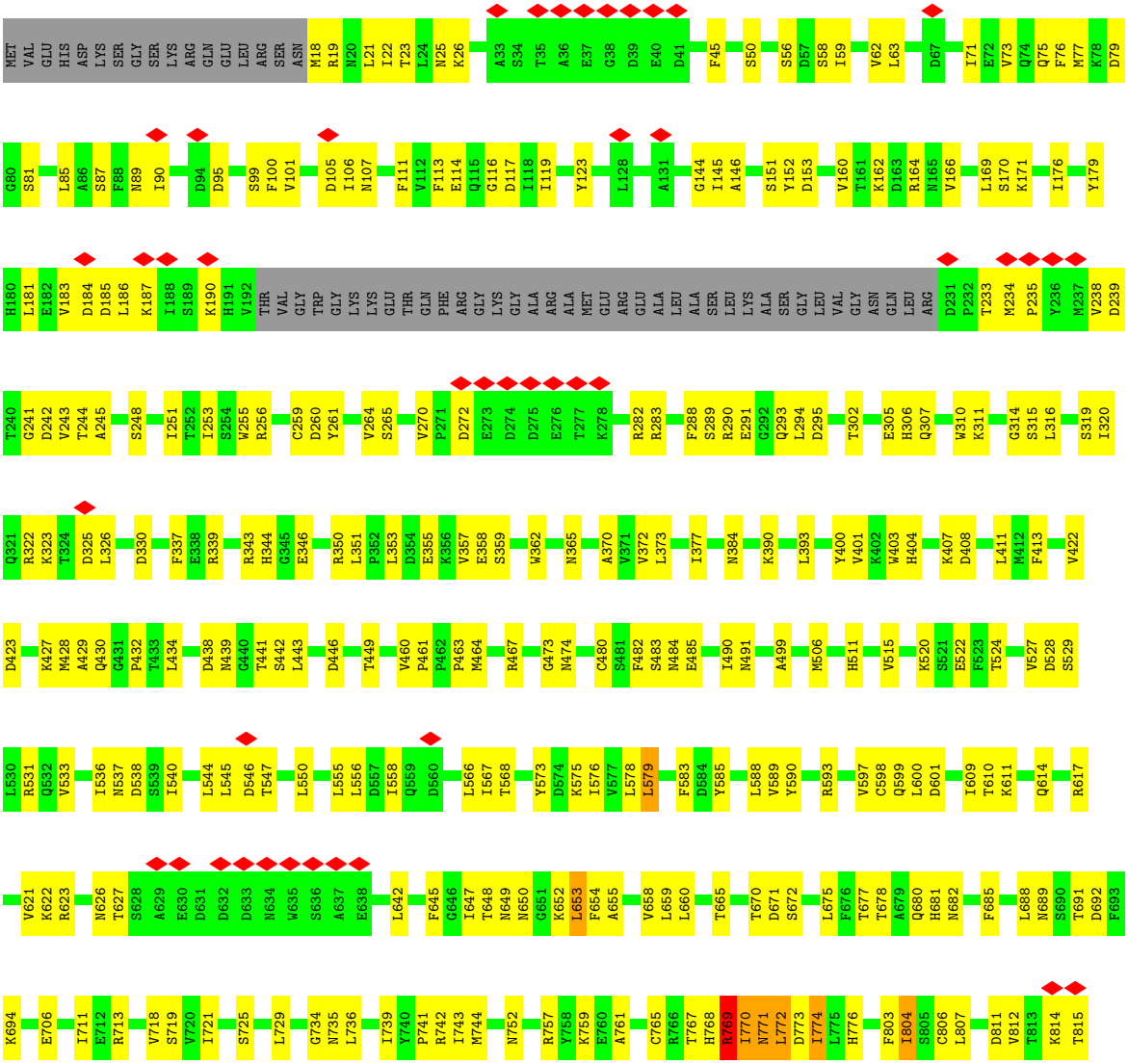
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	C	1	18	10	5	3	0

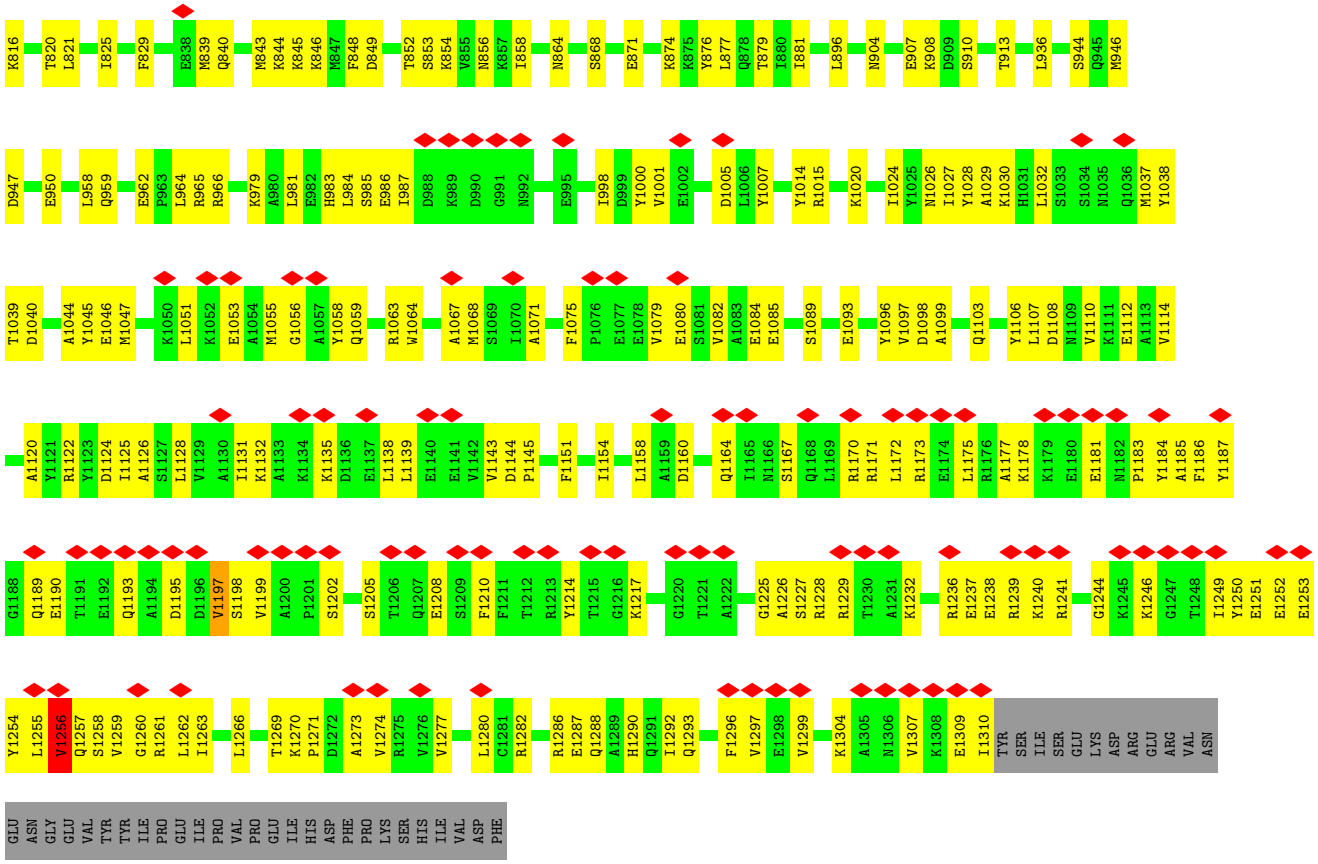
3 Residue-property plots (i)

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

- Molecule 1: Elongator complex protein 1

Chain A: 10% 57% 35% 7%

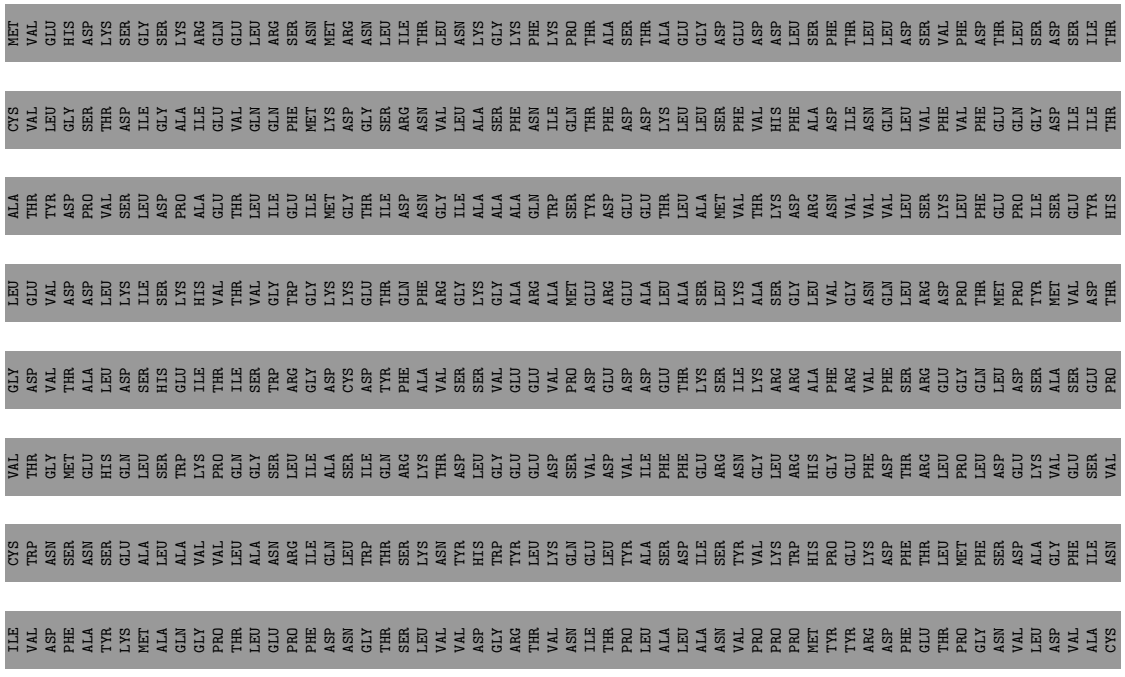


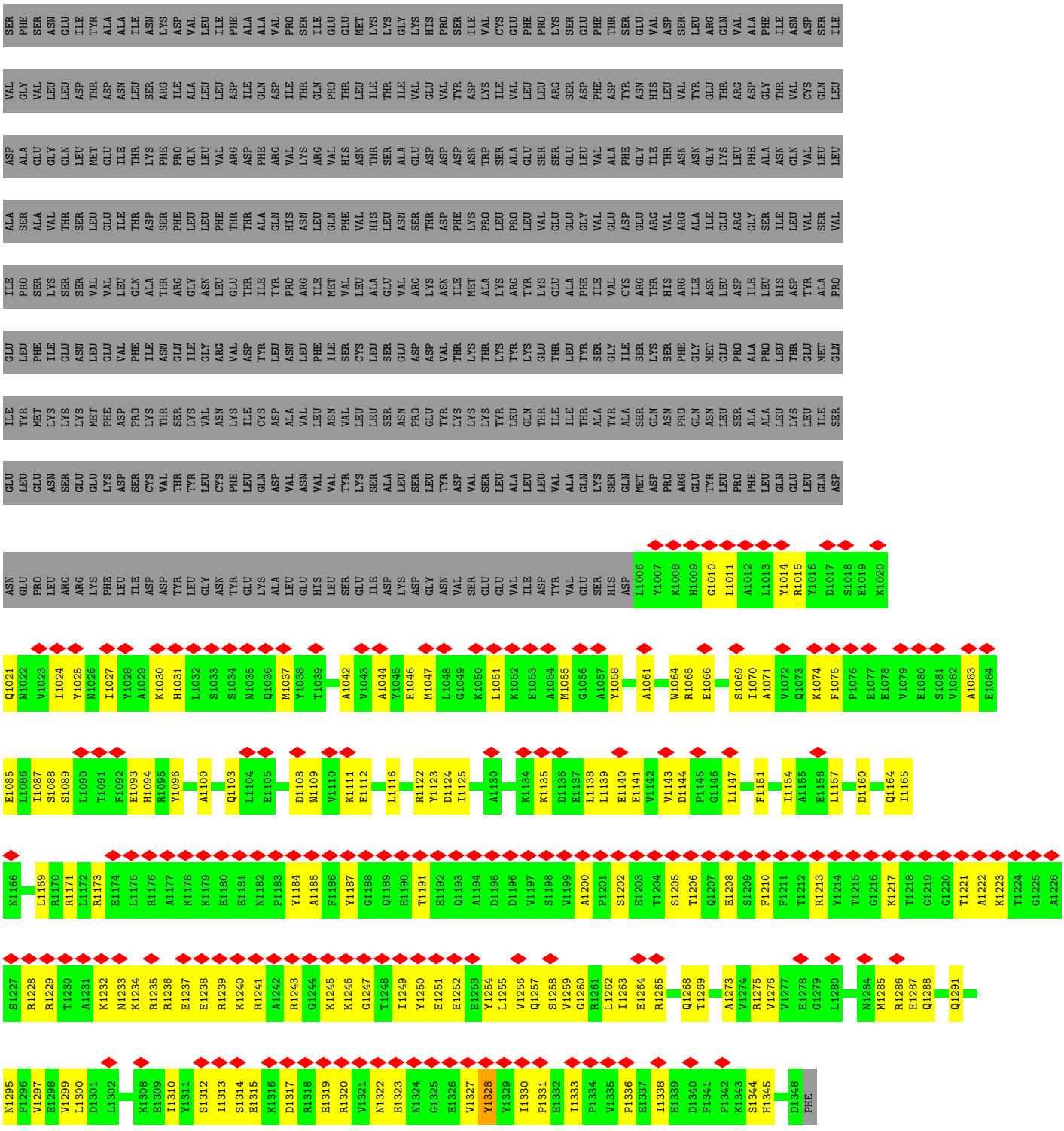


• Molecule 1: Elongator complex protein 1

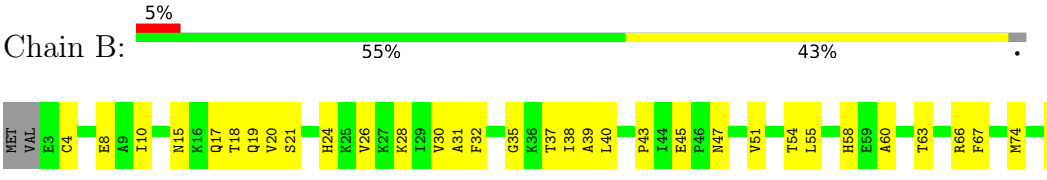
Chain D:

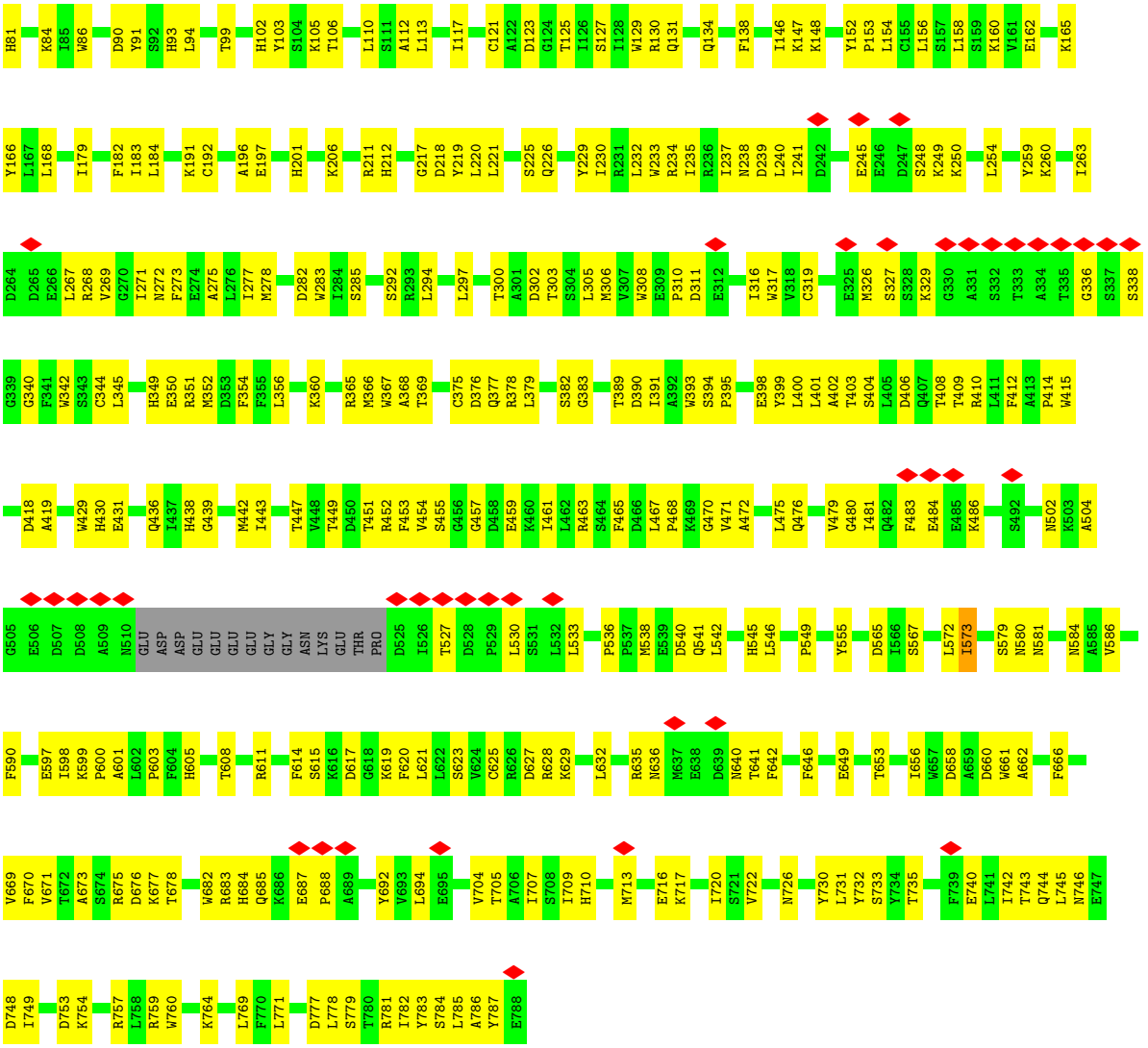






• Molecule 2: Elongator complex protein 2

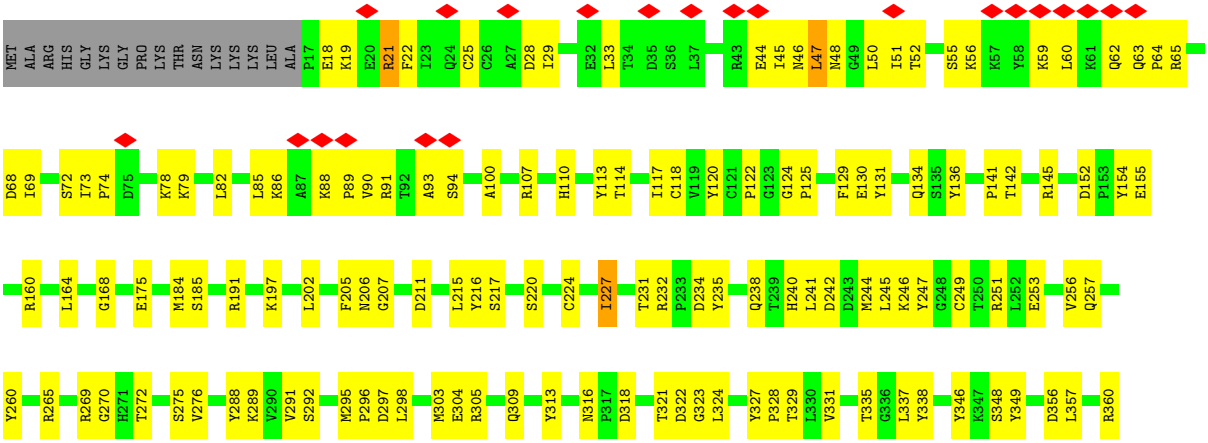


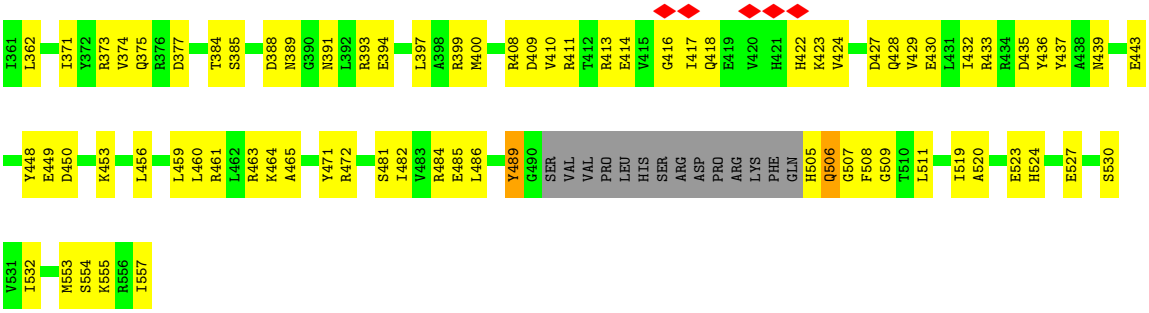


• Molecule 3: Elongator complex protein 3

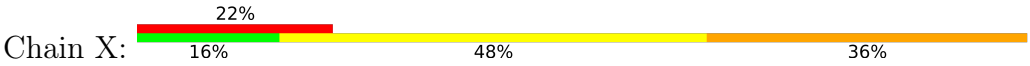
Chain C:



