



Full wwPDB EM Validation Report ⓘ

Oct 6, 2025 – 01:26 PM EDT

PDB ID : 9DVU / pdb_00009dvu
EMDB ID : EMD-47223
Title : CryoEM structure of RpaA bound to PkaiBC DNA and Syn7942 RNAP-SigA holoenzyme
Authors : Fang, M.; Gu, Y.; Matyszewski, M.; Leanca, M.; LiWang, A.; Yuzenkova, Y.; Corbett, K.D.; Golden, S.E.
Deposited on : 2024-10-08
Resolution : 3.70 Å (reported)
Based on initial model : 8SYI

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:

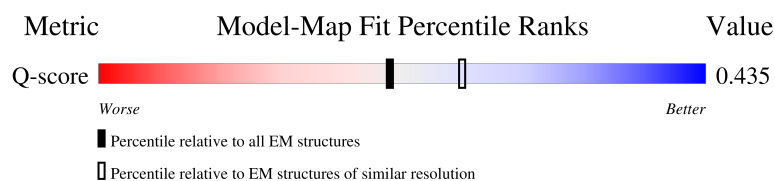
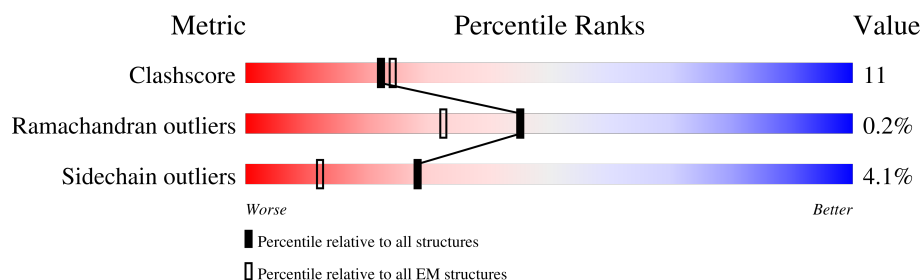
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 3.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1	105	
2	2	105	
3	A	309	
3	B	309	

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Mol	Chain	Length	Quality of chain
4	C	1100	<div><div></div><div>67%26%5%</div></div>
5	D	624	<div><div></div><div>73%25%</div></div>
6	E	76	<div><div></div><div>42%61%11%28%</div></div>
7	F	1318	<div><div></div><div>12%65%25%8%</div></div>
8	G	399	<div><div></div><div>58%18%23%</div></div>
9	R	249	<div><div></div><div>73%20%5%</div></div>
9	S	249	<div><div></div><div>67%22%7%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35249 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	P	0	0
			1253	600	219	373	61		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	52	Total	C	N	O	P	0	0
			1067	509	199	307	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	278	Total	C	N	O	S	0	0
			2147	1346	375	421	5		
3	B	215	Total	C	N	O	S	0	0
			1644	1032	290	318	4		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1042	Total	C	N	O	S	0	0
			8222	5166	1454	1575	27		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	617	Total	C	N	O	S	0	0
			4926	3107	892	906	21		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	55	Total	C	N	O	S	0	0
			451	281	81	87	2		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	1209	Total	C	N	O	S	0	0
			9265	5771	1643	1830	21		

- Molecule 8 is a protein called RNA polymerase sigma factor SigA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	308	Total	C	N	O	S	0	0
			2491	1564	456	466	5		

- Molecule 9 is a protein called DNA-binding dual master transcriptional regulator RpaA.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	R	236	Total	C	N	O	P	S	0	0
			1904	1206	330	358	1	9		
9	S	232	Total	C	N	O	P	S	0	0
			1876	1191	325	350	1	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	121	GLN	ARG	conflict	UNP Q31S42
S	121	GLN	ARG	conflict	UNP Q31S42

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

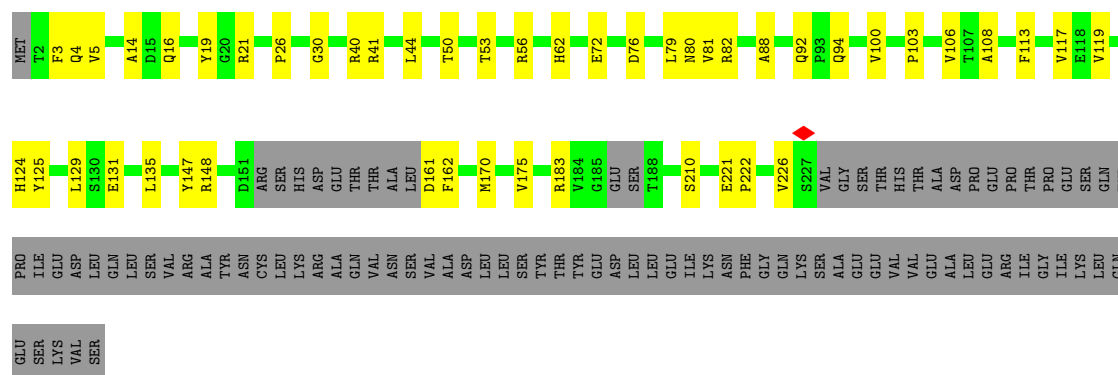
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Zn	0
			1	1	

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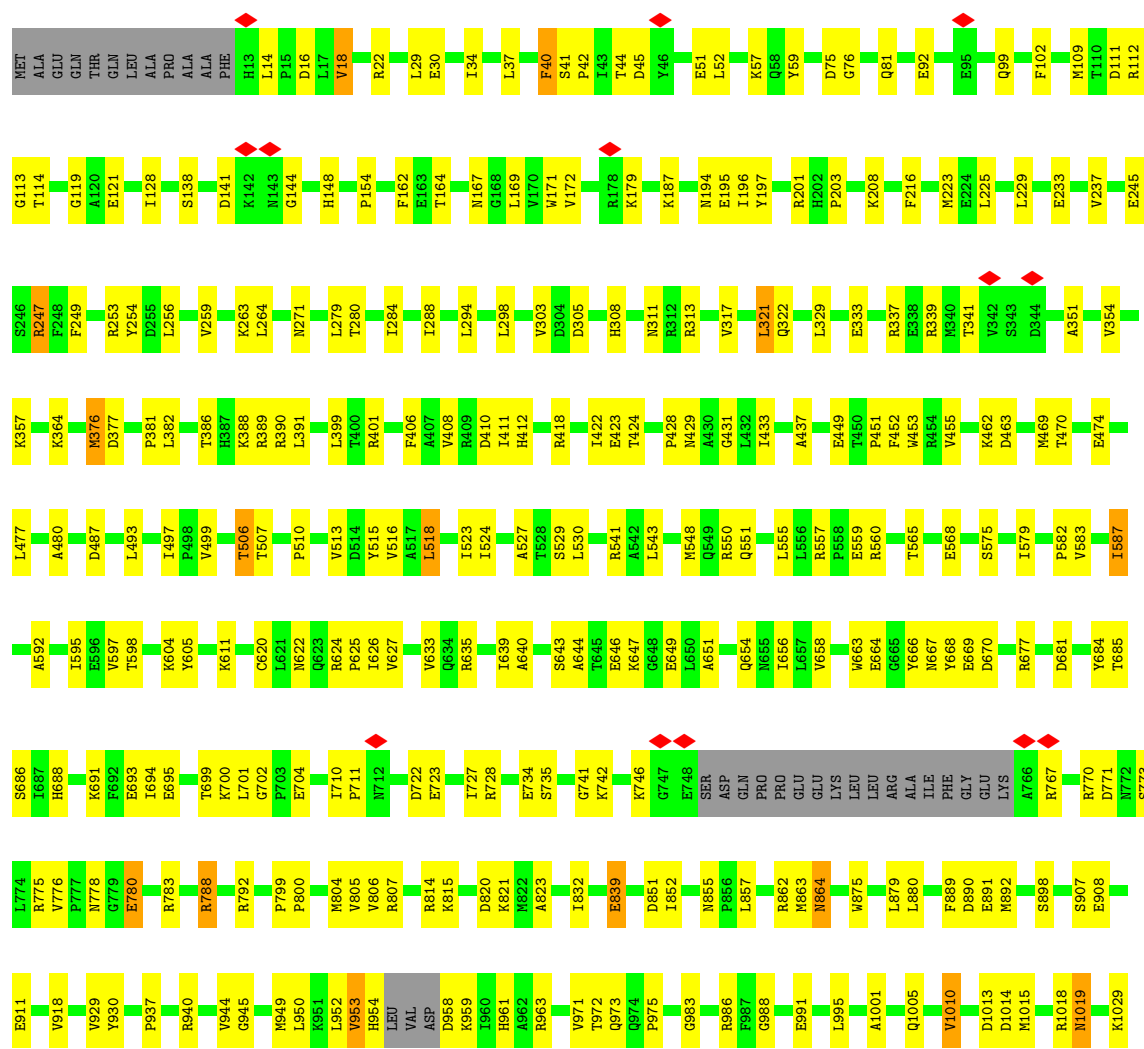
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	F	1	1	1	0

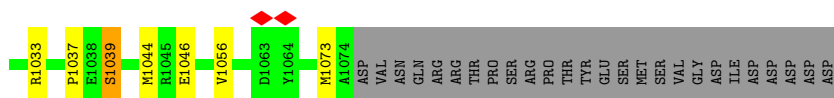
Chain B: 



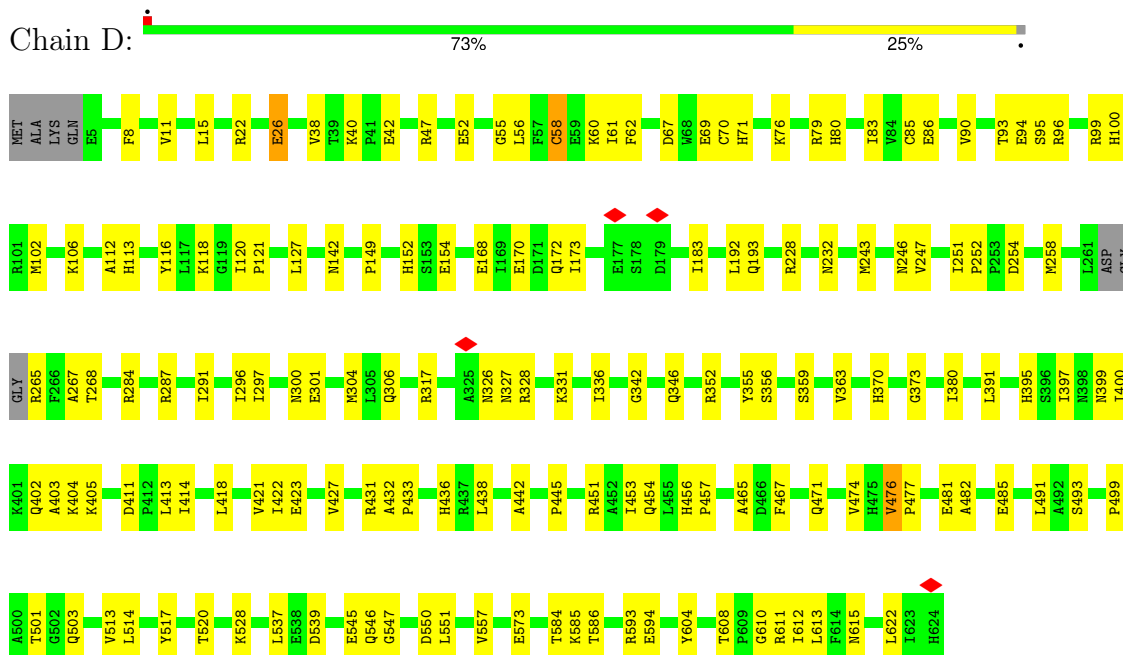
• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain C: 

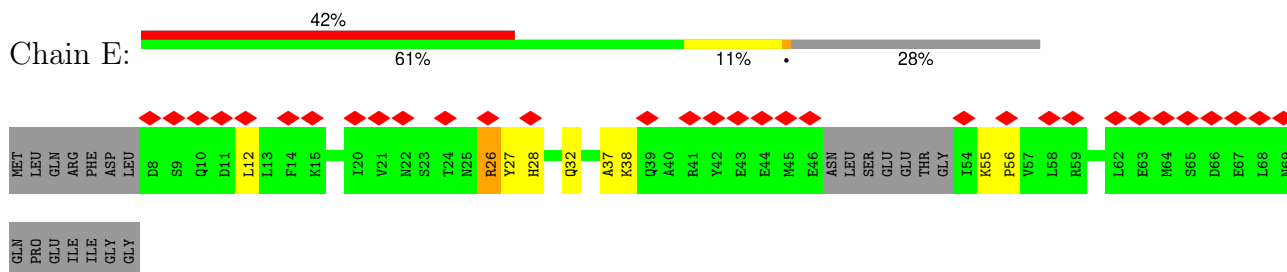




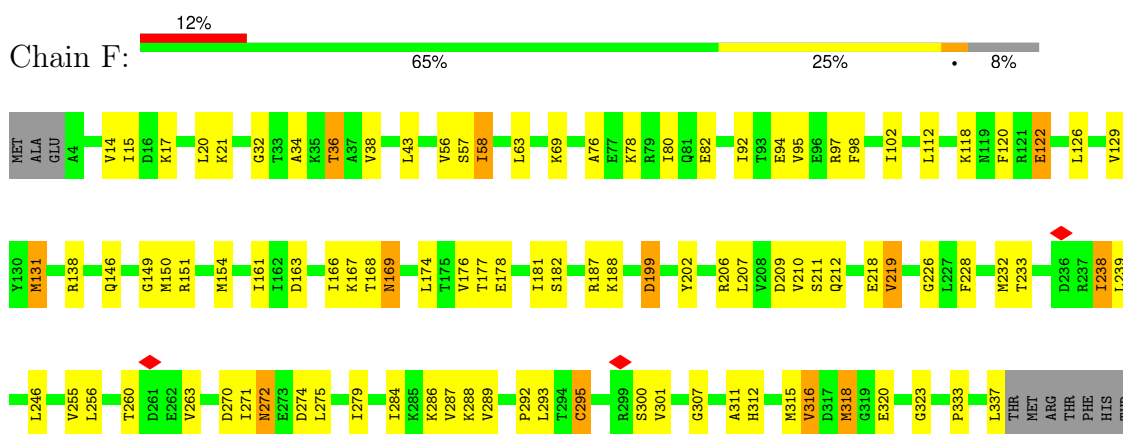
- Molecule 5: DNA-directed RNA polymerase subunit gamma