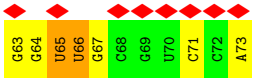




- Molecule 4: Alanine tRNA







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16809	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00855	Depositor
Map size (Å)	340.2, 340.2, 340.2	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 5AD

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	0.24	0/10196	0.45	3/13809 (0.0%)
1	D	0.15	0/2814	0.39	0/3787
2	B	0.25	0/6323	0.43	0/8566
3	C	0.33	0/4322	0.50	0/5835
4	X	0.17	0/1741	0.38	0/2713
All	All	0.25	0/25396	0.44	3/34710 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	ARG	CA-C-N	5.27	128.70	120.68
1	A	350	ARG	C-N-CA	5.27	128.70	120.68
1	A	804	ILE	N-CA-C	-5.25	107.24	111.91

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	10014	0	9909	361	0
1	D	2769	0	2757	119	0
2	B	6177	0	6083	243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4236	0	4241	183	0
4	X	1559	0	787	66	0
5	C	8	0	0	4	0
6	C	18	0	13	0	0
All	All	24781	0	23790	942	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 19.

All (942) 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:A:772:LEU:HD23	1:A:806:CYS:SG	1.94	1.07
1:A:772:LEU:CD2	1:A:806:CYS:SG	2.48	1.01
1:A:1183:PRO:HB2	1:A:1195:ASP:HB2	1.49	0.94
1:A:1139:LEU:HA	1:A:1143:VAL:HB	1.52	0.89
3:C:269:ARG:NH1	5:C:601:SF4:S4	2.47	0.88
2:B:713:MET:HE3	2:B:716:GLU:H	1.40	0.86
2:B:24:HIS:O	2:B:28:LYS:HA	1.78	0.84
1:A:772:LEU:HD21	1:A:803:PHE:HD1	1.42	0.82
2:B:709:ILE:HG12	2:B:720:ILE:HG22	1.63	0.80
3:C:413:ARG:NH1	3:C:449:GLU:OE2	2.15	0.79
1:A:1096:TYR:HB2	1:A:1120:ALA:HB2	1.64	0.79
2:B:605:HIS:ND1	2:B:625:CYS:SG	2.56	0.79
1:A:1250:TYR:HB2	1:A:1254:TYR:HE2	1.45	0.78
1:A:343:ARG:HH21	1:A:346:GLU:HG2	1.48	0.78
2:B:365:ARG:NH2	2:B:540:ASP:OD1	2.19	0.76
1:A:1056:GLY:HA2	1:A:1059:GLN:HE21	1.51	0.76
1:A:853:SER:OG	1:A:856:ASN:ND2	2.17	0.76
3:C:21:ARG:HG3	3:C:62:GLN:HE22	1.50	0.75
3:C:63:GLN:NE2	4:X:26:G:O2'	2.20	0.75
1:A:1286:ARG:HH22	1:D:1046:GLU:HG3	1.52	0.75
1:A:377:ILE:HG22	1:A:393:LEU:HB2	1.68	0.75
1:A:575:LYS:HB2	1:A:593:ARG:HD3	1.70	0.74
3:C:175:GLU:OE2	3:C:251:ARG:NH2	2.20	0.74
3:C:18:GLU:O	3:C:62:GLN:NE2	2.21	0.73
3:C:51:ILE:HG21	3:C:64:PRO:HG3	1.71	0.73
4:X:14:A:N1	4:X:15:G:N2	2.36	0.73
1:A:947:ASP:HB3	1:A:950:GLU:HG3	1.71	0.73
1:A:768:HIS:O	1:A:769:ARG:C	2.32	0.72
1:A:307:GLN:HG3	1:A:359:SER:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:MET:HE1	3:C:265:ARG:HG3	1.72	0.72
1:A:1037:MET:HE3	1:A:1039:THR:H	1.54	0.72
1:A:1128:LEU:HD22	1:D:1065:ARG:HD2	1.71	0.72
1:A:959:GLN:HA	1:A:966:ARG:HH21	1.53	0.72
1:A:741:PRO:HG2	1:A:744:MET:HG3	1.72	0.72
3:C:443:GLU:OE2	3:C:463:ARG:NH1	2.23	0.72
2:B:605:HIS:HE2	2:B:623:SER:HG	1.38	0.71
1:A:1258:SER:HA	1:A:1261:ARG:HE	1.56	0.71
4:X:65:U:O2'	4:X:66:U:OP1	2.06	0.71
3:C:373:ARG:NH1	3:C:377:ASP:OD2	2.22	0.71
1:A:184:ASP:HA	1:A:187:LYS:HE2	1.73	0.70
1:A:706:GLU:HB3	1:A:743:ILE:HD13	1.71	0.70
2:B:43:PRO:HB2	2:B:366:MET:HE1	1.74	0.70
2:B:598:ILE:HG12	2:B:600:PRO:HD2	1.73	0.70
1:A:1032:LEU:HD13	1:A:1040:ASP:HB3	1.74	0.70
4:X:55:U:N3	4:X:58:A:N7	2.39	0.70
3:C:356:ASP:O	3:C:360:ARG:HG3	1.92	0.69
3:C:227:ILE:HG23	3:C:249:CYS:HA	1.74	0.69
3:C:65:ARG:NH2	4:X:28:U:OP2	2.26	0.69
1:D:1051:LEU:HD12	1:D:1074:LYS:HD3	1.74	0.69
1:A:1181:GLU:OE1	1:A:1202:SER:OG	2.11	0.69
4:X:54:U:N3	4:X:58:A:C6	2.60	0.69
1:A:291:GLU:O	1:A:293:GLN:NE2	2.24	0.69
2:B:79:GLU:HA	2:B:106:THR:HG23	1.75	0.68
1:D:1291:GLN:O	1:D:1295:ASN:ND2	2.26	0.68
1:A:1063:ARG:HH12	1:D:1275:ARG:HH22	1.39	0.68
1:A:1114:VAL:HG13	1:A:1126:ALA:HB1	1.76	0.68
2:B:197:GLU:OE1	2:B:197:GLU:N	2.27	0.68
2:B:376:ASP:OD1	2:B:377:GLN:N	2.26	0.68
1:A:1068:MET:HE1	1:A:1106:TYR:HB3	1.74	0.68
1:D:1313:ILE:HD12	1:D:1320:ARG:HH12	1.58	0.68
1:A:536:ILE:HD11	1:A:588:LEU:HB2	1.75	0.68
3:C:313:TYR:HH	3:C:321:THR:HG1	1.42	0.67
2:B:245:GLU:O	2:B:250:LYS:NZ	2.23	0.67
3:C:89:PRO:HA	3:C:93:ALA:HB3	1.77	0.67
3:C:100:ALA:O	3:C:145:ARG:NH2	2.27	0.67
1:D:1259:VAL:HG21	1:D:1310:ILE:HG21	1.75	0.67
3:C:56:LYS:HD3	3:C:59:LYS:HA	1.74	0.67
3:C:155:GLU:N	3:C:155:GLU:OE1	2.27	0.67
3:C:292:SER:OG	3:C:313:TYR:OH	2.12	0.67
1:A:322:ARG:NH2	1:A:355:GLU:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:HB2	1:A:114:GLU:HB3	1.78	0.66
2:B:573:ILE:HG23	2:B:590:PHE:HB2	1.76	0.66
2:B:152:TYR:HB2	3:C:216:TYR:HE1	1.59	0.66
2:B:636:ASN:ND2	2:B:641:THR:OG1	2.28	0.66
1:D:1200:ALA:HB3	1:D:1205:SER:HB3	1.77	0.66
2:B:235:ILE:HG13	2:B:271:ILE:HD13	1.77	0.66
3:C:191:ARG:NH1	3:C:247:TYR:OH	2.28	0.66
3:C:211:ASP:N	3:C:211:ASP:OD1	2.29	0.66
1:A:253:ILE:HG12	1:A:264:VAL:HG22	1.78	0.66
3:C:110:HIS:CD2	5:C:601:SF4:S1	2.89	0.66
1:D:1085:GLU:O	1:D:1088:SER:OG	2.13	0.66
1:D:1229:ARG:HB3	1:D:1232:LYS:HB2	1.78	0.66
4:X:30:C:H2'	4:X:31:C:C6	2.31	0.65
4:X:31:C:N4	4:X:37:A:OP2	2.27	0.65
4:X:13:C:H2'	4:X:14:A:C8	2.32	0.65
4:X:32:C:O2	4:X:36:C:H5'	1.97	0.65
1:A:19:ARG:HG2	1:A:428:MET:HE1	1.78	0.65
1:D:1286:ARG:NH1	1:D:1287:GLU:OE2	2.30	0.65
2:B:620:PHE:HB3	2:B:632:LEU:HD11	1.78	0.64
1:A:752:ASN:HB3	1:A:761:ALA:HB2	1.79	0.64
1:A:962:GLU:HG2	1:A:965:ARG:H	1.62	0.64
1:A:1240:LYS:NZ	4:X:55:U:O4	2.30	0.64
2:B:311:ASP:N	2:B:316:ILE:O	2.19	0.64
3:C:184:MET:HA	3:C:184:MET:HE3	1.78	0.64
3:C:418:GLN:OE1	3:C:422:HIS:ND1	2.29	0.64
3:C:362:LEU:HB3	3:C:400:MET:HE1	1.79	0.64
2:B:391:ILE:H	2:B:757:ARG:HG2	1.61	0.64
1:A:1241:ARG:HH11	1:A:1249:ILE:HG21	1.62	0.64
2:B:483:PHE:O	2:B:486:LYS:NZ	2.31	0.64
1:A:1175:LEU:HG	1:A:1177:ALA:H	1.63	0.64
2:B:565:ASP:OD2	2:B:614:PHE:N	2.30	0.64
3:C:272:THR:O	3:C:275:SER:OG	2.15	0.64
3:C:142:THR:HG23	3:C:145:ARG:HH21	1.63	0.64
1:A:187:LYS:HA	1:A:190:LYS:HE3	1.79	0.64
1:A:1172:LEU:HD23	1:A:1252:GLU:HG2	1.80	0.64
2:B:152:TYR:HB2	3:C:216:TYR:CE1	2.33	0.63
3:C:21:ARG:NH1	3:C:55:SER:O	2.31	0.63
2:B:459:GLU:OE2	2:B:463:ARG:NH1	2.30	0.63
1:A:243:VAL:HB	1:A:282:ARG:HA	1.81	0.63
2:B:260:LYS:HA	2:B:269:VAL:O	1.98	0.63
2:B:660:ASP:OD1	2:B:661:TRP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:NH1	1:A:353:LEU:O	2.31	0.63
1:D:1143:VAL:O	1:D:1147:LEU:N	2.28	0.63
2:B:635:ARG:NH2	2:B:640:ASN:OD1	2.27	0.63
3:C:409:ASP:OD1	3:C:410:VAL:N	2.32	0.63
1:D:1066:GLU:OE2	1:D:1069:SER:OG	2.17	0.63
1:A:473:GLY:H	1:A:491:ASN:HD21	1.45	0.63
4:X:2:G:H2'	4:X:3:G:H8	1.64	0.63
2:B:21:SER:HB3	2:B:32:PHE:HB3	1.81	0.62
2:B:366:MET:HG2	2:B:378:ARG:HB2	1.81	0.62
3:C:443:GLU:OE1	3:C:484:ARG:NH2	2.32	0.62
1:A:1172:LEU:HD22	1:A:1189:GLN:HG2	1.81	0.62
1:A:544:LEU:HB2	1:A:579:LEU:HD13	1.81	0.62
4:X:31:C:O2	4:X:40:G:N2	2.32	0.62
3:C:481:SER:OG	3:C:524:HIS:ND1	2.32	0.62
2:B:349:HIS:HB2	2:B:354:PHE:HE2	1.64	0.62
2:B:468:PRO:HG2	2:B:471:VAL:HG12	1.82	0.62
2:B:710:HIS:HE2	2:B:769:LEU:HD22	1.64	0.62
3:C:130:GLU:HG2	3:C:131:TYR:CD2	2.34	0.62
1:A:316:LEU:HA	1:A:337:PHE:O	1.99	0.62
2:B:306:MET:HE2	2:B:308:TRP:CE2	2.34	0.62
1:D:1125:ILE:HD12	1:D:1125:ILE:H	1.64	0.62
1:A:105:ASP:OD1	1:A:106:ILE:N	2.33	0.61
1:A:1124:ASP:OD1	1:A:1124:ASP:N	2.33	0.61
3:C:117:ILE:HD11	5:C:601:SF4:S3	2.38	0.61
1:A:307:GLN:N	1:A:307:GLN:OE1	2.33	0.61
3:C:295:MET:HG2	3:C:327:TYR:O	2.00	0.61
2:B:382:SER:OG	2:B:383:GLY:N	2.29	0.61
2:B:731:LEU:HD21	2:B:760:TRP:HZ2	1.65	0.61
1:D:1187:TYR:HB3	1:D:1232:LYS:HD3	1.82	0.61
1:D:1291:GLN:OE1	1:D:1295:ASN:ND2	2.32	0.61
1:A:765:CYS:HB2	1:A:770:ILE:HG12	1.82	0.61
1:D:1184:TYR:H	1:D:1239:ARG:HB3	1.65	0.61
2:B:282:ASP:OD1	2:B:283:TRP:N	2.28	0.61
3:C:427:ASP:O	3:C:428:GLN:NE2	2.34	0.61
1:D:1027:ILE:HA	1:D:1030:LYS:HD3	1.83	0.61
3:C:45:ILE:HD11	3:C:50:LEU:HB2	1.83	0.61
1:A:144:GLY:HA3	1:A:162:LYS:HE3	1.83	0.60
2:B:329:LYS:NZ	2:B:338:SER:O	2.34	0.60
2:B:484:GLU:HB2	2:B:486:LYS:HG3	1.84	0.60
2:B:764:LYS:NZ	2:B:787:TYR:O	2.28	0.60
3:C:241:LEU:HG	3:C:288:TYR:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:LEU:O	1:A:1055:MET:HG3	2.02	0.60
2:B:673:ALA:HB1	2:B:704:VAL:HG13	1.83	0.60
2:B:694:LEU:HD23	2:B:694:LEU:H	1.66	0.60
3:C:29:ILE:HG13	3:C:51:ILE:HG12	1.82	0.60
1:A:876:TYR:O	1:A:879:THR:OG1	2.19	0.60
2:B:19:GLN:HG2	2:B:66:ARG:HH21	1.66	0.60
1:A:307:GLN:NE2	1:A:357:VAL:O	2.35	0.60
1:A:623:ARG:HG3	1:A:642:LEU:HD13	1.84	0.60
1:A:1228:ARG:HG3	1:A:1229:ARG:HE	1.67	0.60
2:B:45:GLU:HG2	2:B:47:ASN:H	1.67	0.59
1:D:1015:ARG:NH1	1:D:1025:TYR:OH	2.32	0.59
1:D:1111:LYS:NZ	1:D:1141:GLU:OE2	2.33	0.59
1:D:1165:ILE:HG21	1:D:1299:VAL:HG23	1.84	0.59
2:B:617:ASP:OD1	2:B:619:LYS:NZ	2.33	0.59
4:X:60:U:H5”	4:X:61:C:H5	1.66	0.59
1:A:351:LEU:HD13	1:A:373:LEU:HD21	1.83	0.59
1:A:626:ASN:OD1	1:A:627:THR:N	2.36	0.59
1:A:1014:TYR:HD2	1:A:1024:ILE:HD11	1.68	0.59
2:B:211:ARG:NH2	2:B:292:SER:O	2.35	0.59
2:B:230:ILE:HB	2:B:277:ILE:HB	1.84	0.59
4:X:23:C:H2’	4:X:24:G:C8	2.38	0.59
1:A:1269:THR:O	1:A:1273:ALA:N	2.28	0.59
1:A:772:LEU:CD2	1:A:803:PHE:HD1	2.14	0.59
1:A:772:LEU:HD21	1:A:803:PHE:CD1	2.32	0.59
1:A:1005:ASP:OD1	1:A:1007:TYR:OH	2.11	0.59
3:C:89:PRO:O	3:C:94:SER:N	2.32	0.59
1:D:1055:MET:HE2	1:D:1070:ILE:HG13	1.85	0.59
4:X:65:U:HO2’	4:X:66:U:P	2.25	0.59
2:B:597:GLU:O	2:B:599:LYS:NZ	2.36	0.59
1:D:1171:ARG:HD3	1:D:1250:TYR:HE1	1.67	0.59
3:C:322:ASP:OD2	3:C:484:ARG:NH1	2.31	0.58
3:C:251:ARG:HH11	3:C:289:LYS:NZ	2.01	0.58
2:B:342:TRP:HE1	2:B:360:LYS:HG3	1.68	0.58
3:C:245:LEU:HD21	3:C:532:ILE:HD11	1.85	0.58
1:D:1228:ARG:HB3	1:D:1319:GLU:HB2	1.86	0.58
1:A:463:PRO:HG2	3:C:437:TYR:HB3	1.84	0.58
1:A:692:ASP:O	1:A:694:LYS:NZ	2.37	0.58
1:A:773:ASP:O	1:A:774:ILE:C	2.46	0.58
1:A:1246:LYS:HE2	1:A:1254:TYR:CD1	2.39	0.58
2:B:662:ALA:HB3	2:B:669:VAL:HG13	1.86	0.58
4:X:48:C:O2’	4:X:50:U:OP2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:HA	2:B:340:GLY:HA3	1.86	0.58
3:C:324:LEU:HB3	3:C:371:ILE:HD13	1.85	0.58
3:C:422:HIS:HB3	3:C:424:VAL:HG23	1.86	0.58
2:B:749:ILE:O	2:B:783:TYR:OH	2.18	0.58
3:C:231:THR:OG1	3:C:232:ARG:N	2.36	0.58
1:D:1221:THR:OG1	1:D:1222:ALA:N	2.37	0.58
1:A:1236:ARG:HB3	1:A:1239:ARG:HH22	1.67	0.57
3:C:450:ASP:OD2	3:C:453:LYS:NZ	2.37	0.57
1:D:1269:THR:O	1:D:1273:ALA:N	2.24	0.57
1:A:319:SER:OG	1:A:320:ILE:N	2.37	0.57
1:A:678:THR:OG1	1:A:682:ASN:OD1	2.21	0.57
1:A:1256:VAL:HG12	1:A:1257:GLN:H	1.69	0.57
2:B:389:THR:OG1	2:B:443:ILE:O	2.22	0.57
3:C:110:HIS:CE1	3:C:117:ILE:HD12	2.39	0.57
1:A:652:LYS:HG2	1:A:659:LEU:HD11	1.87	0.57
1:A:1135:LYS:HB3	1:A:1138:LEU:HD13	1.87	0.57
3:C:46:ASN:O	3:C:48:ASN:N	2.37	0.57
1:A:849:ASP:HB3	1:A:852:THR:HG22	1.85	0.57
1:A:985:SER:OG	1:A:986:GLU:OE2	2.22	0.57
3:C:120:TYR:CE1	3:C:295:MET:HE1	2.39	0.57
3:C:124:GLY:HA2	3:C:134:GLN:HA	1.86	0.57
3:C:296:PRO:HD2	3:C:328:PRO:HA	1.86	0.57
1:A:1167:SER:O	1:A:1171:ARG:NH1	2.37	0.57
2:B:779:SER:OG	2:B:781:ARG:NH1	2.37	0.57
3:C:113:TYR:OH	3:C:270:GLY:O	2.23	0.57
3:C:388:ASP:OD1	3:C:388:ASP:N	2.33	0.57
2:B:201:HIS:CG	2:B:225:SER:HG	2.22	0.57
2:B:671:VAL:HG13	2:B:707:ILE:HD12	1.87	0.57
2:B:414:PRO:HA	2:B:429:TRP:HA	1.87	0.56
2:B:586:VAL:HG12	2:B:603:PRO:HB3	1.85	0.56
1:A:164:ARG:HG2	1:A:181:LEU:HD23	1.87	0.56
1:A:555:LEU:HB2	1:A:567:ILE:HB	1.86	0.56
1:A:811:ASP:OD1	1:A:812:VAL:N	2.36	0.56
1:A:1020:LYS:O	1:A:1024:ILE:HG13	2.06	0.56
1:A:1024:ILE:HA	1:A:1027:ILE:HG12	1.87	0.56
2:B:4:CYS:HB3	2:B:786:ALA:HB3	1.87	0.56
2:B:233:TRP:HB3	2:B:271:ILE:HD11	1.87	0.56
2:B:769:LEU:HD12	2:B:785:LEU:HD23	1.87	0.56
1:D:1140:GLU:HA	1:D:1144:ASP:HB2	1.88	0.56
1:D:1249:ILE:HD13	1:D:1323:GLU:HA	1.87	0.56
1:A:325:ASP:OD1	1:A:326:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:HIS:HD2	1:A:407:LYS:HB3	1.70	0.56
1:A:1205:SER:HA	1:A:1251:GLU:HG3	1.86	0.56
3:C:22:PHE:HE1	3:C:64:PRO:HB3	1.69	0.56
4:X:15:G:H4'	4:X:16:U:O5'	2.06	0.56
1:A:672:SER:O	1:A:672:SER:OG	2.21	0.56
1:D:1344:SER:OG	1:D:1345:HIS:N	2.38	0.56
1:D:1124:ASP:N	1:D:1124:ASP:OD1	2.36	0.56
1:D:1138:LEU:HA	1:D:1141:GLU:HB3	1.86	0.56
1:A:56:SER:HB2	1:A:77:MET:HE1	1.88	0.56
1:A:772:LEU:HD21	1:A:803:PHE:HA	1.88	0.56
3:C:418:GLN:O	3:C:423:LYS:N	2.38	0.56
1:D:1123:TYR:HE2	1:D:1276:VAL:HG22	1.70	0.56
2:B:67:PHE:CD1	2:B:74:MET:HB2	2.41	0.56
1:D:1164:GLN:HB3	1:D:1262:LEU:HD11	1.88	0.56
2:B:248:SER:O	2:B:250:LYS:NZ	2.34	0.55
1:A:461:PRO:HA	1:A:736:LEU:HD12	1.87	0.55
1:A:1241:ARG:HB2	4:X:53:G:H5"	1.87	0.55
2:B:60:ALA:N	2:B:80:ASP:OD2	2.37	0.55
3:C:465:ALA:HB2	3:C:482:ILE:HD11	1.88	0.55
4:X:54:U:C2	4:X:58:A:N6	2.74	0.55
4:X:63:G:H2'	4:X:64:G:C8	2.41	0.55
1:A:295:ASP:OD2	1:A:339:ARG:NH1	2.39	0.55
1:A:864:ASN:O	1:A:868:SER:OG	2.24	0.55
2:B:55:LEU:HD11	2:B:94:LEU:HD13	1.88	0.55
2:B:130:ARG:CZ	2:B:184:LEU:HD21	2.36	0.55
3:C:185:SER:O	3:C:185:SER:OG	2.15	0.55
1:A:241:GLY:HA2	1:A:302:THR:HG22	1.89	0.55
1:A:430:GLN:HE22	1:A:719:SER:HB2	1.72	0.55
1:A:1307:VAL:O	1:A:1310:ILE:HG12	2.06	0.55
1:A:259:CYS:O	1:A:290:ARG:NH1	2.40	0.55
2:B:504:ALA:HA	2:B:549:PRO:HB3	1.89	0.55
3:C:251:ARG:HH11	3:C:289:LYS:HZ1	1.54	0.55
1:A:401:VAL:HG22	1:A:413:PHE:HB3	1.89	0.55
1:A:839:MET:SD	1:A:840:GLN:N	2.80	0.55
1:A:959:GLN:OE1	1:A:966:ARG:NH2	2.40	0.55
3:C:21:ARG:HG3	3:C:62:GLN:NE2	2.21	0.55
1:A:626:ASN:HB2	1:A:691:THR:HG23	1.88	0.55
2:B:165:LYS:HG2	2:B:183:ILE:HG22	1.88	0.55
1:A:58:SER:HB2	1:A:77:MET:HA	1.89	0.55
1:A:482:PHE:HB2	1:A:585:TYR:HD2	1.72	0.55
2:B:220:LEU:HD22	2:B:232:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:ARG:C	2:B:677:LYS:H	2.15	0.55
4:X:7:A:O2'	4:X:8:U:OP1	2.23	0.55
1:A:234:MET:HB3	1:A:235:PRO:HD3	1.89	0.54
1:A:1058:TYR:HB3	1:A:1067:ALA:HB2	1.87	0.54
2:B:541:GLN:HA	2:B:545:HIS:CE1	2.41	0.54
1:D:1213:ARG:HH12	1:D:1258:SER:HA	1.72	0.54
2:B:777:ASP:C	2:B:778:LEU:HD23	2.31	0.54
1:A:767:THR:O	3:C:448:TYR:OH	2.20	0.54
3:C:409:ASP:OD1	3:C:411:ARG:N	2.39	0.54
1:A:979:LYS:O	1:A:983:HIS:ND1	2.39	0.54
3:C:129:PHE:HB3	3:C:131:TYR:CE1	2.42	0.54
3:C:433:ARG:NH2	3:C:523:GLU:OE2	2.29	0.54
1:A:306:HIS:NE2	1:A:358:GLU:O	2.39	0.54
1:A:384:ASN:HD21	1:A:734:GLY:HA3	1.73	0.54
1:A:1189:GLN:H	1:A:1255:LEU:HA	1.72	0.54
1:A:75:GLN:NE2	1:A:77:MET:SD	2.71	0.54
1:A:589:VAL:HG11	1:A:621:VAL:HG11	1.88	0.54
1:A:590:TYR:CZ	1:A:598:CYS:HB3	2.43	0.54
2:B:461:ILE:HG22	2:B:555:TYR:HA	1.89	0.54
1:A:146:ALA:HB3	1:A:160:VAL:HG13	1.88	0.54
1:A:432:PRO:HD2	1:A:484:ASN:HD21	1.73	0.54
1:A:742:ARG:NE	3:C:430:GLU:OE2	2.35	0.54
1:A:1250:TYR:HD2	1:A:1254:TYR:CD2	2.26	0.54
3:C:328:PRO:HD2	3:C:375:GLN:HA	1.90	0.54
2:B:297:LEU:HD11	2:B:305:LEU:HD21	1.89	0.54
3:C:331:VAL:HG23	3:C:337:LEU:HB3	1.89	0.53
1:D:1243:ARG:HD3	1:D:1249:ILE:HG13	1.90	0.53
1:A:675:LEU:HD11	1:A:685:PHE:CE2	2.44	0.53
2:B:131:GLN:HA	2:B:138:PHE:HA	1.91	0.53
3:C:348:SER:OG	3:C:349:TYR:N	2.41	0.53
1:A:599:GLN:HB2	1:A:609:ILE:HD11	1.90	0.53
2:B:717:LYS:HB3	2:B:735:THR:HG22	1.91	0.53
3:C:141:PRO:HG2	4:X:33:U:H4'	1.90	0.53
1:A:550:LEU:HD13	1:A:573:TYR:HA	1.89	0.53
1:A:1259:VAL:HG12	1:A:1263:ILE:HG13	1.90	0.53
1:A:1282:ARG:O	1:A:1282:ARG:NH1	2.42	0.53
2:B:17:GLN:NE2	3:C:206:ASN:O	2.32	0.53
2:B:685:GLN:HE22	2:B:688:PRO:HD2	1.74	0.53
3:C:389:ASN:OD1	3:C:391:ASN:N	2.41	0.53
1:A:480:CYS:SG	1:A:484:ASN:HA	2.49	0.53
2:B:17:GLN:HG3	2:B:63:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PHE:HD1	2:B:431:GLU:HA	1.72	0.53
2:B:687:GLU:HB3	2:B:688:PRO:HD3	1.89	0.53
1:D:1157:LEU:HD21	1:D:1265:ARG:NH2	2.24	0.53
2:B:720:ILE:HG13	2:B:732:TYR:HB2	1.91	0.53
3:C:69:ILE:O	3:C:72:SER:OG	2.23	0.53
3:C:107:ARG:HG2	3:C:125:PRO:HG3	1.91	0.53
3:C:152:ASP:OD1	3:C:154:TYR:N	2.42	0.53
4:X:13:C:H2'	4:X:14:A:H8	1.73	0.53
4:X:48:C:H41	4:X:60:U:H1'	1.74	0.53
1:A:272:ASP:OD1	1:A:272:ASP:N	2.42	0.53
1:A:365:ASN:ND2	1:A:408:ASP:OD2	2.42	0.53
1:A:653:LEU:HD11	1:A:660:LEU:HD12	1.89	0.53
1:A:681:HIS:CE1	1:A:713:ARG:HG3	2.44	0.53
1:D:1171:ARG:NH1	1:D:1245:LYS:O	2.41	0.53
1:A:153:ASP:OD2	1:A:290:ARG:NH2	2.29	0.53
1:A:490:ILE:HD11	1:A:533:VAL:HB	1.91	0.53
1:A:614:GLN:OE1	1:A:650:ASN:ND2	2.42	0.53
1:A:772:LEU:HD11	1:A:803:PHE:CD1	2.44	0.53
2:B:37:THR:OG1	2:B:38:ILE:N	2.41	0.53
3:C:22:PHE:CE1	3:C:64:PRO:HB3	2.43	0.53
3:C:25:CYS:HA	3:C:28:ASP:OD2	2.09	0.53
3:C:505:HIS:CG	3:C:506:GLN:H	2.27	0.53
3:C:520:ALA:HA	3:C:524:HIS:HB2	1.89	0.52
1:D:1191:THR:H	1:D:1206:THR:HG21	1.73	0.52
2:B:134:GLN:H	2:B:134:GLN:CD	2.16	0.52
3:C:471:TYR:CD1	3:C:471:TYR:C	2.87	0.52
1:D:1235:ARG:HH12	1:D:1320:ARG:HB2	1.73	0.52
1:A:186:LEU:HD21	1:A:282:ARG:HH21	1.75	0.52
1:A:536:ILE:HB	1:A:540:ILE:HB	1.92	0.52
2:B:352:MET:HE3	2:B:352:MET:HA	1.90	0.52
3:C:73:ILE:HB	3:C:78:LYS:HG3	1.91	0.52
3:C:141:PRO:O	3:C:145:ARG:HG3	2.09	0.52
1:D:1320:ARG:HB3	1:D:1322:ASN:OD1	2.09	0.52
2:B:404:SER:OG	2:B:406:ASP:O	2.27	0.52
3:C:256:VAL:HG22	3:C:276:VAL:HG11	1.91	0.52
1:A:244:THR:OG1	1:A:245:ALA:N	2.42	0.52
2:B:8:GLU:OE1	2:B:784:SER:OG	2.26	0.52
3:C:19:LYS:HA	3:C:62:GLN:HE21	1.74	0.52
3:C:232:ARG:NH2	3:C:269:ARG:O	2.42	0.52
1:A:1183:PRO:HG3	1:A:1198:SER:HA	1.91	0.52
2:B:90:ASP:HB3	2:B:93:HIS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:ARG:HH21	3:C:60:LEU:HB2	1.73	0.52
1:D:1058:TYR:HE2	1:D:1066:GLU:HB3	1.74	0.52
1:A:742:ARG:HE	3:C:430:GLU:CD	2.17	0.52
4:X:23:C:H2'	4:X:24:G:H8	1.73	0.52
1:A:260:ASP:OD1	1:A:260:ASP:N	2.34	0.52
1:A:531:ARG:HD3	1:A:546:ASP:HB2	1.91	0.52
1:A:981:LEU:HD21	1:A:1000:TYR:HB3	1.90	0.52
1:A:1246:LYS:HA	1:A:1254:TYR:CE2	2.44	0.52
2:B:628:ARG:HA	2:B:656:ILE:HG13	1.92	0.52
1:D:1108:ASP:OD1	1:D:1108:ASP:N	2.36	0.52
1:D:1171:ARG:HD3	1:D:1250:TYR:CE1	2.45	0.52
1:D:1236:ARG:CZ	1:D:1251:GLU:HB3	2.40	0.52
1:A:853:SER:HG	1:A:856:ASN:ND2	2.08	0.52
1:A:1250:TYR:HB2	1:A:1254:TYR:CE2	2.36	0.52
1:A:21:LEU:HB2	1:A:390:LYS:HB3	1.92	0.52
2:B:19:GLN:HE21	2:B:66:ARG:CZ	2.22	0.52
3:C:508:PHE:O	3:C:509:GLY:C	2.53	0.52
4:X:31:C:H2'	4:X:32:C:H5'	1.90	0.52
1:A:183:VAL:HG13	1:A:270:VAL:HG12	1.91	0.51
1:A:370:ALA:HB2	1:A:403:TRP:HZ2	1.76	0.51
4:X:54:U:N3	4:X:58:A:N6	2.59	0.51
1:D:1083:ALA:O	1:D:1087:ILE:HG13	2.10	0.51
1:A:22:ILE:HG21	1:A:427:LYS:HD3	1.93	0.51
1:A:1026:ASN:O	1:A:1030:LYS:HG2	2.10	0.51
1:A:1198:SER:HB2	1:A:1227:SER:N	2.26	0.51
4:X:27:C:H2'	4:X:28:U:C6	2.45	0.51
1:A:1089:SER:O	1:A:1093:GLU:N	2.36	0.51
1:A:1184:TYR:HB3	1:A:1193:GLN:HB3	1.92	0.51
2:B:356:LEU:HD13	2:B:366:MET:SD	2.50	0.51
2:B:394:SER:HB3	2:B:399:TYR:CD1	2.45	0.51
1:D:1169:LEU:HD12	1:D:1246:LYS:HE3	1.92	0.51
1:D:1256:VAL:HA	1:D:1259:VAL:HG22	1.93	0.51
2:B:21:SER:HB2	2:B:345:LEU:HD21	1.92	0.51
2:B:218:ASP:OD2	2:B:234:ARG:NH2	2.43	0.51
2:B:300:THR:OG1	2:B:302:ASP:OD1	2.18	0.51
1:D:1235:ARG:NH1	1:D:1237:GLU:OE2	2.44	0.51
1:D:1259:VAL:HG11	1:D:1310:ILE:HD13	1.92	0.51
4:X:29:U:H2'	4:X:30:C:C6	2.45	0.51
2:B:360:LYS:NZ	3:C:155:GLU:OE2	2.38	0.51
1:A:1097:VAL:HG13	1:A:1098:ASP:H	1.75	0.51
1:A:1158:LEU:HD11	1:A:1296:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:LEU:HB3	2:B:749:ILE:HG13	1.92	0.51
2:B:408:THR:HG21	2:B:410:ARG:HH21	1.74	0.50
2:B:658:ASP:CG	2:B:757:ARG:HH22	2.18	0.50
2:B:103:TYR:HB3	2:B:121:CYS:SG	2.51	0.50
3:C:117:ILE:HD12	3:C:118:CYS:H	1.76	0.50
3:C:234:ASP:OD1	3:C:235:TYR:N	2.45	0.50
3:C:377:ASP:HB2	4:X:34:U:O2	2.11	0.50
1:D:1252:GLU:O	1:D:1256:VAL:HG22	2.11	0.50
2:B:45:GLU:HG2	2:B:47:ASN:N	2.26	0.50
1:D:1229:ARG:NH2	1:D:1317:ASP:OD2	2.45	0.50
1:D:1240:LYS:O	1:D:1243:ARG:NE	2.29	0.50
3:C:414:GLU:OE1	3:C:417:ILE:N	2.30	0.50
3:C:432:ILE:HD13	3:C:449:GLU:HB3	1.93	0.50
2:B:398:GLU:HB3	2:B:481:ILE:HD11	1.93	0.50
1:D:1208:GLU:HG2	1:D:1210:PHE:H	1.76	0.50
4:X:14:A:N6	4:X:15:G:H21	2.10	0.50
4:X:15:G:N1	4:X:21:A:N1	2.60	0.50
1:A:815:THR:OG1	1:A:816:LYS:NZ	2.39	0.50
1:A:256:ARG:NH2	1:A:260:ASP:OD2	2.45	0.50
2:B:707:ILE:HG22	2:B:722:VAL:HG12	1.94	0.50
1:A:735:ASN:HB2	3:C:436:TYR:HB3	1.94	0.50
1:A:45:PHE:HB3	1:A:63:LEU:HD12	1.94	0.50
2:B:403:THR:OG1	2:B:442:MET:HB3	2.11	0.50
3:C:408:ARG:HA	3:C:413:ARG:HD3	1.94	0.50
1:A:244:THR:HG21	1:A:305:GLU:HG2	1.94	0.49
3:C:238:GLN:HG2	3:C:471:TYR:CE2	2.47	0.49
1:D:1154:ILE:HG21	1:D:1276:VAL:HG11	1.94	0.49
1:D:1327:VAL:HG23	1:D:1328:TYR:H	1.77	0.49
1:A:50:SER:OG	1:A:400:TYR:OH	2.19	0.49
1:A:446:ASP:HB3	1:A:449:THR:HB	1.94	0.49
1:A:694:LYS:H	1:A:825:ILE:HD11	1.77	0.49
2:B:465:PHE:HE2	2:B:502:ASN:HB2	1.77	0.49
2:B:579:SER:HB2	2:B:584:ASN:HB2	1.94	0.49
1:D:1160:ASP:O	1:D:1164:GLN:HG2	2.12	0.49
4:X:43:G:H2'	4:X:44:A:C8	2.47	0.49
1:A:871:GLU:HA	1:A:874:LYS:HD2	1.94	0.49
1:A:1071:ALA:O	1:A:1075:PHE:N	2.45	0.49
2:B:294:LEU:HD23	2:B:310:PRO:HG3	1.94	0.49
1:D:1139:LEU:HA	1:D:1143:VAL:HG12	1.94	0.49
1:A:682:ASN:OD1	1:A:682:ASN:N	2.43	0.49
2:B:90:ASP:OD1	2:B:91:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:GLU:OE2	4:X:56:C:H5”	2.12	0.49
2:B:74:MET:HE2	2:B:86:TRP:HB2	1.95	0.49
3:C:118:CYS:CB	5:C:601:SF4:S4	2.97	0.49
1:D:1191:THR:HG21	1:D:1257:GLN:NE2	2.28	0.49
4:X:14:A:H61	4:X:15:G:H21	1.59	0.49
2:B:467:LEU:HG	2:B:472:ALA:HB2	1.95	0.49
1:D:1064:TRP:H	1:D:1064:TRP:CD1	2.29	0.49
1:A:843:MET:HA	1:A:846:LYS:HG2	1.95	0.49
1:A:1286:ARG:NH2	1:D:1046:GLU:HG3	2.24	0.49
3:C:292:SER:HG	3:C:313:TYR:HH	1.57	0.49
1:A:160:VAL:HG11	1:A:251:ILE:HG21	1.95	0.48
1:A:1280:LEU:HD21	1:A:1288:GLN:HG3	1.95	0.48
2:B:350:GLU:O	2:B:351:ARG:HD3	2.13	0.48
2:B:415:TRP:CE2	2:B:536:PRO:HD3	2.47	0.48
2:B:598:ILE:HD11	2:B:641:THR:HA	1.94	0.48
1:D:1135:LYS:HG3	1:D:1138:LEU:HB2	1.95	0.48
4:X:31:C:H3’	4:X:32:C:H6	1.77	0.48
1:A:79:ASP:OD1	1:A:81:SER:OG	2.19	0.48
1:A:353:LEU:HD12	1:A:353:LEU:H	1.77	0.48
1:A:771:ASN:O	1:A:773:ASP:N	2.46	0.48
1:A:1197:VAL:HG22	1:A:1198:SER:H	1.78	0.48
2:B:160:LYS:HG3	2:B:166:TYR:CZ	2.48	0.48
2:B:259:TYR:HB2	2:B:271:ILE:HG23	1.95	0.48
2:B:418:ASP:OD1	2:B:419:ALA:N	2.46	0.48
2:B:628:ARG:NH1	2:B:653:THR:O	2.46	0.48
2:B:733:SER:O	2:B:740:GLU:N	2.30	0.48
1:D:1233:ASN:OD1	1:D:1233:ASN:N	2.41	0.48
1:A:583:PHE:CD2	1:A:622:LYS:HD3	2.47	0.48
1:A:1154:ILE:HG13	1:A:1292:ILE:HG12	1.94	0.48
1:A:1186:PHE:HA	1:A:1229:ARG:HA	1.95	0.48
1:A:1256:VAL:C	1:A:1258:SER:H	2.21	0.48
1:A:311:LYS:HB2	1:A:362:TRP:CE2	2.48	0.48
1:A:323:LYS:O	1:A:330:ASP:HA	2.13	0.48
1:A:665:THR:OG1	1:A:677:THR:OG1	2.10	0.48
2:B:81:HIS:N	2:B:81:HIS:CD2	2.80	0.48
2:B:221:LEU:HB3	2:B:235:ILE:HD11	1.95	0.48
1:A:62:VAL:HG13	1:A:73:VAL:HG12	1.96	0.48
2:B:567:SER:OG	2:B:572:LEU:O	2.29	0.48
1:D:1229:ARG:NH2	1:D:1237:GLU:OE1	2.43	0.48
1:A:1189:GLN:NE2	1:A:1254:TYR:O	2.47	0.48
1:A:1190:GLU:HB3	1:A:1307:VAL:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:LYS:HE2	4:X:48:C:H5	1.79	0.48
2:B:326:MET:HE3	2:B:327:SER:N	2.27	0.48
3:C:25:CYS:SG	3:C:51:ILE:HG23	2.54	0.48
1:D:1263:ILE:HG13	1:D:1264:GLU:N	2.28	0.48
1:A:848:PHE:HE1	1:A:853:SER:HB3	1.78	0.48
2:B:162:GLU:OE1	2:B:165:LYS:NZ	2.35	0.48
2:B:394:SER:HB3	2:B:399:TYR:CE1	2.48	0.48
4:X:54:U:C4	4:X:58:A:C6	3.02	0.48
1:A:1175:LEU:HG	1:A:1177:ALA:N	2.29	0.48
2:B:30:VAL:HG21	2:B:356:LEU:HD23	1.95	0.48
3:C:205:PHE:CZ	3:C:207:GLY:HA3	2.48	0.48
1:A:537:ASN:N	1:A:585:TYR:O	2.47	0.48
1:A:896:LEU:HD22	1:A:936:LEU:HD21	1.96	0.48
2:B:15:ASN:HB2	2:B:20:VAL:HG11	1.96	0.48
3:C:260:TYR:CZ	3:C:309:GLN:HB3	2.49	0.48
1:D:1058:TYR:CE2	1:D:1066:GLU:HB3	2.49	0.48
1:D:1314:SER:OG	1:D:1315:GLU:N	2.47	0.48
1:A:467:ARG:HB2	1:A:506:MET:HE1	1.94	0.48
2:B:35:GLY:HA3	2:B:778:LEU:HD21	1.96	0.48
2:B:277:ILE:HD12	2:B:317:TRP:HB2	1.95	0.48
2:B:352:MET:HE2	2:B:368:ALA:HB1	1.96	0.48
3:C:331:VAL:HG12	3:C:385:SER:O	2.14	0.48
1:A:358:GLU:HB2	1:A:372:VAL:HG23	1.94	0.47
1:A:807:LEU:HD21	1:A:858:ILE:HD13	1.95	0.47
1:A:1122:ARG:NH2	1:A:1124:ASP:OD2	2.46	0.47
2:B:586:VAL:HB	2:B:601:ALA:HB1	1.96	0.47
3:C:65:ARG:N	3:C:68:ASP:OD2	2.47	0.47
1:A:89:ASN:C	1:A:90:ILE:HD13	2.39	0.47
1:A:169:LEU:HA	1:A:176:ILE:H	1.78	0.47
3:C:82:LEU:HD21	3:C:168:GLY:HA2	1.96	0.47
1:D:1058:TYR:HA	1:D:1061:ALA:HB3	1.95	0.47
1:D:1217:LYS:HG2	1:D:1257:GLN:HA	1.97	0.47
1:D:1243:ARG:NH1	1:D:1249:ILE:O	2.47	0.47
2:B:77:ALA:HB2	2:B:110:LEU:HD22	1.96	0.47
2:B:454:VAL:HG11	2:B:573:ILE:HD12	1.96	0.47
3:C:461:ARG:NE	3:C:485:GLU:OE1	2.46	0.47
1:D:1312:SER:O	1:D:1330:ILE:HD11	2.14	0.47
1:A:434:LEU:O	1:A:438:ASP:HB3	2.15	0.47
1:A:681:HIS:CE1	1:A:713:ARG:HH11	2.32	0.47
2:B:580:ASN:OD1	2:B:580:ASN:N	2.46	0.47
3:C:356:ASP:OD2	3:C:399:ARG:NH2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HB2	1:A:117:ASP:HB2	1.95	0.47
1:A:538:ASP:C	1:A:558:ILE:HD11	2.40	0.47
1:A:1027:ILE:HG13	1:A:1028:TYR:N	2.29	0.47
1:A:1210:PHE:CG	1:A:1210:PHE:O	2.68	0.47
2:B:18:THR:OG1	2:B:285:SER:O	2.33	0.47
2:B:666:PHE:O	2:B:683:ARG:NH2	2.46	0.47
3:C:74:PRO:O	3:C:78:LYS:N	2.41	0.47
1:D:1109:ASN:ND2	1:D:1112:GLU:OE2	2.47	0.47
1:A:675:LEU:HD11	1:A:685:PHE:CD2	2.50	0.47
1:A:711:ILE:HD11	1:A:739:ILE:HD13	1.95	0.47
1:A:910:SER:O	1:A:913:THR:OG1	2.31	0.47
1:A:1028:TYR:CZ	1:A:1032:LEU:HD11	2.50	0.47
2:B:127:SER:HB2	2:B:129:TRP:HE1	1.79	0.47
2:B:153:PRO:O	3:C:216:TYR:OH	2.26	0.47
2:B:263:ILE:HD12	2:B:267:LEU:HD23	1.97	0.47
2:B:581:ASN:N	2:B:581:ASN:OD1	2.48	0.47
3:C:59:LYS:HB2	3:C:59:LYS:HE3	1.66	0.47
2:B:753:ASP:HB2	2:B:777:ASP:HB2	1.97	0.47
1:A:439:ASN:OD1	1:A:441:THR:OG1	2.33	0.47
1:A:908:LYS:HE2	1:A:908:LYS:HB3	1.72	0.47
1:A:1199:VAL:C	1:A:1225:GLY:HA2	2.40	0.47
2:B:627:ASP:O	2:B:628:ARG:HG2	2.15	0.47
3:C:242:ASP:OD1	3:C:472:ARG:NH1	2.47	0.47
1:D:1259:VAL:O	1:D:1263:ILE:HG23	2.15	0.47
1:D:1297:VAL:HA	1:D:1300:LEU:HD12	1.96	0.47
4:X:48:C:N4	4:X:60:U:H1'	2.29	0.47
1:A:524:THR:HG21	1:A:527:VAL:HB	1.97	0.47
2:B:238:ASN:OD1	2:B:239:ASP:N	2.48	0.47
1:D:1071:ALA:O	1:D:1075:PHE:N	2.47	0.47
1:A:1199:VAL:O	1:A:1227:SER:N	2.48	0.46
2:B:367:TRP:HB3	2:B:375:CYS:SG	2.56	0.46
3:C:456:LEU:HD21	3:C:459:LEU:HB3	1.96	0.46
1:A:854:LYS:O	1:A:858:ILE:HG22	2.15	0.46
1:A:877:LEU:O	1:A:881:ILE:HG12	2.15	0.46
2:B:105:LYS:HG3	2:B:123:ASP:HB2	1.96	0.46
2:B:661:TRP:CE3	2:B:670:PHE:HB3	2.50	0.46
3:C:22:PHE:HB2	3:C:62:GLN:CD	2.40	0.46
3:C:52:THR:HG21	4:X:10:G:H1'	1.96	0.46
1:D:1044:ALA:HA	1:D:1047:MET:HE2	1.96	0.46
3:C:260:TYR:CE2	3:C:309:GLN:HB3	2.51	0.46
1:A:71:ILE:O	1:A:87:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:LEU:O	1:A:773:ASP:C	2.58	0.46
1:A:1064:TRP:CD1	1:A:1064:TRP:H	2.32	0.46
2:B:58:HIS:CE1	2:B:84:LYS:HG3	2.50	0.46
2:B:232:LEU:HB2	2:B:275:ALA:HB3	1.96	0.46
2:B:402:ALA:O	2:B:409:THR:OG1	2.30	0.46
3:C:33:LEU:HD21	3:C:47:LEU:HD22	1.97	0.46
1:A:166:VAL:HG22	1:A:179:TYR:O	2.16	0.46
1:A:170:SER:OG	1:A:171:LYS:N	2.48	0.46
1:A:520:LYS:HD2	1:A:527:VAL:HG12	1.98	0.46
3:C:29:ILE:HG13	3:C:51:ILE:CG1	2.46	0.46
3:C:202:LEU:HD13	3:C:224:CYS:HB2	1.97	0.46
1:A:648:THR:OG1	1:A:649:ASN:N	2.49	0.46
1:A:804:ILE:HG22	1:A:804:ILE:O	2.16	0.46
1:A:1103:GLN:HA	1:A:1107:LEU:HB2	1.97	0.46
1:A:1187:TYR:HA	1:A:1253:GLU:HB2	1.96	0.46
2:B:182:PHE:HB3	2:B:192:CYS:HB2	1.97	0.46
2:B:217:GLY:HA3	2:B:240:LEU:HD13	1.96	0.46
2:B:438:HIS:CG	2:B:439:GLY:H	2.33	0.46
1:D:1027:ILE:O	1:D:1031:HIS:ND1	2.48	0.46
1:A:820:THR:HB	1:A:829:PHE:HE1	1.81	0.46
3:C:205:PHE:CD2	3:C:216:TYR:HD2	2.34	0.46
3:C:296:PRO:O	3:C:329:THR:OG1	2.27	0.46
1:D:1247:GLY:C	1:D:1249:ILE:H	2.22	0.46
4:X:58:A:H2	4:X:61:C:C2	2.33	0.46
1:A:1080:GLU:O	1:A:1084:GLU:HG2	2.16	0.46
3:C:152:ASP:OD1	3:C:152:ASP:C	2.58	0.46
1:D:1268:GLN:HG3	1:D:1269:THR:N	2.30	0.46
1:A:843:MET:SD	1:A:843:MET:N	2.87	0.46
1:A:1185:ALA:H	1:A:1195:ASP:HB3	1.81	0.46
2:B:206:LYS:HG2	2:B:226:GLN:HG3	1.97	0.46
2:B:241:ILE:HG21	2:B:268:ARG:HH12	1.81	0.46
3:C:433:ARG:NE	3:C:435:ASP:OD2	2.49	0.46
4:X:27:C:H2'	4:X:28:U:H6	1.80	0.46
1:A:377:ILE:HD13	1:A:411:LEU:HD11	1.98	0.46
1:A:1131:ILE:HD13	1:D:1069:SER:HB2	1.98	0.46
2:B:722:VAL:HG22	2:B:730:TYR:HB2	1.96	0.46
3:C:240:HIS:O	3:C:244:MET:HG3	2.16	0.46
3:C:554:SER:OG	3:C:555:LYS:N	2.48	0.46
1:D:1089:SER:O	1:D:1093:GLU:N	2.34	0.46
1:A:774:ILE:O	1:A:776:HIS:N	2.49	0.45
2:B:179:ILE:HB	2:B:196:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:LYS:HE2	3:C:91:ARG:HB2	1.98	0.45
1:D:1171:ARG:HH11	1:D:1250:TYR:HE1	1.64	0.45
1:D:1259:VAL:HG23	1:D:1336:PRO:HG2	1.98	0.45
1:A:179:TYR:OH	1:A:185:ASP:OD2	2.29	0.45
1:A:377:ILE:HD11	1:A:401:VAL:HG11	1.98	0.45
3:C:85:LEU:HB2	3:C:86:LYS:HE3	1.98	0.45
4:X:44:A:H2'	4:X:45:G:C8	2.52	0.45
1:A:1047:MET:HE2	1:A:1047:MET:N	2.31	0.45
1:A:1241:ARG:NH2	4:X:53:G:H4'	2.31	0.45
3:C:78:LYS:HB3	3:C:79:LYS:NZ	2.31	0.45
1:A:25:ASN:N	1:A:423:ASP:OD1	2.50	0.45
1:A:311:LYS:HB3	1:A:315:SER:O	2.16	0.45
1:A:681:HIS:ND1	1:A:713:ARG:HG3	2.31	0.45
2:B:391:ILE:HG23	2:B:400:LEU:HD21	1.98	0.45
2:B:394:SER:HG	2:B:399:TYR:H	1.60	0.45
1:D:1223:LYS:HA	1:D:1223:LYS:HD2	1.85	0.45
1:A:59:ILE:O	1:A:76:PHE:N	2.49	0.45
2:B:608:THR:O	2:B:625:CYS:HB2	2.16	0.45
3:C:122:PRO:HA	3:C:335:THR:HG22	1.98	0.45
3:C:331:VAL:HG13	3:C:384:THR:HB	1.96	0.45
3:C:449:GLU:HG3	3:C:456:LEU:HA	1.98	0.45
1:D:1213:ARG:HB2	1:D:1217:LYS:NZ	2.32	0.45
4:X:16:U:O2	4:X:19:G:H1'	2.16	0.45
1:A:1096:TYR:HA	1:A:1099:ALA:HB3	1.98	0.45