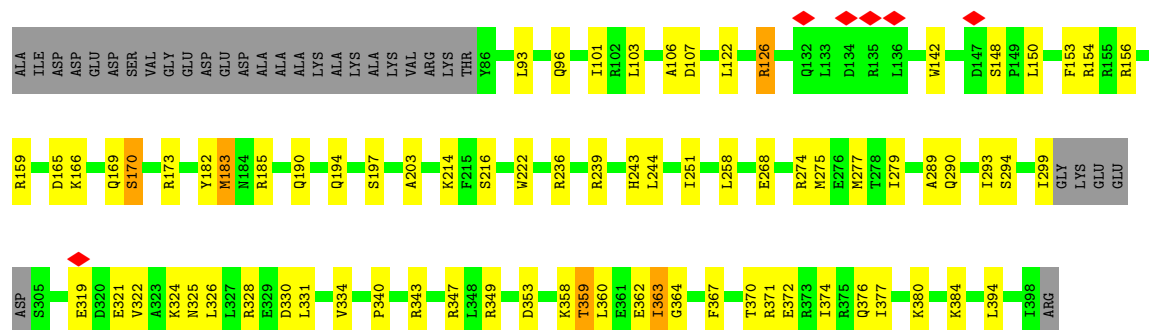


- Molecule 6: DNA-directed RNA polymerase subunit omega



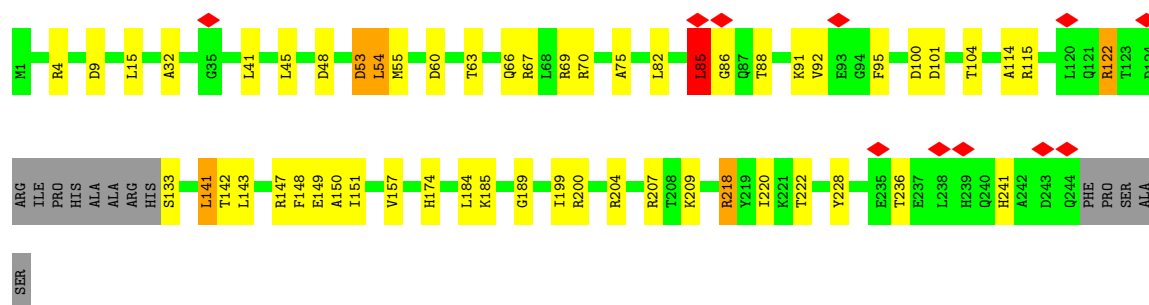
- Molecule 7: DNA-directed RNA polymerase subunit beta'





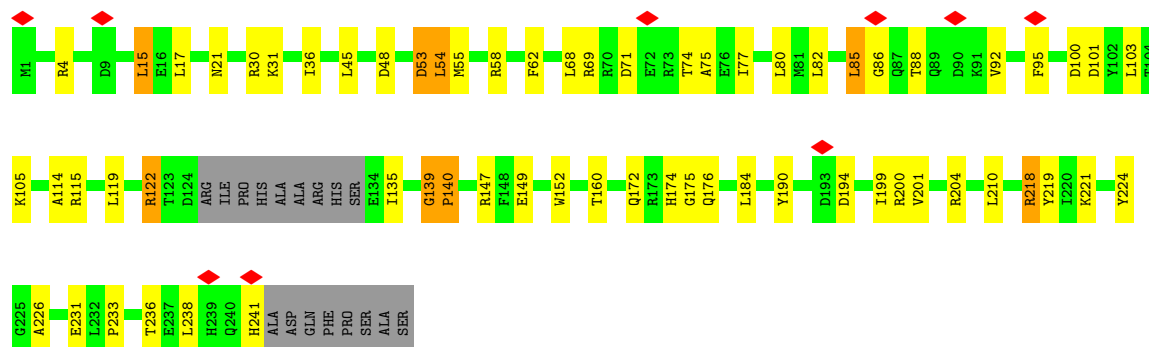
• Molecule 9: DNA-binding dual master transcriptional regulator RpaA

Chain R: 73% 20% 5%



• Molecule 9: DNA-binding dual master transcriptional regulator RpaA

Chain S: 67% 22% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.017	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	478.72, 478.72, 478.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1968, 1.1968, 1.1968	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHD, ZN, 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	1	0.36	0/1403	0.53	0/2165
2	2	0.35	0/1198	0.50	0/1846
3	A	0.26	0/2178	0.41	0/2961
3	B	0.26	0/1670	0.38	0/2274
4	C	0.31	0/8376	0.45	0/11340
5	D	0.28	0/5019	0.38	0/6793
6	E	0.17	0/454	0.45	0/608
7	F	0.23	0/9383	0.40	0/12707
8	G	0.23	0/2521	0.44	0/3389
9	R	0.27	0/1927	0.57	0/2612
9	S	0.27	0/1899	0.53	0/2574
All	All	0.27	0/36028	0.44	0/49269

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
3	B	0	1
4	C	0	5
6	E	0	1
7	F	0	1
8	G	0	2
9	R	0	3
9	S	0	2
All	All	0	15