2:B:272:ASN:OD1	2:B:273:PHE:N	2.49	0.45
2:B:730:TYR:CD1	2:B:744:GLN:HB2	2.52	0.45
4:X:61:C:H2'	4:X:62:C:C6	2.51	0.45
1:A:302:THR:O	1:A:302:THR:OG1	2.29	0.45
1:A:529:SER:O	1:A:545:LEU:HB2	2.16	0.45
1:A:1046:GLU:OE1	1:A:1058:TYR:OH	2.32	0.45
2:B:393:TRP:HD1	2:B:759:ARG:HB3	1.81	0.45
2:B:395:PRO:HD3	2:B:447:THR:HG21	1.98	0.45
1:D:1185:ALA:HB3	1:D:1239:ARG:CZ	2.47	0.45
1:A:233:THR:OG1	1:A:235:PRO:HD2	2.16	0.45
1:A:358:GLU:N	1:A:358:GLU:OE1	2.50	0.45
1:A:1260:GLY:HA2	1:A:1263:ILE:HB	1.99	0.45
2:B:254:LEU:HD23	2:B:254:LEU:HA	1.79	0.45
3:C:313:TYR:OH	3:C:321:THR:OG1	2.21	0.45
1:D:1044:ALA:HA	1:D:1047:MET:CE	2.47	0.45
1:D:1187:TYR:O	1:D:1202:SER:HB2	2.17	0.45
1:D:1234:LYS:HD3	1:D:1317:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1295:ASN:O	1:D:1299:VAL:HG12	2.17	0.45
1:A:645:PHE:HA	1:A:654:PHE:O	2.17	0.45
2:B:40:LEU:O	2:B:51:VAL:HG23	2.16	0.45
2:B:481:ILE:HD12	2:B:481:ILE:HA	1.88	0.45
2:B:742:ILE:HG22	2:B:743:THR:HG22	1.98	0.45
3:C:47:LEU:O	3:C:51:ILE:N	2.39	0.45
1:D:1025:TYR:HD2	1:D:1047:MET:HG3	1.82	0.45
1:A:25:ASN:OD1	1:A:26:LYS:N	2.50	0.44
1:A:721:ILE:O	1:A:725:SER:N	2.50	0.44
1:A:1110:VAL:O	1:A:1114:VAL:HG23	2.17	0.44
3:C:527:GLU:O	3:C:557:ILE:N	2.48	0.44
1:D:1010:GLY:HA2	1:D:1014:TYR:CD1	2.52	0.44
4:X:49:A:N6	4:X:59:U:H3	2.14	0.44
1:A:1250:TYR:HD2	1:A:1254:TYR:HD2	1.63	0.44
3:C:394:GLU:OE1	3:C:394:GLU:N	2.46	0.44
1:A:111:PHE:HD2	1:A:119:ILE:HB	1.82	0.44
1:A:1015:ARG:HG2	1:D:1286:ARG:HH12	1.82	0.44
1:A:1237:GLU:O	1:A:1239:ARG:N	2.50	0.44
2:B:218:ASP:HA	2:B:235:ILE:O	2.18	0.44
3:C:110:HIS:HE1	3:C:117:ILE:HD12	1.81	0.44
4:X:28:U:H2'	4:X:29:U:H6	1.82	0.44
4:X:47:U:H4'	4:X:48:C:O5'	2.16	0.44
1:A:116:GLY:HA2	1:A:145:ILE:HD11	2.00	0.44
1:A:404:HIS:HB3	1:A:407:LYS:O	2.17	0.44
1:A:962:GLU:HG2	1:A:965:ARG:HB3	1.99	0.44
2:B:229:TYR:CZ	2:B:278:MET:HE1	2.52	0.44
2:B:344:CYS:O	2:B:345:LEU:HD13	2.16	0.44
2:B:369:THR:HB	2:B:375:CYS:HB2	1.99	0.44
2:B:684:HIS:HB2	2:B:692:TYR:CE2	2.51	0.44
2:B:733:SER:HB2	2:B:742:ILE:HD11	2.00	0.44
1:A:839:MET:SD	1:A:840:GLN:HG2	2.57	0.44
1:A:958:LEU:O	1:A:966:ARG:NE	2.51	0.44
1:A:1103:GLN:O	1:A:1108:ASP:N	2.51	0.44
2:B:760:TRP:CD2	2:B:771:LEU:HD13	2.53	0.44
3:C:145:ARG:NH1	3:C:160:ARG:HD3	2.32	0.44
3:C:303:MET:HE3	3:C:357:LEU:HB2	1.98	0.44
1:D:1024:ILE:O	1:D:1027:ILE:HG12	2.18	0.44
1:D:1191:THR:HG22	1:D:1254:TYR:CE1	2.53	0.44
1:A:944:SER:OG	1:A:946:MET:HG3	2.18	0.44
2:B:408:THR:HA	2:B:436:GLN:O	2.18	0.44
2:B:453:PHE:CE1	2:B:465:PHE:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1184:TYR:N	1:D:1239:ARG:HB3	2.30	0.44
1:A:265:SER:OG	1:A:283:ARG:NH2	2.48	0.44
1:A:578:LEU:HD12	1:A:579:LEU:H	1.82	0.44
1:A:1005:ASP:HA	1:A:1007:TYR:CZ	2.52	0.44
2:B:156:LEU:HD22	2:B:168:LEU:HD11	2.00	0.44
2:B:218:ASP:OD1	2:B:219:TYR:N	2.51	0.44
3:C:464:LYS:HB2	3:C:524:HIS:CE1	2.53	0.44
4:X:2:G:H2'	4:X:3:G:C8	2.47	0.44
1:A:256:ARG:NE	1:A:260:ASP:OD1	2.51	0.44
1:A:609:ILE:HD12	1:A:642:LEU:HD23	2.00	0.44
1:A:1068:MET:HE3	1:A:1079:VAL:O	2.18	0.44
3:C:197:LYS:HD3	3:C:197:LYS:HA	1.82	0.44
3:C:304:GLU:HG3	3:C:305:ARG:N	2.33	0.44
3:C:505:HIS:CG	3:C:506:GLN:N	2.85	0.44
1:A:590:TYR:CE1	1:A:598:CYS:HB3	2.53	0.44
1:A:600:LEU:HD12	1:A:601:ASP:H	1.83	0.44
1:A:1082:VAL:HA	1:A:1085:GLU:OE1	2.18	0.44
1:A:1252:GLU:CD	1:A:1253:GLU:H	2.25	0.44
1:A:1262:LEU:O	1:A:1266:LEU:HG	2.17	0.44
2:B:611:ARG:HG2	2:B:658:ASP:OD1	2.18	0.44
2:B:726:ASN:OD1	2:B:726:ASN:N	2.47	0.44
3:C:291:VAL:HG22	3:C:323:GLY:HA3	1.99	0.44
4:X:52:G:O6	4:X:61:C:N4	2.50	0.44
1:A:772:LEU:C	1:A:774:ILE:N	2.75	0.43
1:A:844:LYS:HA	1:A:844:LYS:HD3	1.51	0.43
2:B:211:ARG:HG2	2:B:212:HIS:H	1.83	0.43
2:B:382:SER:OG	2:B:431:GLU:OE2	2.32	0.43
2:B:467:LEU:HD12	2:B:468:PRO:HD2	2.00	0.43
1:A:1296:PHE:HA	1:A:1299:VAL:HG12	2.00	0.43
2:B:237:ILE:HG22	2:B:238:ASN:H	1.82	0.43
1:A:765:CYS:CB	1:A:770:ILE:HG12	2.46	0.43
1:A:1270:LYS:HB3	1:A:1271:PRO:HD3	2.00	0.43
2:B:619:LYS:HA	2:B:635:ARG:HB3	2.00	0.43
3:C:253:GLU:HA	3:C:291:VAL:O	2.19	0.43
1:D:1094:HIS:HA	1:D:1096:TYR:CE1	2.53	0.43
1:D:1285:MET:SD	1:D:1288:GLN:HB2	2.59	0.43
1:A:432:PRO:HD2	1:A:484:ASN:ND2	2.32	0.43
2:B:377:GLN:HB3	2:B:538:MET:HE3	2.01	0.43
2:B:449:THR:HG22	2:B:452:ARG:HB2	1.99	0.43
1:D:1171:ARG:HG3	1:D:1241:ARG:HH11	1.83	0.43
1:A:1037:MET:SD	1:A:1038:TYR:N	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LYS:HD2	2:B:206:LYS:HA	1.83	0.43
3:C:136:TYR:HE1	4:X:34:U:O4	2.01	0.43
3:C:507:GLY:O	3:C:511:LEU:HG	2.19	0.43
1:A:544:LEU:HD13	1:A:576:ILE:HD12	2.00	0.43
1:A:1122:ARG:HH21	1:A:1124:ASP:CG	2.25	0.43
2:B:403:THR:OG1	2:B:404:SER:N	2.51	0.43
3:C:44:GLU:HG2	3:C:45:ILE:HG12	2.00	0.43
4:X:55:U:C2	4:X:57:G:H2'	2.54	0.43
1:A:711:ILE:HD12	1:A:729:LEU:HD22	2.00	0.43
1:A:984:LEU:O	1:A:987:ILE:HG12	2.19	0.43
2:B:211:ARG:HG2	2:B:212:HIS:N	2.33	0.43
2:B:219:TYR:CD2	2:B:235:ILE:HD13	2.53	0.43
2:B:305:LEU:HD23	2:B:305:LEU:C	2.43	0.43
2:B:449:THR:HG23	2:B:451:THR:H	1.84	0.43
3:C:184:MET:HE1	3:C:191:ARG:NH1	2.34	0.43
1:A:152:TYR:HB2	1:A:259:CYS:SG	2.58	0.43
1:A:962:GLU:CG	1:A:965:ARG:H	2.28	0.43
1:A:1198:SER:HB2	1:A:1227:SER:H	1.83	0.43
1:A:1232:LYS:HD3	1:A:1232:LYS:HA	1.79	0.43
1:A:1274:VAL:HA	1:A:1277:VAL:HG22	2.01	0.43
2:B:394:SER:OG	2:B:399:TYR:N	2.38	0.43
1:A:1214:TYR:CD2	4:X:19:G:H5"	2.53	0.43
2:B:229:TYR:CE1	2:B:278:MET:HE1	2.54	0.43
3:C:241:LEU:HG	3:C:288:TYR:CE2	2.51	0.43
3:C:304:GLU:HG3	3:C:305:ARG:H	1.82	0.43
4:X:32:C:O2	4:X:32:C:H2'	2.19	0.43
1:A:430:GLN:NE2	1:A:442:SER:OG	2.52	0.42
1:A:1029:ALA:HB2	1:A:1044:ALA:HB3	2.01	0.42
2:B:146:ILE:C	2:B:148:LYS:H	2.27	0.42
2:B:191:LYS:HA	2:B:191:LYS:HD3	1.82	0.42
2:B:530:LEU:H	2:B:530:LEU:HD23	1.84	0.42
2:B:629:LYS:HG2	2:B:649:GLU:O	2.19	0.42
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.77	0.42
3:C:460:LEU:HD12	3:C:486:LEU:HD13	2.00	0.42
1:D:1042:ALA:HB1	1:D:1058:TYR:CE1	2.55	0.42
1:A:556:LEU:HD13	1:A:566:LEU:HA	2.01	0.42
1:A:588:LEU:HD23	1:A:589:VAL:N	2.34	0.42
1:A:689:ASN:ND2	1:A:821:LEU:O	2.51	0.42
3:C:257:GLN:HA	3:C:295:MET:H	1.85	0.42
1:D:1010:GLY:HA2	1:D:1014:TYR:HD1	1.84	0.42
1:D:1103:GLN:CD	1:D:1112:GLU:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1122:ARG:HB3	1:D:1125:ILE:HD13	2.01	0.42
1:A:567:ILE:HG22	1:A:568:THR:H	1.84	0.42
1:A:757:ARG:C	1:A:759:LYS:H	2.28	0.42
1:A:1263:ILE:HA	1:A:1266:LEU:CD1	2.50	0.42
2:B:102:HIS:CG	2:B:103:TYR:H	2.37	0.42
2:B:627:ASP:O	2:B:629:LYS:HG3	2.18	0.42
2:B:730:TYR:CE1	2:B:744:GLN:HB2	2.54	0.42
1:A:622:LYS:HG2	1:A:688:LEU:HD23	2.01	0.42
1:A:772:LEU:O	1:A:774:ILE:N	2.52	0.42
1:A:1293:GLN:O	1:A:1297:VAL:HG13	2.19	0.42
2:B:117:ILE:HG12	2:B:129:TRP:HB2	2.01	0.42
2:B:414:PRO:HD3	2:B:429:TRP:CZ3	2.54	0.42
3:C:215:LEU:HD12	3:C:215:LEU:HA	1.84	0.42
3:C:530:SER:HA	3:C:554:SER:HA	2.02	0.42
1:A:242:ASP:H	1:A:302:THR:HA	1.84	0.42
1:A:310:TRP:HE1	1:A:314:GLY:C	2.27	0.42
1:A:429:ALA:HB3	1:A:443:LEU:O	2.20	0.42
1:A:1171:ARG:HB2	1:A:1250:TYR:OH	2.20	0.42
2:B:546:LEU:HD23	2:B:546:LEU:HA	1.79	0.42
3:C:298:LEU:HD23	3:C:298:LEU:HA	1.74	0.42
4:X:51:C:H2'	4:X:52:G:C8	2.54	0.42
1:A:18:MET:SD	1:A:18:MET:N	2.92	0.42
1:A:164:ARG:HB3	1:A:181:LEU:HB3	2.00	0.42
1:A:1263:ILE:HA	1:A:1266:LEU:HD11	2.01	0.42
2:B:431:GLU:OE1	2:B:542:LEU:HD21	2.18	0.42
1:D:1173:ARG:HH22	1:D:1250:TYR:HB3	1.85	0.42
1:A:547:THR:OG1	1:A:550:LEU:O	2.25	0.42
1:A:655:ALA:O	1:A:658:VAL:HG22	2.19	0.42
2:B:676:ASP:HB2	2:B:678:THR:HG22	2.00	0.42
1:A:99:SER:OG	1:A:100:PHE:N	2.52	0.42
1:A:811:ASP:HB3	1:A:815:THR:HG23	2.01	0.42
1:A:1045:TYR:CE2	1:A:1053:GLU:HB3	2.55	0.42
1:A:1144:ASP:HB2	1:A:1145:PRO:HD3	2.01	0.42
2:B:329:LYS:HG3	2:B:336:GLY:O	2.19	0.42
2:B:682:TRP:CD1	2:B:682:TRP:N	2.87	0.42
3:C:130:GLU:HG2	3:C:131:TYR:HD2	1.85	0.42
3:C:489:TYR:N	3:C:489:TYR:CD1	2.87	0.42
1:D:1338:ILE:HD12	1:D:1338:ILE:HA	1.86	0.42
1:A:467:ARG:NH2	1:A:511:HIS:HB3	2.35	0.42
2:B:533:LEU:HD11	2:B:538:MET:HG2	2.02	0.42
2:B:781:ARG:O	2:B:782:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:397:LEU:HD23	3:C:397:LEU:HA	1.80	0.42
4:X:55:U:H2'	4:X:57:G:C8	2.55	0.42
1:A:151:SER:HA	1:A:255:TRP:CD1	2.54	0.42
1:A:460:VAL:HG13	1:A:464:MET:HG3	2.01	0.42
1:A:670:THR:OG1	1:A:671:ASP:N	2.53	0.42
2:B:10:ILE:HG12	2:B:781:ARG:HG3	2.02	0.42
2:B:389:THR:OG1	2:B:390:ASP:N	2.52	0.42
2:B:632:LEU:HD23	2:B:646:PHE:HD2	1.85	0.42
3:C:289:LYS:HB2	3:C:289:LYS:HE2	1.81	0.42
3:C:297:ASP:OD1	3:C:346:TYR:OH	2.32	0.42
1:A:998:ILE:HA	1:A:1001:VAL:HG22	2.01	0.41
2:B:442:MET:HE1	2:B:455:SER:HB2	2.01	0.41
2:B:475:LEU:O	2:B:479:VAL:N	2.53	0.41
3:C:318:ASP:O	3:C:439:ASN:ND2	2.52	0.41
1:D:1265:ARG:HA	1:D:1268:GLN:HG2	2.02	0.41
4:X:10:G:C2	4:X:26:G:H1'	2.55	0.41
4:X:62:C:N4	4:X:63:G:O6	2.53	0.41
1:A:964:LEU:HD12	1:A:987:ILE:HA	2.03	0.41
1:A:1160:ASP:O	1:A:1164:GLN:HG2	2.20	0.41
2:B:470:GLY:O	2:B:527:THR:HG22	2.20	0.41
2:B:760:TRP:CZ3	2:B:771:LEU:HB2	2.55	0.41
1:A:528:ASP:HB2	1:A:546:ASP:O	2.20	0.41
1:A:773:ASP:OD2	1:A:807:LEU:HA	2.20	0.41
1:A:1304:LYS:HD2	1:A:1309:GLU:OE2	2.20	0.41
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.88	0.41
2:B:158:LEU:HB3	2:B:168:LEU:HD13	2.03	0.41
2:B:379:LEU:HD13	2:B:430:HIS:CE1	2.55	0.41
2:B:621:LEU:HB2	2:B:642:PHE:HE2	1.86	0.41
2:B:781:ARG:C	2:B:782:ILE:HD13	2.45	0.41
3:C:160:ARG:NH2	4:X:33:U:H2'	2.35	0.41
1:A:23:THR:HG23	1:A:422:VAL:HG23	2.01	0.41
1:A:556:LEU:HD13	1:A:556:LEU:HA	1.92	0.41
1:A:617:ARG:NH2	1:A:647:ILE:HD12	2.35	0.41
1:A:654:PHE:HA	1:A:658:VAL:O	2.21	0.41
1:A:1132:LYS:HD3	1:A:1132:LYS:HA	1.91	0.41
2:B:350:GLU:C	2:B:351:ARG:HH11	2.28	0.41
2:B:442:MET:HA	2:B:457:GLY:HA2	2.02	0.41
2:B:635:ARG:HG2	2:B:636:ASN:N	2.34	0.41
2:B:731:LEU:HD23	2:B:731:LEU:HA	1.81	0.41
3:C:217:SER:HA	3:C:220:SER:HB3	2.02	0.41
1:D:1100:ALA:HB2	1:D:1116:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1331:PRO:HB2	1:D:1333:ILE:HD12	2.01	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.71	0.41
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.76	0.41
1:A:248:SER:HB3	1:A:306:HIS:CG	2.56	0.41
1:A:522:GLU:OE1	1:A:522:GLU:HA	2.19	0.41
2:B:84:LYS:NZ	2:B:99:THR:OG1	2.50	0.41
3:C:238:GLN:HG2	3:C:471:TYR:CD2	2.56	0.41
3:C:553:MET:HE3	3:C:553:MET:HA	2.03	0.41
1:D:1260:GLY:HA2	1:D:1263:ILE:HG12	2.03	0.41
1:A:845:LYS:HE2	1:A:845:LYS:HB2	1.81	0.41
1:A:1028:TYR:CE2	1:A:1032:LEU:HD11	2.55	0.41
1:A:1232:LYS:HE3	1:A:1244:GLY:N	2.35	0.41
3:C:409:ASP:OD1	3:C:409:ASP:C	2.63	0.41
1:D:1011:LEU:HD23	1:D:1021:GLN:HE22	1.84	0.41
1:D:1025:TYR:CD2	1:D:1047:MET:HG3	2.56	0.41
1:A:18:MET:HE3	1:A:718:VAL:HG21	2.02	0.41
1:A:261:TYR:HD1	1:A:289:SER:HA	1.86	0.41
1:A:811:ASP:OD2	1:A:814:LYS:HG2	2.21	0.41
1:A:1287:GLU:HA	1:A:1290:HIS:CD2	2.55	0.41
2:B:147:LYS:HE3	2:B:147:LYS:HB3	1.97	0.41
2:B:705:THR:HG21	2:B:754:LYS:HE2	2.03	0.41
3:C:429:VAL:HA	3:C:449:GLU:O	2.20	0.41
4:X:7:A:C4	4:X:67:G:N2	2.89	0.41
1:A:429:ALA:O	1:A:443:LEU:HD12	2.21	0.41
1:A:597:VAL:HG12	1:A:609:ILE:HB	2.02	0.41
1:A:1058:TYR:CB	1:A:1067:ALA:HB2	2.50	0.41
1:A:1197:VAL:HG22	1:A:1198:SER:N	2.35	0.41
2:B:54:THR:O	2:B:54:THR:OG1	2.37	0.41
3:C:374:VAL:HG21	3:C:393:ARG:HB2	2.02	0.41
3:C:414:GLU:OE2	3:C:416:GLY:N	2.48	0.41
3:C:519:ILE:HG23	3:C:523:GLU:HB2	2.01	0.41
1:A:742:ARG:HA	1:A:742:ARG:HD3	1.91	0.41
1:A:1103:GLN:HG2	1:A:1112:GLU:HB2	2.02	0.41
1:A:1170:ARG:NH1	1:A:1173:ARG:HB3	2.35	0.41
1:A:1199:VAL:O	1:A:1226:ALA:N	2.54	0.41
2:B:28:LYS:H	2:B:28:LYS:HG2	1.53	0.41
2:B:112:ALA:HA	2:B:117:ILE:HA	2.02	0.41
2:B:338:SER:O	2:B:338:SER:OG	2.38	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.91	0.41
3:C:19:LYS:O	3:C:22:PHE:HB3	2.20	0.41
3:C:90:VAL:HA	3:C:94:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:LEU:HD23	3:C:164:LEU:HA	1.88	0.41
3:C:251:ARG:HB2	3:C:289:LYS:HG3	2.03	0.41
3:C:297:ASP:OD2	3:C:349:TYR:CG	2.74	0.41
1:D:1066:GLU:O	1:D:1070:ILE:HG12	2.20	0.41
4:X:9:G:N2	4:X:45:G:N7	2.68	0.41
4:X:23:C:O2'	4:X:24:G:P	2.79	0.41
1:A:343:ARG:HG3	1:A:344:HIS:N	2.36	0.41
1:A:483:SER:O	1:A:485:GLU:HG3	2.21	0.41
1:A:678:THR:C	1:A:680:GLN:H	2.29	0.41
1:A:964:LEU:HB3	1:A:987:ILE:HG22	2.03	0.41
2:B:249:LYS:N	2:B:249:LYS:HD2	2.36	0.41
2:B:476:GLN:O	2:B:480:GLY:HA2	2.21	0.41
1:D:1237:GLU:HG2	1:D:1238:GLU:H	1.85	0.41
1:A:62:VAL:HG22	1:A:73:VAL:HG12	2.02	0.40
3:C:338:TYR:HE1	3:C:384:THR:HG21	1.86	0.40
1:D:1122:ARG:NH2	1:D:1125:ILE:HD11	2.36	0.40
4:X:31:C:H3'	4:X:32:C:C6	2.55	0.40
1:A:288:PHE:CE2	1:A:294:LEU:HD13	2.56	0.40
1:A:474:ASN:N	1:A:491:ASN:OD1	2.54	0.40
1:A:499:ALA:HB3	1:A:515:VAL:HG11	2.03	0.40
1:A:904:ASN:ND2	1:A:907:GLU:H	2.19	0.40
2:B:130:ARG:NE	2:B:184:LEU:HD11	2.36	0.40
2:B:615:SER:HA	2:B:661:TRP:CD1	2.56	0.40
2:B:684:HIS:HB2	2:B:692:TYR:CZ	2.56	0.40
3:C:21:ARG:CG	3:C:62:GLN:HE22	2.28	0.40
3:C:110:HIS:O	3:C:114:THR:HG23	2.21	0.40
3:C:245:LEU:HG	3:C:288:TYR:CZ	2.56	0.40
3:C:245:LEU:HG	3:C:288:TYR:OH	2.22	0.40
1:A:107:ASN:HB3	1:A:123:TYR:CZ	2.57	0.40
1:A:372:VAL:HG12	1:A:377:ILE:HG13	2.02	0.40
1:A:610:THR:OG1	1:A:611:LYS:N	2.55	0.40
1:A:876:TYR:HB3	1:A:879:THR:OG1	2.21	0.40
1:A:979:LYS:HE3	1:A:979:LYS:HB3	1.84	0.40
2:B:113:LEU:HD23	2:B:113:LEU:HA	1.84	0.40
2:B:746:ASN:HB2	2:B:748:ASP:OD1	2.21	0.40
3:C:246:LYS:HE2	3:C:246:LYS:HB2	1.90	0.40
1:D:1103:GLN:NE2	1:D:1109:ASN:HB3	2.37	0.40
1:D:1213:ARG:NH1	1:D:1258:SER:HA	2.35	0.40
1:A:238:VAL:HG23	1:A:239:ASP:H	1.86	0.40
2:B:19:GLN:HG2	2:B:66:ARG:NH2	2.35	0.40
2:B:31:ALA:HA	2:B:39:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1185:ALA:H	1:D:1239:ARG:HD3	1.87	0.40
4:X:27:C:C2	4:X:28:U:C5	3.09	0.40
1:A:404:HIS:CD2	1:A:407:LYS:HB3	2.53	0.40
1:A:1125:ILE:H	1:A:1125:ILE:HG12	1.67	0.40
1:A:1151:PHE:O	1:A:1154:ILE:HG12	2.22	0.40
2:B:306:MET:HE1	2:B:319:CYS:HB2	2.03	0.40
2:B:390:ASP:H	2:B:403:THR:CG2	2.34	0.40
3:C:316:ASN:C	3:C:318:ASP:H	2.30	0.40
1:D:1037:MET:HE2	1:D:1037:MET:HB2	1.86	0.40
1:D:1241:ARG:HA	1:D:1241:ARG:HD3	1.98	0.40
1:D:1255:LEU:HD11	1:D:1310:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1251/1349 (93%)	1109 (89%)	136 (11%)	6 (0%)	24 60
1	D	341/1349 (25%)	313 (92%)	28 (8%)	0	100 100
2	B	768/788 (98%)	679 (88%)	89 (12%)	0	100 100
3	C	523/557 (94%)	472 (90%)	50 (10%)	1 (0%)	43 75
All	All	2883/4043 (71%)	2573 (89%)	303 (10%)	7 (0%)	44 75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	47	LEU
1	A	769	ARG
1	A	1256	VAL
1	A	1178	LYS

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Mol	Chain	Res	Type
1	A	1197	VAL
1	A	1238	GLU
1	A	772	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1115/1196 (93%)	1107 (99%)	8 (1%)	76	79
1	D	293/1196 (24%)	291 (99%)	2 (1%)	76	79
2	B	678/692 (98%)	675 (100%)	3 (0%)	84	84
3	C	464/490 (95%)	460 (99%)	4 (1%)	70	76
All	All	2550/3574 (71%)	2533 (99%)	17 (1%)	73	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	579	LEU
1	A	653	LEU
1	A	769	ARG
1	A	770	ILE
1	A	771	ASN
1	A	774	ILE
1	A	1256	VAL
2	B	26	VAL
2	B	125	THR
2	B	573	ILE
3	C	21	ARG
3	C	227	ILE
3	C	489	TYR
3	C	506	GLN
1	D	1151	PHE
1	D	1328	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	143	ASN
1	A	375	ASN
1	A	430	GLN
1	A	484	ASN
1	A	599	GLN
1	A	649	ASN
1	A	650	ASN
1	A	730	GLN
1	A	786	ASN
1	A	887	GLN
1	A	891	ASN
1	A	956	GLN
1	A	1022	ASN
1	A	1059	GLN
1	A	1103	GLN
1	A	1166	ASN
2	B	98	GLN
2	B	358	ASN
2	B	438	HIS
2	B	541	GLN
2	B	545	HIS
2	B	636	ASN
3	C	62	GLN
3	C	63	GLN
3	C	206	ASN
3	C	478	GLN
3	C	506	GLN
1	D	1267	ASN
1	D	1288	GLN
1	D	1345	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	X	72/73 (98%)	34 (47%)	6 (8%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	X	5	A
4	X	8	U
4	X	9	G
4	X	10	G
4	X	14	A
4	X	15	G
4	X	16	U
4	X	17	U
4	X	18	G
4	X	20	U
4	X	21	A
4	X	22	G
4	X	24	G
4	X	25	C
4	X	32	C
4	X	34	U
4	X	35	G
4	X	36	C
4	X	37	A
4	X	39	G
4	X	44	A
4	X	47	U
4	X	48	C
4	X	49	A
4	X	53	G
4	X	55	U
4	X	58	A
4	X	59	U
4	X	60	U
4	X	61	C
4	X	65	U
4	X	66	U
4	X	71	C
4	X	73	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	X	4	C
4	X	7	A
4	X	15	G
4	X	23	C
4	X	47	U