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	183	ARG	Sidechain
4	C	247	ARG	Sidechain
4	C	253	ARG	Sidechain
4	C	339	ARG	Sidechain
4	C	624	ARG	Sidechain
4	C	788	ARG	Sidechain
6	E	26	ARG	Sidechain
7	F	1221	LYS	Mainchain
8	G	126	ARG	Sidechain
8	G	359	THR	Peptide
9	R	122	ARG	Sidechain
9	R	141	LEU	Peptide
9	R	218	ARG	Sidechain
9	S	122	ARG	Sidechain
9	S	218	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1253	0	694	50	0
2	2	1067	0	586	35	0
3	A	2147	0	2134	33	0
3	B	1644	0	1632	35	0
4	C	8222	0	8196	192	0
5	D	4926	0	4951	112	0
6	E	451	0	458	6	0
7	F	9265	0	9364	238	0
8	G	2491	0	2549	67	0
9	R	1904	0	1913	50	0
9	S	1876	0	1891	70	0
10	D	1	0	0	0	0
11	D	1	0	0	0	0
11	F	1	0	0	0	0
All	All	35249	0	34368	776	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (776) 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)
5:D:304:MET:HE2	8:G:190:GLN:HB3	1.36	1.07
3:B:147:TYR:H	3:B:170:MET:HE3	1.33	0.94
4:C:109:MET:HE3	4:C:113:GLY:HA2	1.51	0.91
1:1:29:DT:H3'	9:S:204:ARG:HH12	1.36	0.89
4:C:259:VAL:HG21	4:C:313:ARG:HD2	1.54	0.89
4:C:411:ILE:HG13	7:F:187:ARG:HD2	1.54	0.88
1:1:17:DG:OP1	9:R:222:THR:OG1	1.94	0.84
7:F:642:ASN:HD22	8:G:106:ALA:HB3	1.42	0.83
9:R:70:ARG:NH2	9:S:172:GLN:O	2.13	0.81
3:A:34:THR:HG22	3:B:41:ARG:HE	1.46	0.80
3:B:44:LEU:HB3	5:D:546:GLN:HE22	1.46	0.80
4:C:1019:ASN:ND2	8:G:321:GLU:OE1	2.14	0.80
3:B:170:MET:HE1	5:D:546:GLN:HG3	1.65	0.79
7:F:371:ARG:HH21	7:F:387:GLU:HB2	1.48	0.78
7:F:95:VAL:HG11	7:F:983:PHE:CE2	2.19	0.78
9:R:92:VAL:HA	9:R:95:PHE:HD2	1.48	0.78
7:F:209:ASP:OD2	7:F:1221:LYS:NZ	2.18	0.77
5:D:300:ASN:HD21	5:D:304:MET:HE3	1.49	0.77
7:F:605:LYS:HB2	7:F:632:LEU:HB2	1.66	0.77
9:R:114:ALA:HB2	9:S:95:PHE:HE1	1.49	0.77
7:F:657:GLU:HA	7:F:671:THR:HG23	1.67	0.77
4:C:480:ALA:HB3	4:C:516:VAL:HG22	1.67	0.76
1:1:16:DG:OP2	9:R:200:ARG:NH2	2.18	0.76
7:F:448:ASP:N	7:F:448:ASP:OD1	2.17	0.75
7:F:69:LYS:NZ	7:F:149:GLY:O	2.20	0.75
8:G:101:ILE:HD13	8:G:169:GLN:HG2	1.69	0.74
4:C:523:ILE:HD13	7:F:176:VAL:HG13	1.70	0.73
4:C:821:LYS:HD3	4:C:952:LEU:HD12	1.69	0.73
4:C:229:LEU:HD13	4:C:247:ARG:HH21	1.54	0.73
1:1:23:DG:OP1	3:A:287:LYS:NZ	2.16	0.73
4:C:114:THR:HG21	4:C:376:MET:HE1	1.69	0.73
9:R:207:ARG:NH2	9:R:220:ILE:O	2.22	0.72
7:F:32:GLY:O	7:F:36:THR:OG1	2.07	0.72
8:G:126:ARG:HB2	8:G:142:TRP:CE2	2.25	0.72
3:B:147:TYR:N	3:B:170:MET:HE3	2.04	0.72
9:R:95:PHE:HE1	9:S:114:ALA:HB2	1.55	0.72
9:S:53:PHD:OP1	9:S:105:LYS:NZ	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:76:ASP:OD1	5:D:604:TYR:OH	2.07	0.71
9:R:122:ARG:HD3	9:S:122:ARG:HD3	1.72	0.71
2:2:57:DG:H2'	2:2:58:DA:C8	2.26	0.71
4:C:22:ARG:HA	4:C:109:MET:HE1	1.72	0.70
4:C:449:GLU:HG2	4:C:470:THR:HG22	1.72	0.70
4:C:410:ASP:HA	7:F:187:ARG:HD3	1.74	0.70
9:S:15:LEU:HD21	9:S:31:LYS:HB3	1.73	0.70
7:F:1103:GLN:NE2	7:F:1134:THR:OG1	2.20	0.70
9:R:100:ASP:HB3	9:S:122:ARG:HH21	1.56	0.70
4:C:76:GLY:O	4:C:119:GLY:N	2.25	0.69
4:C:1073:MET:HB3	5:D:100:HIS:CD2	2.27	0.69
7:F:729:ALA:HB1	7:F:740:LEU:HD11	1.73	0.69
4:C:424:THR:HG21	7:F:187:ARG:NH2	2.07	0.69
5:D:8:PHE:O	7:F:1228:ARG:NH2	2.21	0.69
5:D:585:LYS:NZ	5:D:594:GLU:OE1	2.25	0.69
1:1:27:DT:OP2	9:S:200:ARG:NH2	2.26	0.69
3:A:92:GLN:O	3:A:94:GLN:NE2	2.26	0.69
1:1:54:DT:H2''	1:1:55:DA:C8	2.28	0.68
8:G:359:THR:N	8:G:362:GLU:OE1	2.24	0.68
3:B:92:GLN:O	3:B:94:GLN:NE2	2.26	0.68
5:D:85:CYS:SG	5:D:86:GLU:N	2.66	0.68
7:F:985:ARG:HH22	7:F:987:LYS:HE3	1.57	0.68
7:F:1200:GLU:OE1	7:F:1203:ARG:NH1	2.27	0.68
9:S:4:ARG:NH1	9:S:45:LEU:O	2.27	0.67
1:1:20:DA:H2''	1:1:21:DA:C8	2.30	0.67
4:C:548:MET:HE3	4:C:823:ALA:HB1	1.75	0.66
4:C:487:ASP:HB3	4:C:493:LEU:HD21	1.77	0.66
7:F:389:ASN:HD21	7:F:406:LEU:HD12	1.61	0.66
7:F:1165:MET:HG3	7:F:1170:MET:HB2	1.75	0.66
4:C:469:MET:HE3	4:C:474:GLU:HB3	1.76	0.66
7:F:907:ASP:OD1	7:F:907:ASP:N	2.25	0.66
4:C:333:GLU:OE2	4:C:337:ARG:NH2	2.27	0.66
4:C:646:GLU:HG2	4:C:647:LYS:HG3	1.78	0.66
5:D:517:TYR:HE2	7:F:131:MET:HG2	1.61	0.66
1:1:29:DT:H3'	9:S:204:ARG:NH1	2.09	0.66
5:D:152:HIS:CE1	5:D:154:GLU:HG2	2.30	0.66
9:S:140:PRO:HB3	9:S:238:LEU:HD21	1.77	0.66