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Mol	Chain	Res	Type
4	X	65	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
5	SF4	C	601	3	0,12,12	-	-	-		
6	5AD	C	602	-	20,20,20	0.72	0	27,30,30	0.89	1 (3%)

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
5	SF4	C	601	3	-	-	0/6/5/5
6	5AD	C	602	-	-	3/4/20/20	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	602	5AD	C3'-C2'-C1'	-2.78	96.14	101.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	602	5AD	C2'-C1'-N9-C8
6	C	602	5AD	C2'-C1'-N9-C4
6	C	602	5AD	O4'-C1'-N9-C8

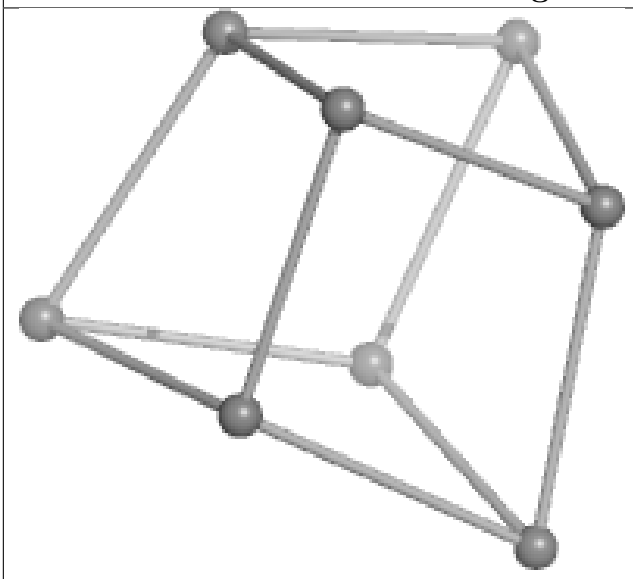
There are no ring outliers.

1 monomer is involved in 4 short contacts:

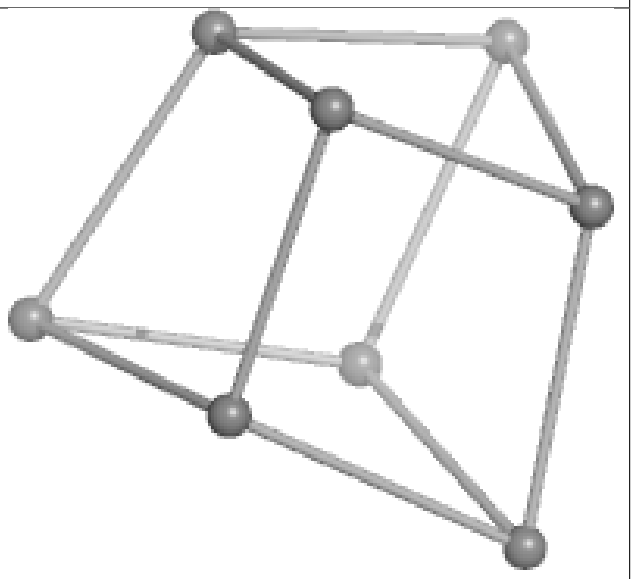
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	SF4	4	0

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 then 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.

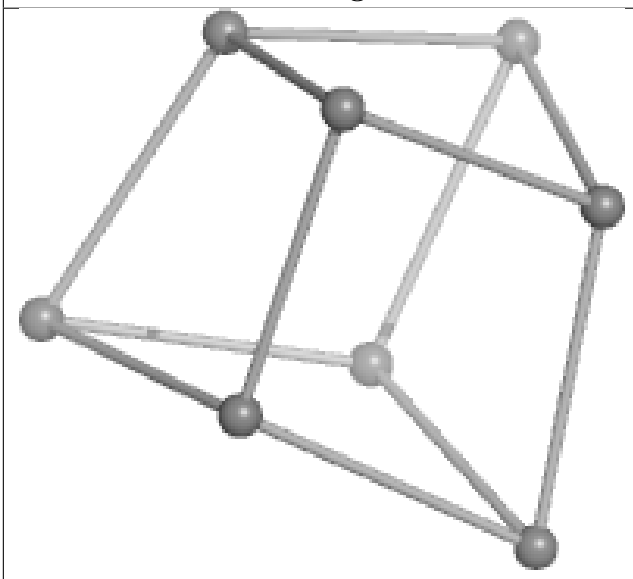
Ligand SF4 C 601



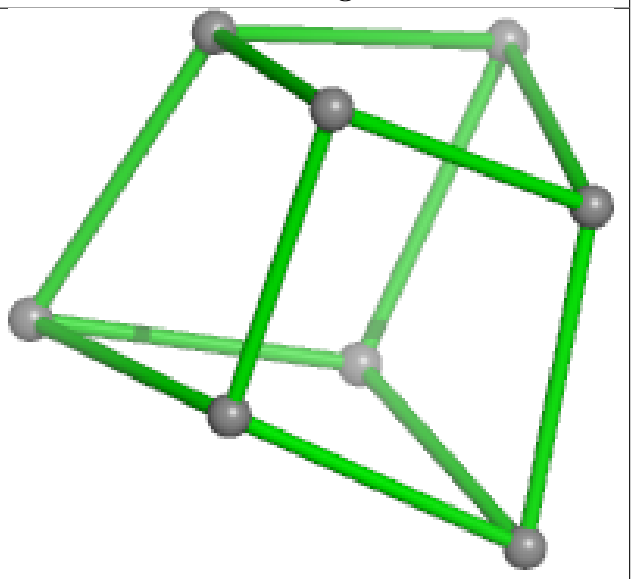
Bond lengths



Bond angles

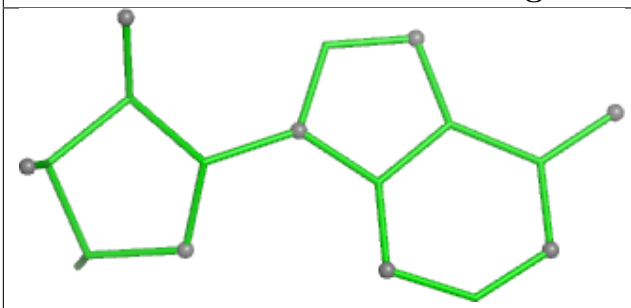


Torsions

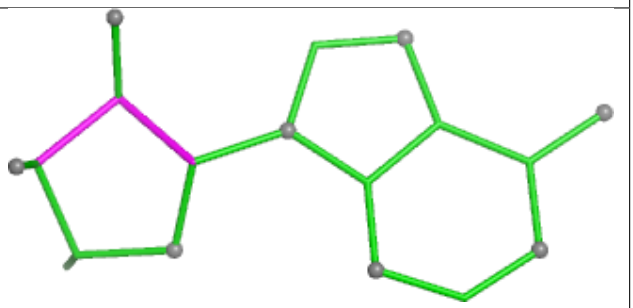


Rings

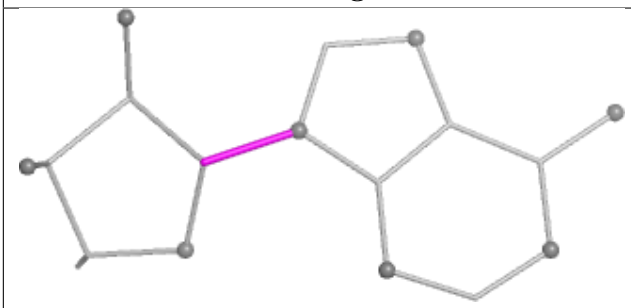
Ligand 5AD C 602



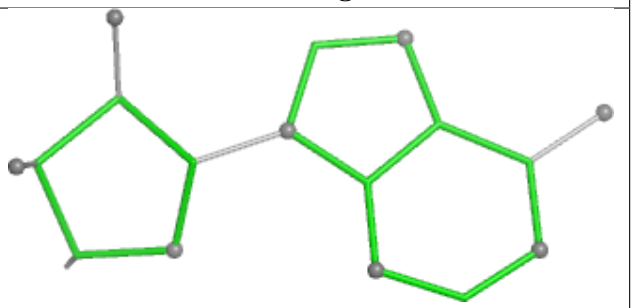
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

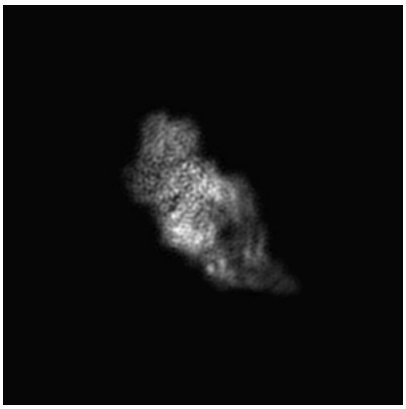
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15623. These allow visual inspection of the internal detail of the map and identification of artifacts.

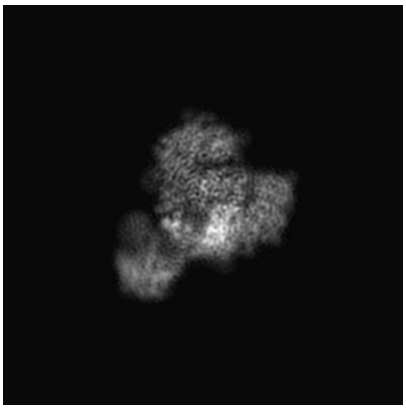
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

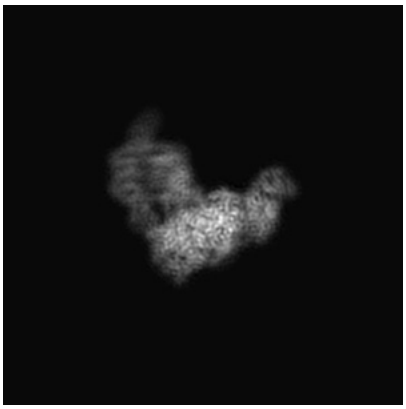
6.1.1 Primary map



X

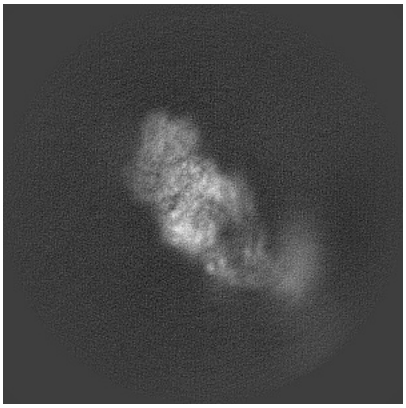


Y

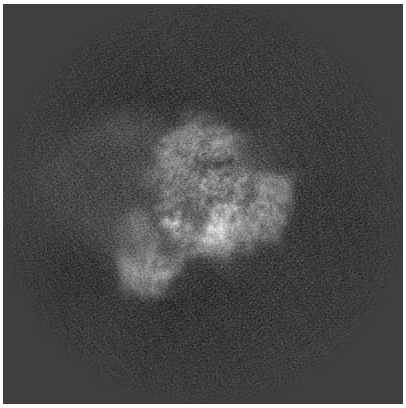


Z

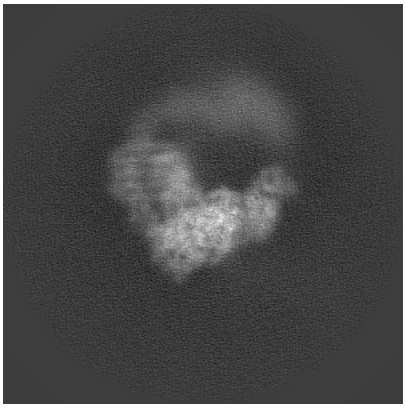
6.1.2 Raw map



X



Y

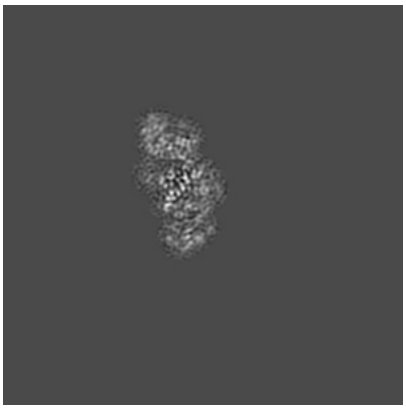


Z

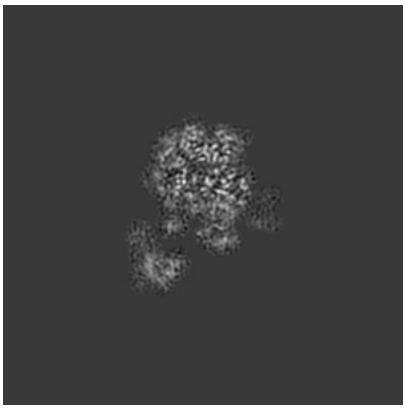
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

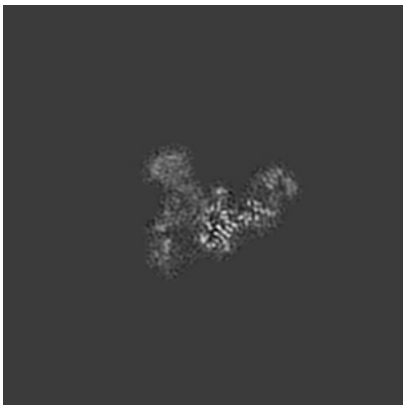
6.2.1 Primary map



X Index: 210

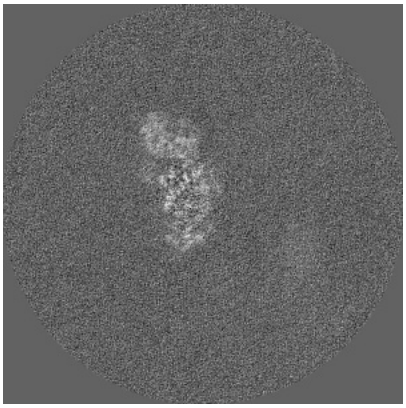


Y Index: 210

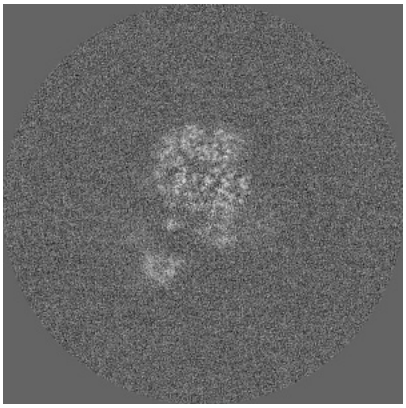


Z Index: 210

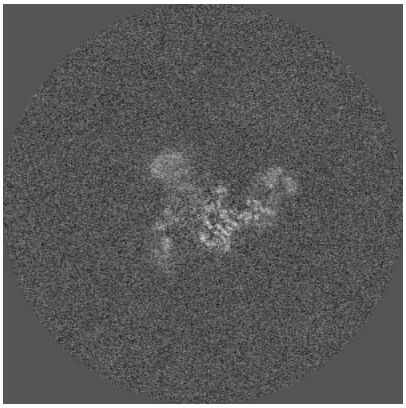
6.2.2 Raw map



X Index: 210



Y Index: 210

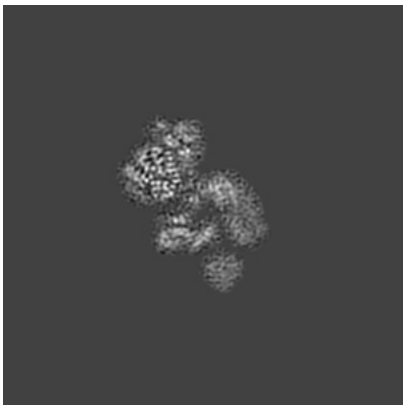


Z Index: 210

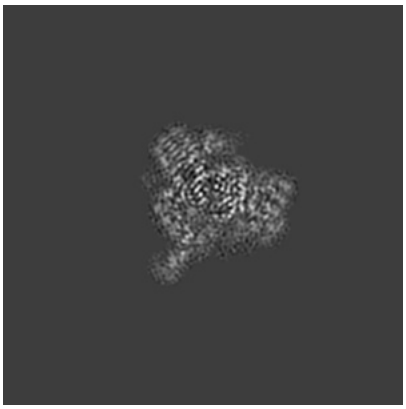
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

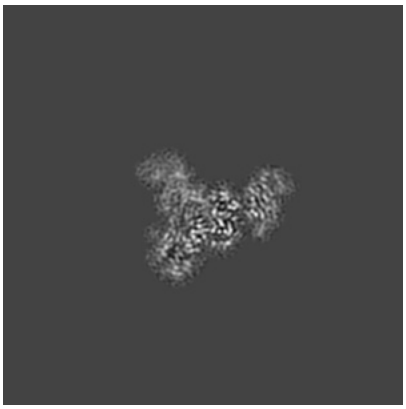
6.3.1 Primary map



X Index: 188

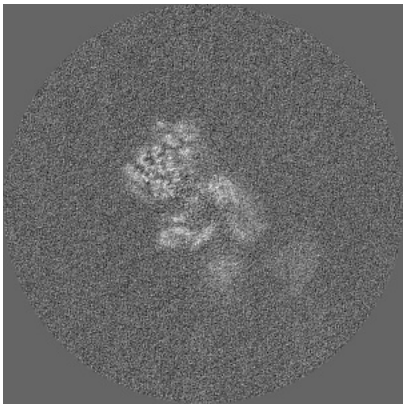


Y Index: 190

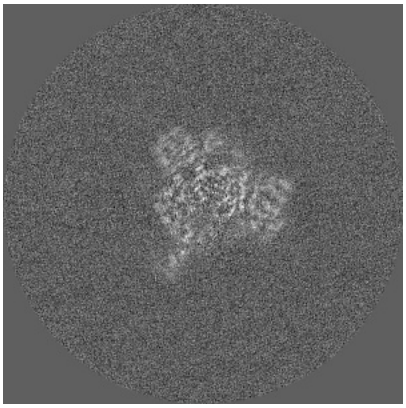


Z Index: 224

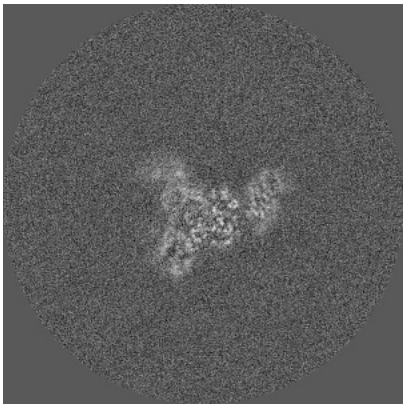
6.3.2 Raw map



X Index: 188



Y Index: 190

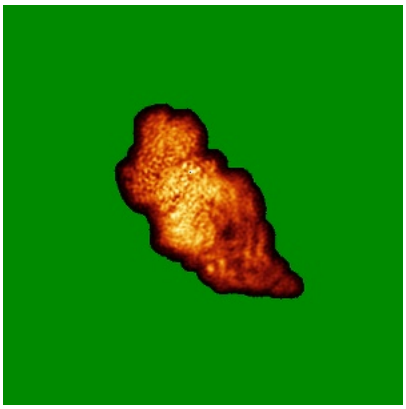


Z Index: 224

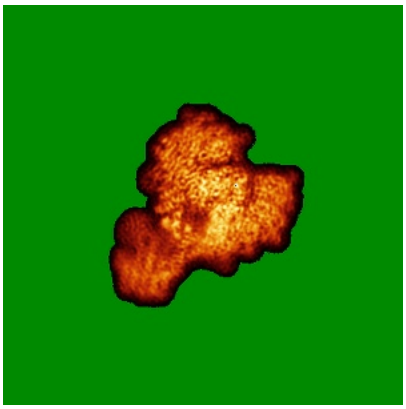
The images above show the largest variance slices of the map in three orthogonal directions.

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

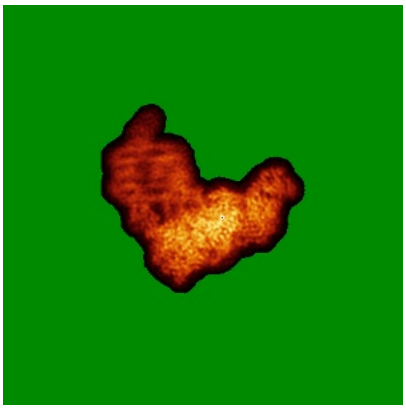
6.4.1 Primary map



X

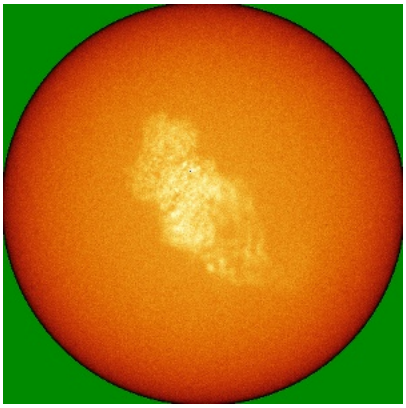


Y

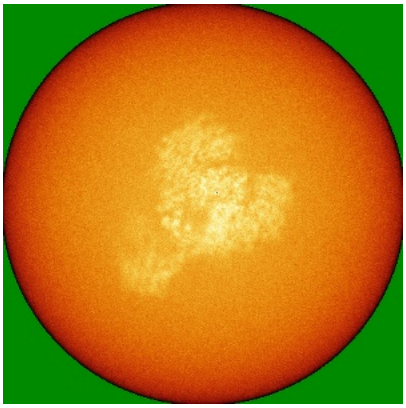


Z

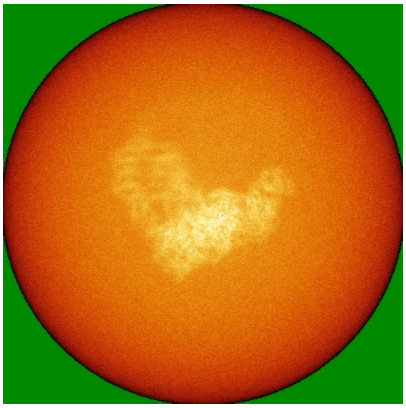
6.4.2 Raw map



X



Y

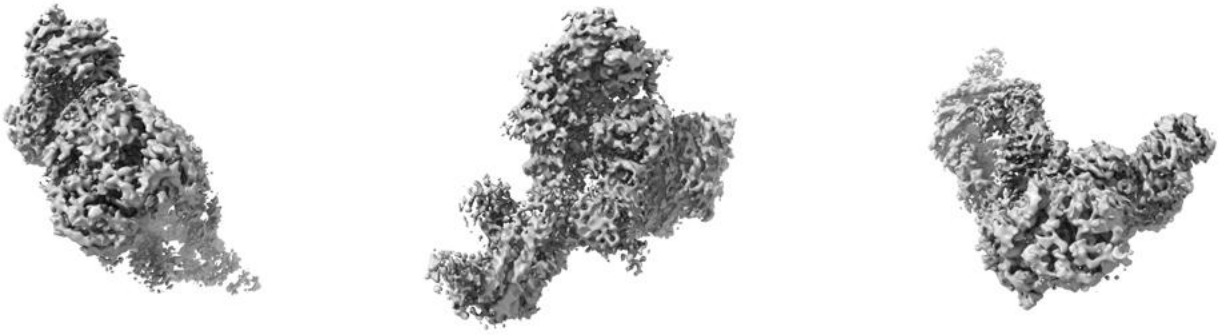


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00855. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

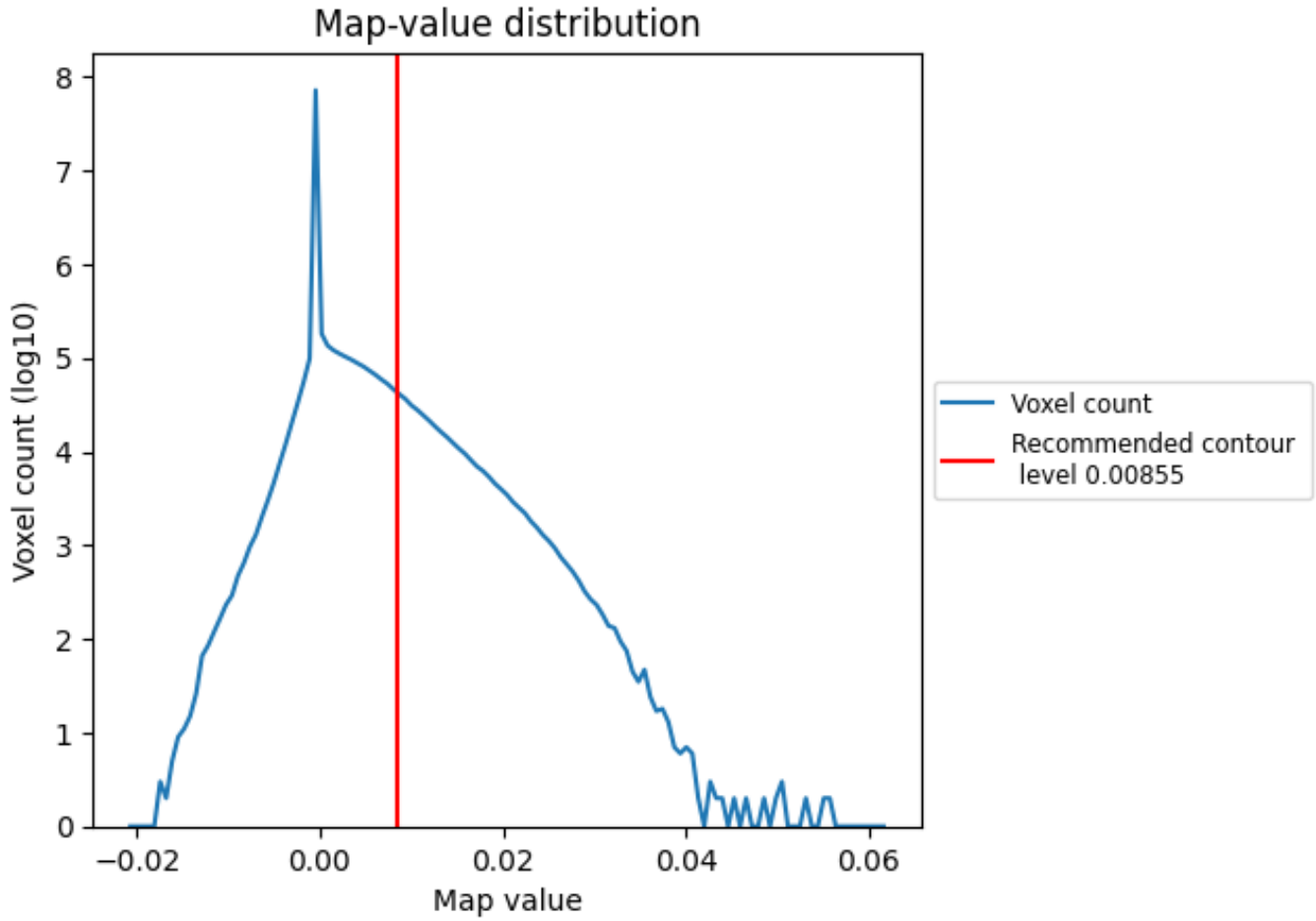
6.6 Mask visualisation (i)