4:C:424:THR:HG21	7:F:187:ARG:HH22	1.61	0.66
7:F:563:VAL:HG11	7:F:571:ARG:HH21	1.60	0.66
4:C:29:LEU:O	4:C:59:TYR:OH	2.13	0.65
3:B:170:MET:HE1	5:D:546:GLN:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:714:GLY:N	7:F:723:ALA:O	2.29	0.65
7:F:292:PRO:HG2	7:F:1127:GLU:HB3	1.78	0.65
7:F:711:VAL:HG11	7:F:717:VAL:HG22	1.79	0.65
7:F:515:LEU:O	7:F:869:ILE:N	2.25	0.64
2:2:58:DA:H2'	2:2:59:DG:C8	2.33	0.64
9:R:4:ARG:NH1	9:R:45:LEU:O	2.31	0.64
3:B:170:MET:HE1	5:D:546:GLN:CD	2.22	0.63
7:F:919:GLY:N	7:F:940:VAL:O	2.27	0.63
5:D:67:ASP:HB3	5:D:95:SER:H	1.63	0.63
1:1:18:DT:H3'	9:R:204:ARG:NH1	2.13	0.63
8:G:275:MET:HB3	8:G:277:MET:HG2	1.79	0.63
4:C:497:ILE:HG13	4:C:510:PRO:HB3	1.81	0.62
5:D:528:LYS:NZ	5:D:547:GLY:O	2.32	0.62
5:D:304:MET:CE	8:G:190:GLN:HB3	2.21	0.62
7:F:628:GLY:H	7:F:752:ASP:HA	1.64	0.62
7:F:151:ARG:HB2	7:F:166:ILE:HB	1.82	0.62
3:A:93:PRO:HA	3:A:141:VAL:O	1.99	0.62
4:C:746:LYS:HD2	4:C:770:ARG:HD2	1.81	0.62
7:F:845:ASP:HA	7:F:848:HIS:HA	1.82	0.62
7:F:997:ARG:NH2	7:F:1109:GLU:OE1	2.24	0.62
7:F:392:LEU:N	7:F:403:PHE:O	2.32	0.62
2:2:89:DC:H2''	2:2:90:DC:H5''	1.82	0.61
5:D:328:ARG:NH2	8:G:294:SER:OG	2.33	0.61
9:R:92:VAL:HA	9:R:95:PHE:CD2	2.34	0.61
4:C:75:ASP:HA	4:C:119:GLY:HA3	1.82	0.61
7:F:228:PHE:CE1	7:F:288:LYS:HB2	2.35	0.61
7:F:516:THR:HG22	7:F:868:VAL:HA	1.83	0.61
7:F:539:ILE:HB	7:F:834:GLU:HB3	1.82	0.61
9:S:92:VAL:HA	9:S:95:PHE:HD2	1.66	0.61
4:C:389:ARG:NH2	4:C:437:ALA:O	2.33	0.61
9:R:95:PHE:CE1	9:S:114:ALA:HB2	2.35	0.61
1:1:65:DA:OP2	8:G:214:LYS:HD3	2.01	0.61
4:C:1046:GLU:HG3	5:D:251:ILE:HD11	1.82	0.60
7:F:634:ILE:HG12	7:F:745:VAL:HG22	1.83	0.60
9:R:122:ARG:HH21	9:S:100:ASP:HB3	1.66	0.60
9:S:69:ARG:HA	9:S:75:ALA:HA	1.84	0.60
2:2:64:DT:H2''	2:2:65:DG:C8	2.37	0.60
9:S:69:ARG:NH1	9:S:75:ALA:O	2.34	0.60
1:1:35:DT:H4'	1:1:36:DC:OP1	2.01	0.60
9:S:36:ILE:HD12	9:S:58:ARG:NH2	2.16	0.60
7:F:910:VAL:HG23	7:F:946:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:232:MET:HE1	7:F:1112:SER:HA	1.83	0.60
7:F:399:ARG:NH1	7:F:401:GLU:OE2	2.31	0.60
8:G:150:LEU:O	8:G:154:ARG:HG3	2.01	0.60
7:F:442:THR:HG22	7:F:982:VAL:HG22	1.83	0.59
7:F:621:GLN:O	7:F:777:ARG:HD3	2.01	0.59
8:G:363:ILE:HD12	8:G:374:ILE:HG21	1.84	0.59
5:D:296:ILE:HD11	8:G:169:GLN:HG3	1.84	0.59
4:C:658:VAL:HG23	4:C:852:ILE:HG23	1.83	0.59
7:F:804:GLU:O	7:F:807:SER:OG	2.20	0.59
8:G:360:LEU:HD13	8:G:371:ARG:HE	1.68	0.59
8:G:372:GLU:O	8:G:376:GLN:NE2	2.36	0.59
4:C:814:ARG:NH2	4:C:958:ASP:OD2	2.36	0.59
7:F:390:PHE:H	7:F:405:ILE:HG12	1.68	0.59
2:2:74:DT:H2'	2:2:75:DT:H71	1.85	0.59
6:E:26:ARG:HH21	7:F:312:HIS:CG	2.20	0.59
2:2:72:DG:H5''	9:S:160:THR:HG22	1.84	0.59
7:F:544:VAL:HG23	7:F:763:GLN:HB2	1.85	0.59
4:C:940:ARG:HH12	7:F:131:MET:HE1	1.67	0.59
4:C:1056:VAL:HG12	5:D:11:VAL:HG22	1.84	0.59
7:F:272:ASN:OD1	7:F:272:ASN:N	2.36	0.59
3:A:34:THR:HG22	3:B:41:ARG:NE	2.15	0.58
7:F:997:ARG:NH1	7:F:1000:GLU:OE2	2.35	0.58
4:C:961:HIS:NE2	4:C:983:GLY:O	2.34	0.58
7:F:716:GLU:HA	7:F:722:THR:HA	1.85	0.58
1:1:67:DG:N2	4:C:233:GLU:OE2	2.35	0.58
5:D:404:LYS:NZ	8:G:319:GLU:OE1	2.30	0.58
4:C:693:GLU:HG3	4:C:807:ARG:HG3	1.84	0.58
4:C:1005:GLN:OE1	4:C:1033:ARG:NH2	2.36	0.58
7:F:642:ASN:HD21	8:G:107:ASP:H	1.52	0.58
7:F:924:ALA:N	7:F:937:SER:OG	2.36	0.58
4:C:424:THR:HG22	4:C:433:ILE:O	2.03	0.58
5:D:400:ILE:HG13	8:G:326:LEU:HD22	1.85	0.58
3:A:101:VAL:HG23	3:A:134:THR:HG22	1.86	0.57
4:C:418:ARG:NH2	4:C:474:GLU:OE2	2.35	0.57
9:R:32:ALA:HB2	9:R:41:LEU:HD12	1.85	0.57
9:R:122:ARG:NH2	9:S:100:ASP:O	2.36	0.57
4:C:530:LEU:HA	4:C:565:THR:HG21	1.87	0.57
9:S:36:ILE:HD12	9:S:58:ARG:HH21	1.69	0.57
1:1:27:DT:H2'	9:S:200:ARG:HH11	1.68	0.57
2:2:73:DC:H2'	2:2:74:DT:H71	1.85	0.57
7:F:924:ALA:HB2	7:F:937:SER:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:72:DG:H5''	9:S:160:THR:CG2	2.35	0.57
4:C:568:GLU:HB3	4:C:649:GLU:HB2	1.85	0.57
7:F:337:LEU:HD12	7:F:995:LEU:HD13	1.87	0.57
5:D:258:MET:HG3	5:D:268:THR:HG22	1.85	0.57
5:D:300:ASN:ND2	5:D:304:MET:HE3	2.17	0.57
9:S:140:PRO:HB3	9:S:238:LEU:CD2	2.34	0.57
3:A:62:HIS:HB2	4:C:783:ARG:HD2	1.85	0.57