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

7 Map analysis

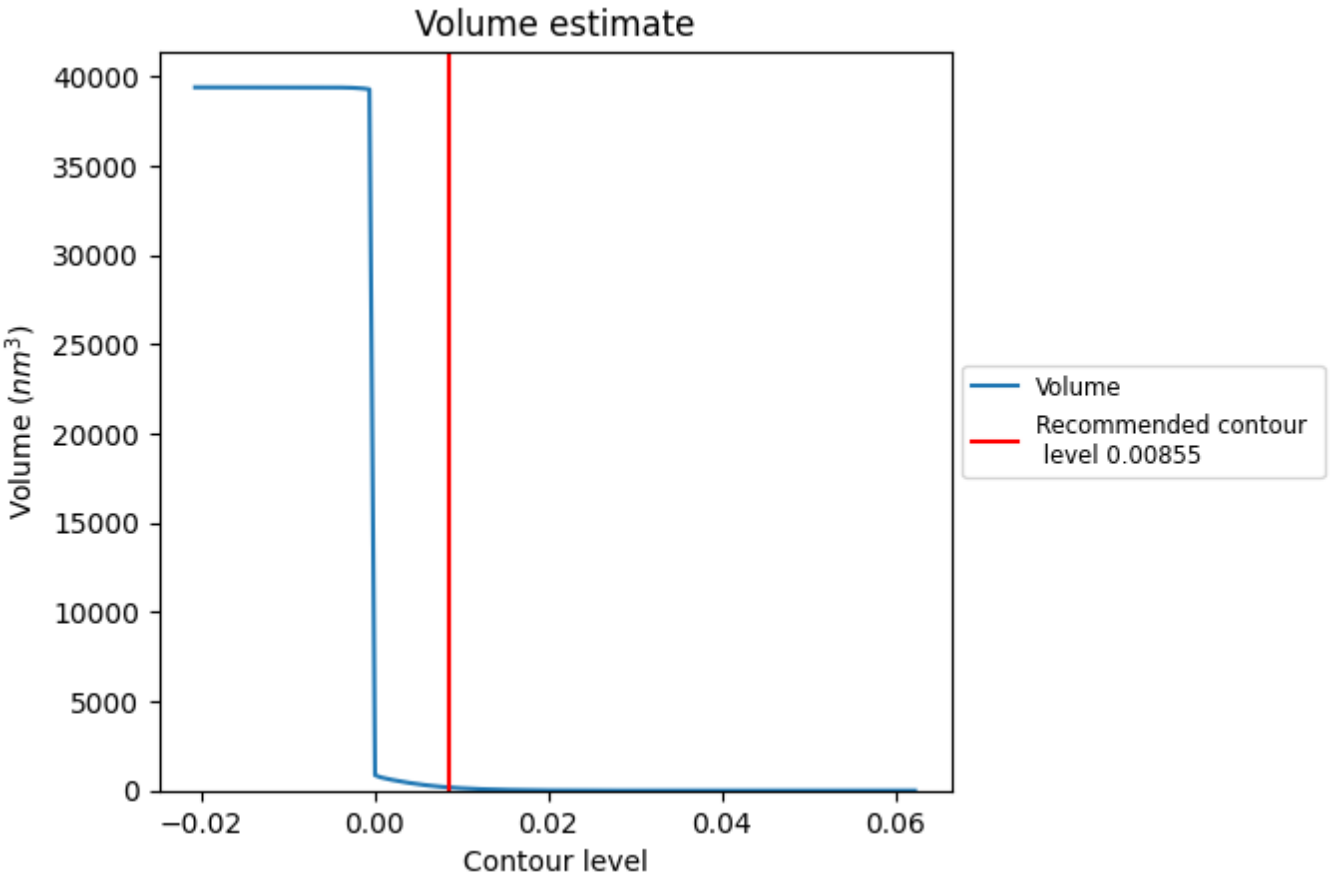
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

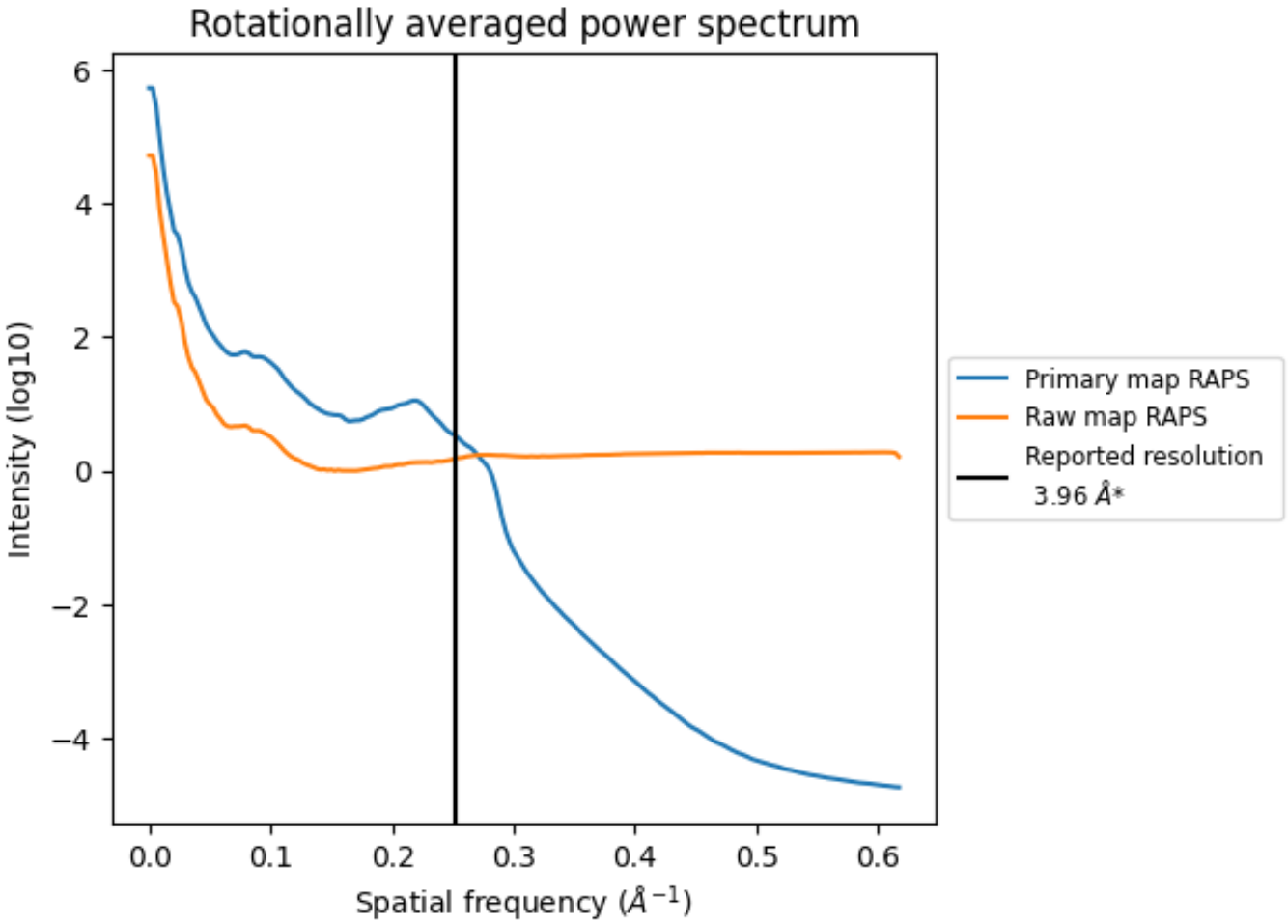
7.2 Volume estimate (i)



The volume at the recommended contour level is 176 nm^3; this corresponds to an approximate mass of 159 kDa.

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

7.3 Rotationally averaged power spectrum (i)

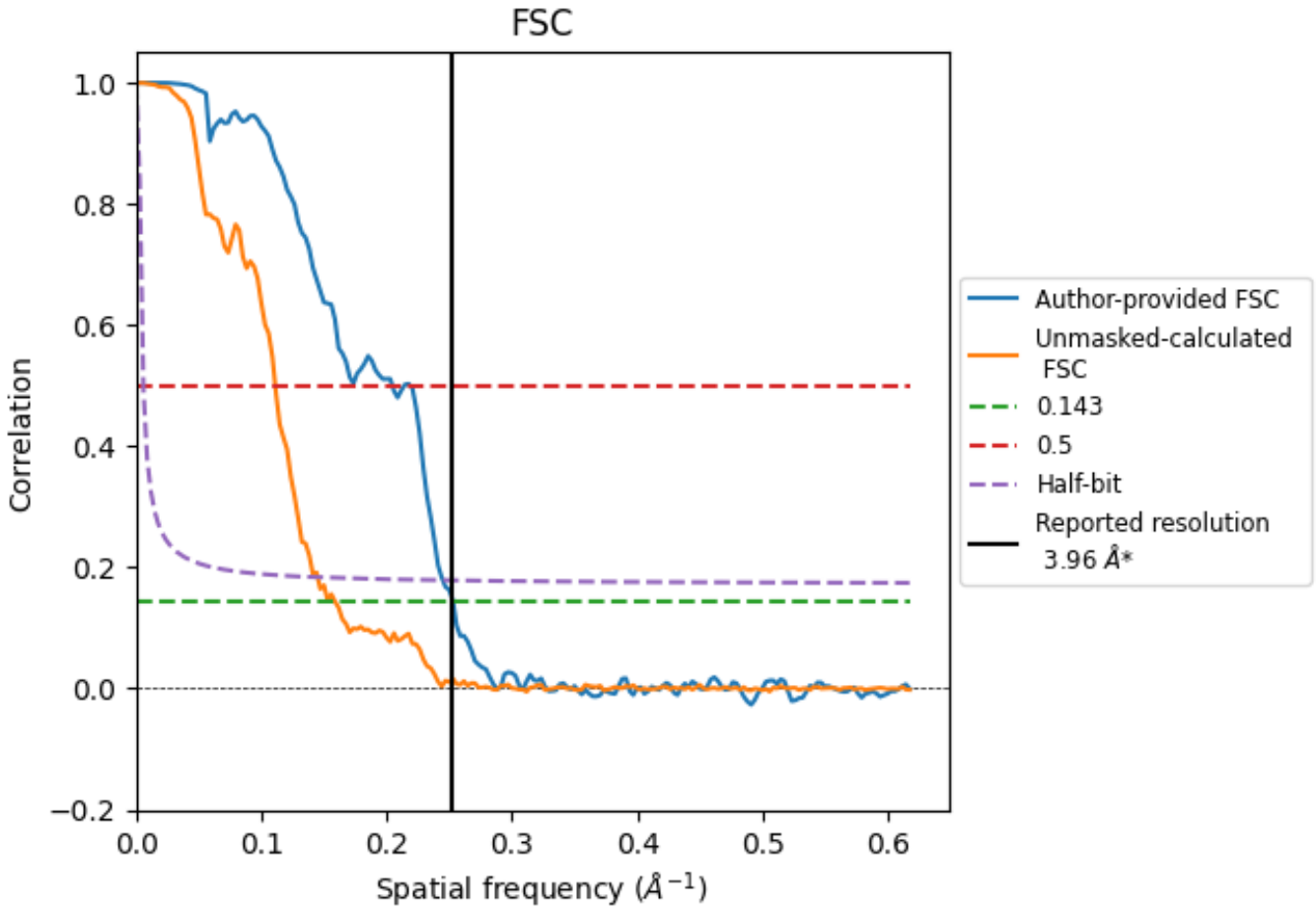


*Reported resolution corresponds to spatial frequency of 0.253 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.253 Å^{-1}

8.2 Resolution estimates (i)

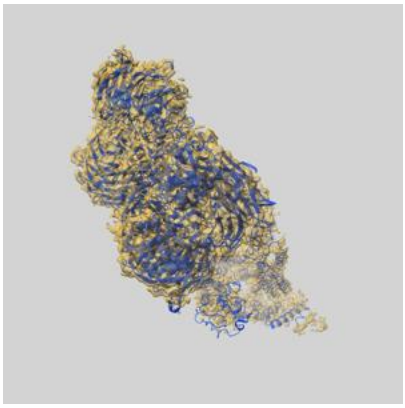
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	3.95	4.89	4.08
Unmasked-calculated*	6.29	9.01	6.90

*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 6.29 differs from the reported value 3.96 by more than 10 %

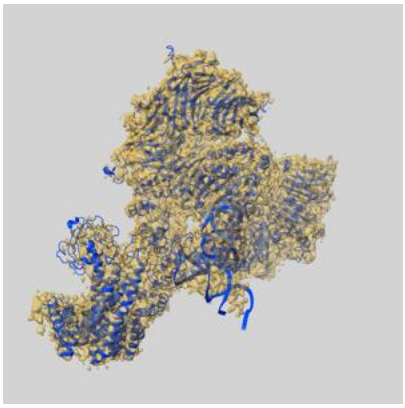
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15623 and PDB model 8ASW. Per-residue inclusion information can be found in section 3 on page 6.

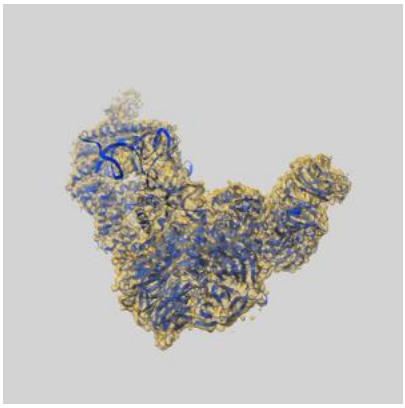
9.1 Map-model overlay



X



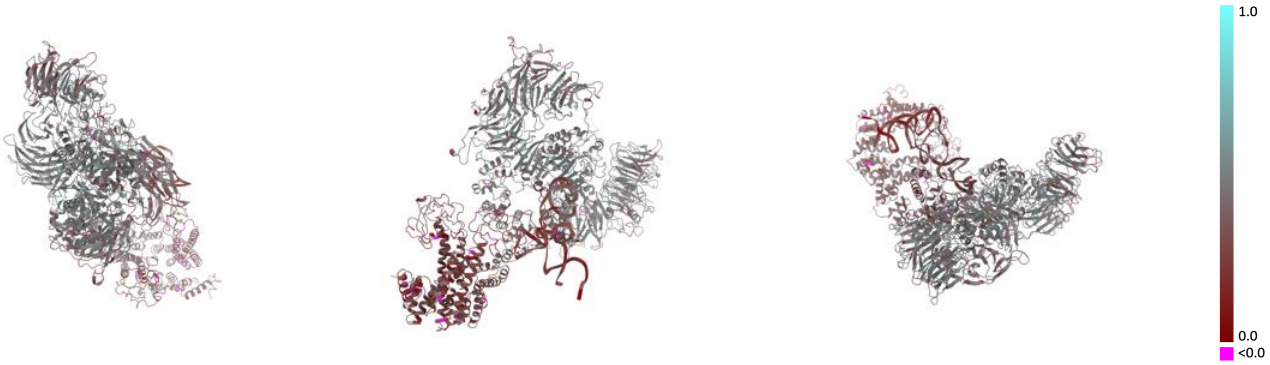
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00855 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

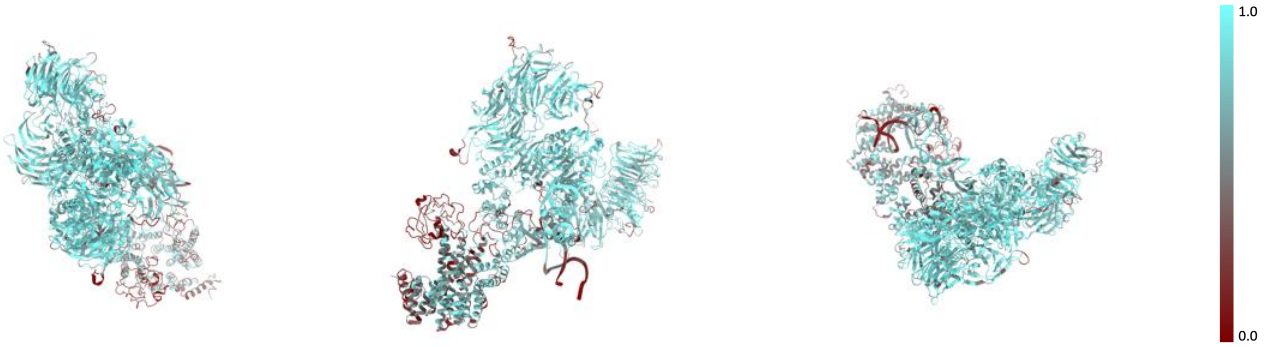
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

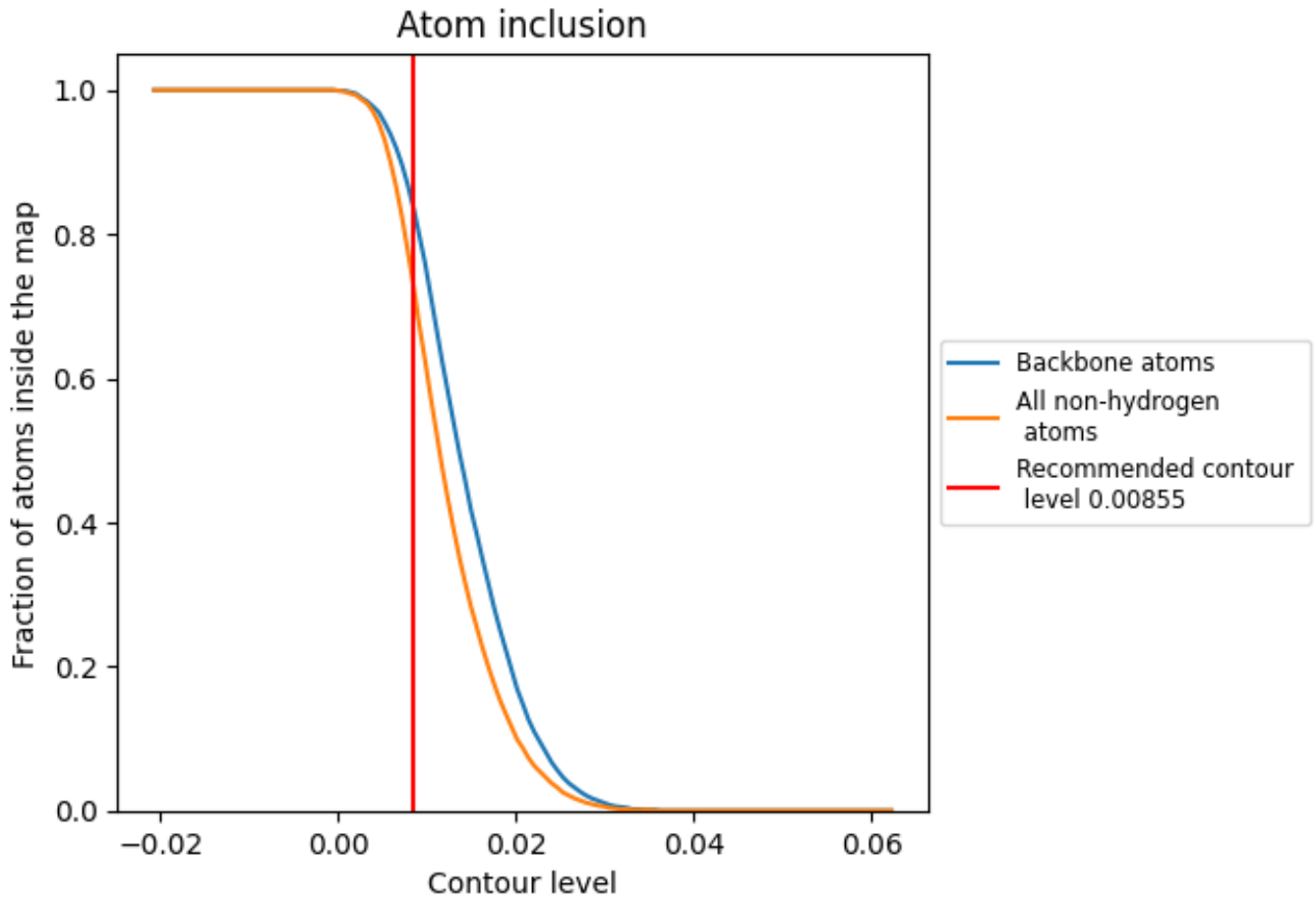
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00855).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.00855) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.4030
A	0.7300	0.4000
B	0.8140	0.4510
C	0.8300	0.4690
D	0.3870	0.2840
X	0.6190	0.2630