7:F:118:LYS:O	7:F:122:GLU:HB2	2.05	0.56
7:F:293:LEU:HG	7:F:1127:GLU:HG2	1.86	0.56
4:C:401:ARG:HH12	4:C:429:ASN:CG	2.13	0.56
4:C:693:GLU:OE2	4:C:807:ARG:NE	2.31	0.56
4:C:792:ARG:NH2	4:C:799:PRO:O	2.38	0.56
7:F:207:LEU:HD21	7:F:1002:LEU:HD13	1.86	0.56
7:F:233:THR:HA	7:F:238:ILE:HA	1.87	0.56
7:F:910:VAL:HG21	7:F:945:PRO:HA	1.87	0.56
9:R:88:THR:O	9:R:92:VAL:HG23	2.06	0.56
1:1:24:DA:P	3:A:285:GLY:HA3	2.45	0.56
7:F:600:THR:OG1	7:F:601:GLY:N	2.36	0.56
4:C:390:ARG:HH12	4:C:423:GLU:HG2	1.70	0.56
7:F:642:ASN:ND2	8:G:106:ALA:HB3	2.18	0.56
7:F:1217:LEU:HD13	7:F:1226:ILE:HD13	1.86	0.56
4:C:45:ASP:HB2	4:C:341:THR:HG22	1.86	0.56
8:G:166:LYS:O	8:G:170:SER:OG	2.23	0.56
8:G:251:ILE:HG12	8:G:275:MET:HE3	1.88	0.56
9:R:101:ASP:OD2	9:R:115:ARG:NH1	2.35	0.56
9:R:66:GLN:OE1	9:S:135:ILE:HD11	2.06	0.56
1:1:31:DA:H1'	1:1:32:DA:H5'	1.88	0.55
9:R:200:ARG:HG2	9:R:228:TYR:OH	2.06	0.55
2:2:93:DT:H2'	2:2:94:DT:C5	2.40	0.55
4:C:857:LEU:HD12	7:F:138:ARG:HB2	1.89	0.55
7:F:202:TYR:OH	7:F:1199:GLN:NE2	2.39	0.55
7:F:641:VAL:HG11	7:F:666:ILE:HD11	1.89	0.55
4:C:557:ARG:O	4:C:654:GLN:NE2	2.39	0.55
7:F:499:LYS:N	7:F:502:ASP:OD2	2.27	0.55
7:F:520:GLY:HA2	7:F:863:VAL:HG23	1.89	0.55
5:D:537:LEU:HD22	5:D:612:ILE:HG23	1.88	0.55
7:F:440:LYS:HG2	7:F:984:GLU:HG2	1.88	0.55
1:1:18:DT:O5'	9:R:204:ARG:NH1	2.36	0.55
5:D:608:THR:HG22	5:D:610:GLY:H	1.72	0.55
3:B:108:ALA:HB1	3:B:119:VAL:HG11	1.89	0.55
7:F:199:ASP:N	7:F:199:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:226:GLY:HA3	7:F:289:VAL:O	2.07	0.54
1:1:58:DC:H2'	1:1:59:DT:H71	1.89	0.54
3:B:40:ARG:NH1	3:B:175:VAL:O	2.40	0.54
3:B:113:PHE:HB3	3:B:117:VAL:HB	1.89	0.54
5:D:422:ILE:HD12	5:D:445:PRO:HB2	1.89	0.54
5:D:514:LEU:HD21	7:F:56:VAL:HG11	1.88	0.54
7:F:694:HIS:CD2	7:F:721:LEU:HD21	2.43	0.54
7:F:1016:ARG:NH2	7:F:1086:GLU:OE1	2.33	0.54
4:C:695:GLU:OE1	4:C:805:VAL:HG22	2.06	0.54
2:2:93:DT:H2'	2:2:94:DT:C6	2.43	0.54
4:C:423:GLU:OE2	4:C:550:ARG:NE	2.37	0.54
5:D:265:ARG:HG2	8:G:290:GLN:OE1	2.08	0.54
5:D:513:VAL:HG21	7:F:17:LYS:HG3	1.90	0.54
7:F:602:GLY:HA2	7:F:636:GLU:HG2	1.89	0.54
7:F:697:ASP:N	7:F:697:ASP:OD1	2.41	0.54
7:F:814:ILE:HG12	7:F:830:LEU:HD22	1.90	0.54
9:S:53:PHD:CG	9:S:54:LEU:N	2.71	0.54
8:G:182:TYR:HB3	8:G:185:ARG:HD2	1.88	0.53
2:2:84:DC:H2''	2:2:85:DT:H5'	1.91	0.53
4:C:864:ASN:OD1	4:C:864:ASN:N	2.40	0.53
7:F:270:ASP:OD1	7:F:270:ASP:N	2.41	0.53
9:S:184:LEU:HG	9:S:199:ILE:HD11	1.89	0.53
4:C:305:ASP:O	4:C:311:ASN:ND2	2.32	0.53
1:1:12:DA:H2''	1:1:13:DA:C8	2.43	0.53
4:C:16:ASP:OD2	4:C:22:ARG:NH1	2.42	0.53
5:D:485:GLU:OE2	7:F:1234:THR:OG1	2.13	0.53
7:F:392:LEU:HB2	7:F:403:PHE:HB2	1.91	0.53
2:2:51:DT:H2''	2:2:52:DA:C8	2.43	0.53
7:F:383:ALA:HB1	7:F:411:ILE:O	2.08	0.53
9:R:141:LEU:HD21	9:R:143:LEU:HD21	1.91	0.53
1:1:17:DG:H2''	1:1:18:DT:H5'	1.90	0.53
7:F:1097:GLU:O	7:F:1101:ARG:HG3	2.09	0.53
4:C:44:THR:HG22	4:C:51:GLU:HG2	1.91	0.53
7:F:169:ASN:OD1	7:F:169:ASN:N	2.42	0.53
7:F:1008:LYS:HG3	7:F:1009:GLU:H	1.73	0.53
8:G:268:GLU:HB3	8:G:279:ILE:HD11	1.91	0.53
9:R:67:ARG:HG2	9:S:176:GLN:NE2	2.24	0.53
7:F:642:ASN:ND2	8:G:107:ASP:H	2.07	0.52
3:B:100:VAL:HG11	3:B:106:VAL:HG22	1.90	0.52
5:D:431:ARG:HD2	5:D:465:ALA:HB2	1.89	0.52
5:D:517:TYR:CE2	7:F:131:MET:HG2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:477:PRO:HB3	5:D:482:ALA:HB1	1.90	0.52
4:C:22:ARG:NH2	4:C:111:ASP:O	2.38	0.52
4:C:317:VAL:O	4:C:321:LEU:HB2	2.09	0.52
5:D:120:ILE:HB	5:D:121:PRO:HD3	1.92	0.52
4:C:663:TRP:HD1	4:C:666:TYR:HD2	1.56	0.52
9:R:69:ARG:NH1	9:R:75:ALA:O	2.42	0.52
4:C:598:THR:HG22	4:C:604:LYS:HG2	1.91	0.52
4:C:722:ASP:O	4:C:723:GLU:HG3	2.10	0.52
7:F:643:LYS:O	7:F:683:LEU:N	2.42	0.52
7:F:485:GLY:HA3	7:F:896:LEU:HD11	1.92	0.52
3:A:43:LEU:HD23	3:A:47:LEU:HD11	1.91	0.51
4:C:711:PRO:HB3	4:C:767:ARG:NH2	2.25	0.51
7:F:519:ARG:HA	7:F:865:PRO:HB3	1.92	0.51
7:F:717:VAL:N	7:F:721:LEU:O	2.44	0.51
7:F:487:VAL:HB	7:F:973:GLN:HG2	1.92	0.51
7:F:463:LYS:HD2	7:F:473:ILE:HD12	1.92	0.51
7:F:850:SER:OG	7:F:875:GLN:HB2	2.10	0.51
8:G:377:ILE:HG23	8:G:380:LYS:HE2	1.92	0.51
9:S:103:LEU:HD13	9:S:115:ARG:HE	1.75	0.51
1:1:25:DG:H2"	1:1:26:DG:C8	2.46	0.51
7:F:63:LEU:HD23	7:F:129:VAL:HG21	1.92	0.51
2:2:80:DC:H2"	2:2:81:DC:C6	2.46	0.51
4:C:890:ASP:OD1	4:C:890:ASP:N	2.41	0.51
4:C:986:ARG:HA	5:D:352:ARG:HA	1.91	0.51
5:D:118:LYS:O	5:D:317:ARG:NH1	2.39	0.51
7:F:271:ILE:HG23	7:F:275:LEU:HB3	1.92	0.51
8:G:359:THR:O	8:G:363:ILE:HG13	2.10	0.51
9:S:53:PHD:CG	9:S:54:LEU:H	2.24	0.51
7:F:78:LYS:O	7:F:82:GLU:HG3	2.10	0.51
9:R:147:ARG:HD2	9:S:175:GLY:O	2.11	0.51
9:S:69:ARG:HH11	9:S:75:ALA:C	2.19	0.51
3:B:53:THR:HG23	3:B:148:ARG:HH22	1.76	0.51
4:C:667:ASN:HB3	4:C:855:ASN:HB2	1.93	0.51
4:C:1013:ASP:OD2	4:C:1039:SER:OG	2.24	0.51
5:D:99:ARG:HB3	5:D:254:ASP:HB2	1.92	0.51
9:R:148:PHE:HE2	9:S:226:ALA:HB2	1.75	0.51
4:C:401:ARG:HD3	4:C:428:PRO:HB2	1.93	0.50
5:D:584:THR:HG22	5:D:593:ARG:HG2	1.92	0.50
7:F:1035:ILE:HG22	7:F:1039:GLY:HA2	1.93	0.50
8:G:384:LYS:HB3	8:G:384:LYS:HZ3	1.76	0.50
9:R:141:LEU:HD11	9:R:150:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:4:ARG:N	9:R:48:ASP:OD2	2.21	0.50
4:C:455:VAL:HG11	4:C:513:VAL:HG23	1.94	0.50
4:C:875:TRP:HB2	4:C:945:GLY:HA2	1.94	0.50
7:F:1180:LEU:HD22	7:F:1184:LYS:HD3	1.92	0.50
7:F:609:VAL:HG22	7:F:629:GLY:HA3	1.94	0.50
4:C:773:SER:OG	4:C:775:ARG:NH1	2.44	0.50
7:F:1222:GLU:O	7:F:1226:ILE:HG12	2.10	0.50
4:C:529:SER:O	4:C:565:THR:HG21	2.12	0.50
5:D:326:ASN:OD1	5:D:327:ASN:N	2.42	0.50
7:F:488:TYR:HE1	7:F:848:HIS:O	1.94	0.50
5:D:193:GLN:HE22	5:D:246:ASN:HD21	1.59	0.50
5:D:232:ASN:ND2	7:F:1211:GLU:HG2	2.27	0.50
1:1:21:DA:H4'	1:1:22:DG:OP1	2.11	0.50
9:S:152:TRP:CD2	9:S:210:LEU:HD22	2.47	0.50
5:D:70:CYS:SG	5:D:85:CYS:HB2	2.51	0.49
4:C:677:ARG:NH1	4:C:851:ASP:OD1	2.46	0.49
9:S:88:THR:O	9:S:92:VAL:HG23	2.12	0.49
4:C:776:VAL:HG12	4:C:780:GLU:HB2	1.94	0.49
5:D:96:ARG:O	5:D:99:ARG:HG2	2.12	0.49
7:F:642:ASN:ND2	8:G:107:ASP:N	2.60	0.49
7:F:1036:GLU:HG3	7:F:1040:THR:HB	1.94	0.49
7:F:1036:GLU:HB2	7:F:1040:THR:H	1.76	0.49
1:1:49:DC:H2'	1:1:50:DT:C6	2.48	0.49
4:C:41:SER:HB3	4:C:42:PRO:HD3	1.93	0.49
4:C:701:LEU:HD12	4:C:701:LEU:H	1.77	0.49
4:C:677:ARG:O	4:C:681:ASP:HB2	2.12	0.49
5:D:112:ALA:H	5:D:306:GLN:HE22	1.60	0.49
5:D:267:ALA:HA	8:G:293:ILE:O	2.13	0.49
4:C:1001:ALA:HB1	7:F:1229:LEU:HD22	1.94	0.49
4:C:194:ASN:OD1	4:C:195:GLU:HG3	2.11	0.49
7:F:442:THR:HB	7:F:980:LEU:HD11	1.95	0.49
7:F:649:ASN:N	7:F:649:ASN:OD1	2.45	0.49
3:A:269:ASP:O	3:A:272:SER:OG	2.29	0.49
7:F:447:THR:HB	7:F:978:LEU:HD11	1.95	0.49
8:G:101:ILE:O	8:G:173:ARG:NH2	2.46	0.49
2:2:55:DG:H2''	2:2:56:DA:C8	2.48	0.49
4:C:187:LYS:HG3	4:C:216:PHE:O	2.12	0.49
1:1:56:DT:OP2	8:G:243:HIS:NE2	2.40	0.49
4:C:411:ILE:HG13	7:F:187:ARG:CD	2.36	0.49
4:C:451:PRO:HB2	4:C:518:LEU:HD13	1.95	0.49
4:C:592:ALA:O	4:C:611:LYS:HE3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:537:LEU:HD23	5:D:557:VAL:HG21	1.93	0.49
7:F:177:THR:O	7:F:181:ILE:HG13	2.13	0.49
7:F:547:ASP:HB2	7:F:827:ARG:HD3	1.95	0.49
7:F:772:LEU:HD21	7:F:830:LEU:HD11	1.94	0.49
7:F:938:GLY:HA2	7:F:953:ALA:HB3	1.95	0.49
9:S:53:PHD:OP3	9:S:55:MET:N	2.45	0.49
9:S:69:ARG:NH2	9:S:77:ILE:O	2.45	0.49
1:1:27:DT:H2'	9:S:200:ARG:NH1	2.27	0.48
3:B:72:GLU:HB3	3:B:76:ASP:HB2	1.95	0.48
4:C:551:GLN:O	4:C:953:VAL:HG22	2.13	0.48
5:D:397:ILE:HG21	5:D:403:ALA:HB2	1.94	0.48
7:F:509:VAL:HG13	7:F:873:GLN:HB3	1.95	0.48
9:S:54:LEU:HD11	9:S:62:PHE:CZ	2.48	0.48
4:C:622:ASN:N	4:C:643:SER:OG	2.45	0.48
7:F:295:CYS:O	7:F:1131:ARG:NH1	2.38	0.48
4:C:382:LEU:O	4:C:386:THR:HG23	2.13	0.48
7:F:705:TYR:OH	7:F:717:VAL:O	2.29	0.48
1:1:29:DT:H2'	1:1:30:DT:C6	2.49	0.48
4:C:688:HIS:ND1	4:C:814:ARG:HG3	2.28	0.48
6:E:28:HIS:O	6:E:32:GLN:HG3	2.13	0.48
8:G:203:ALA:HB2	8:G:222:TRP:HB2	1.95	0.48
4:C:141:ASP:HB3	4:C:144:GLY:H	1.78	0.48
7:F:757:PRO:O	7:F:759:GLN:NE2	2.46	0.48
9:S:147:ARG:NH1	9:S:149:GLU:OE1	2.47	0.48
1:1:50:DT:H2''	1:1:51:DC:H5'	1.96	0.48
4:C:99:GLN:NE2	4:C:351:ALA:HB2	2.29	0.48
7:F:92:ILE:HG22	7:F:380:GLY:HA3	1.96	0.48
7:F:387:GLU:HB3	7:F:407:GLN:NE2	2.28	0.48
7:F:448:ASP:OD1	7:F:956:TYR:OH	2.32	0.48
3:A:27:LEU:HD13	3:A:32:GLY:HA2	1.96	0.48
5:D:611:ARG:O	5:D:615:ASN:ND2	2.40	0.48
7:F:681:ASP:OD1	7:F:681:ASP:N	2.46	0.48
9:R:88:THR:O	9:R:91:LYS:HB2	2.13	0.48
3:B:56:ARG:NH1	3:B:161:ASP:OD1	2.47	0.48
4:C:582:PRO:C	4:C:635:ARG:HG3	2.39	0.48
4:C:959:LYS:HD3	5:D:471:GLN:NE2	2.29	0.48
7:F:333:PRO:HB2	7:F:1119:ILE:HD13	1.95	0.48
7:F:512:GLU:HA	7:F:872:THR:O	2.14	0.48
7:F:600:THR:OG1	7:F:636:GLU:O	2.32	0.48
8:G:325:ASN:O	8:G:328:ARG:HG2	2.14	0.48
9:S:68:LEU:O	9:S:74:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:422:ILE:O	4:C:543:LEU:HD13	2.14	0.47
4:C:963:ARG:NH2	4:C:975:PRO:HB3	2.28	0.47
7:F:1019:VAL:O	7:F:1034:VAL:HA	2.14	0.47
8:G:340:PRO:HA	8:G:343:ARG:NE	2.28	0.47
9:R:53:PHD:HA	9:R:82:LEU:HB2	1.95	0.47
9:S:4:ARG:N	9:S:48:ASP:OD2	2.24	0.47
3:A:296:LEU:HD23	3:A:299:ILE:HD11	1.95	0.47
5:D:399:ASN:OD1	5:D:399:ASN:N	2.47	0.47
7:F:246:LEU:HD11	7:F:287:VAL:HG21	1.95	0.47
7:F:713:ALA:HB2	7:F:725:GLN:HA	1.96	0.47
7:F:1170:MET:SD	7:F:1170:MET:N	2.87	0.47
8:G:331:LEU:O	8:G:334:VAL:HG22	2.14	0.47
1:1:65:DA:H8	8:G:216:SER:OG	1.97	0.47
4:C:14:LEU:HD23	4:C:14:LEU:HA	1.74	0.47
4:C:506:THR:OG1	4:C:507:THR:N	2.47	0.47
4:C:663:TRP:CG	4:C:664:GLU:H	2.33	0.47
5:D:67:ASP:OD1	5:D:67:ASP:N	2.48	0.47
7:F:998:ILE:HG13	7:F:1113:VAL:HG11	1.96	0.47
8:G:258:LEU:HD11	8:G:274:ARG:HG3	1.97	0.47
9:S:82:LEU:HB3	9:S:105:LYS:HE3	1.96	0.47
3:A:56:ARG:NH2	3:A:138:GLU:OE1	2.47	0.47
4:C:626:ILE:HG22	4:C:639:ILE:O	2.15	0.47
4:C:973:GLN:HG3	4:C:1015:MET:SD	2.54	0.47
5:D:304:MET:SD	8:G:194:GLN:HG3	2.55	0.47
5:D:423:GLU:O	6:E:55:LYS:HD2	2.14	0.47
7:F:57:SER:OG	7:F:58:ILE:N	2.48	0.47
7:F:98:PHE:CE1	7:F:163:ASP:HB3	2.50	0.47
7:F:507:GLY:HA2	7:F:875:GLN:HB3	1.97	0.47
7:F:606:TYR:CD2	7:F:782:ASP:HB2	2.50	0.47
7:F:628:GLY:N	7:F:752:ASP:HA	2.30	0.47
7:F:1021:HIS:NE2	7:F:1035:ILE:HD11	2.28	0.47
8:G:349:ARG:NH1	8:G:359:THR:HA	2.30	0.47
9:R:53:PHD:OD1	9:R:54:LEU:N	2.47	0.47
9:R:69:ARG:NH2	9:R:100:ASP:OD2	2.48	0.47
1:1:13:DA:O5'	1:1:13:DA:H8	1.97	0.47
1:1:29:DT:H3'	9:S:204:ARG:HH22	1.80	0.47
4:C:376:MET:HG3	4:C:377:ASP:N	2.29	0.47
5:D:501:THR:HG23	5:D:503:GLN:H	1.80	0.47
7:F:98:PHE:HE1	7:F:163:ASP:HB3	1.79	0.47
7:F:168:THR:OG1	7:F:178:GLU:OE1	2.33	0.47
9:R:88:THR:HA	9:R:91:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:103:LEU:HD13	9:S:115:ARG:NE	2.30	0.47
4:C:225:LEU:HD12	4:C:229:LEU:HG	1.96	0.47
4:C:587:ILE:HD12	4:C:627:VAL:HG21	1.97	0.47
7:F:1011:CYS:SG	7:F:1065:ALA:HB1	2.55	0.47
8:G:321:GLU:HA	8:G:324:LYS:HD3	1.97	0.47
2:2:65:DG:H2"	2:2:66:DA:OP2	2.12	0.47
3:A:206:GLN:HE21	3:A:206:GLN:HB2	1.55	0.47
3:A:224:LYS:O	3:B:210:SER:OG	2.24	0.47
5:D:363:VAL:HB	5:D:467:PHE:CE2	2.50	0.47
3:B:14:ALA:C	3:B:16:GLN:H	2.22	0.46
3:B:82:ARG:NH2	5:D:539:ASP:OD2	2.48	0.46
3:B:108:ALA:HB2	3:B:124:HIS:HB3	1.95	0.46
4:C:284:ILE:O	4:C:288:ILE:HG13	2.14	0.46
4:C:711:PRO:HD2	4:C:771:ASP:HB2	1.97	0.46
7:F:279:ILE:HG23	7:F:284:ILE:HG13	1.97	0.46
1:1:14:DA:H2"	1:1:15:DA:OP2	2.16	0.46
2:2:61:DA:H2"	2:2:62:DA:C8	2.50	0.46
4:C:694:ILE:HD11	4:C:742:LYS:HD3	1.97	0.46
7:F:700:ASP:OD1	7:F:700:ASP:N	2.47	0.46
2:2:88:DA:C5	2:2:89:DC:C4	3.04	0.46
3:A:147:TYR:OH	4:C:815:LYS:NZ	2.46	0.46
4:C:656:ILE:HD11	4:C:949:MET:HG3	1.96	0.46
4:C:668:TYR:CE2	4:C:669:GLU:HG3	2.50	0.46
3:A:108:ALA:HB2	3:A:124:HIS:HB3	1.97	0.46
4:C:201:ARG:NH1	4:C:298:LEU:HD21	2.30	0.46
5:D:62:PHE:HE1	5:D:102:MET:O	1.99	0.46
1:1:63:DA:H2"	1:1:64:DG:C8	2.51	0.46
4:C:280:THR:O	4:C:284:ILE:HD12	2.15	0.46
4:C:308:HIS:HD2	4:C:412:HIS:HE1	1.63	0.46
2:2:78:DG:C2	2:2:79:DA:C4	3.03	0.46
3:A:56:ARG:HD3	3:A:161:ASP:HB3	1.96	0.46
4:C:971:VAL:O	5:D:99:ARG:NH2	2.49	0.46
5:D:499:PRO:HB3	7:F:311:ALA:HB2	1.96	0.46
7:F:275:LEU:O	7:F:279:ILE:HG13	2.15	0.46
7:F:838:ILE:HD11	7:F:855:LEU:HD21	1.97	0.46
7:F:1208:ALA:HA	7:F:1213:LYS:HE3	1.98	0.46
4:C:18:VAL:HG13	4:C:22:ARG:NH1	2.31	0.46
7:F:1004:ALA:HB1	7:F:1074:HIS:HE2	1.79	0.46
7:F:112:LEU:HD23	7:F:150:MET:HB2	1.98	0.46
7:F:307:GLY:O	7:F:316:VAL:HG22	2.16	0.46
7:F:644:ASP:OD1	7:F:645:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:347:ARG:HH21	8:G:353:ASP:CG	2.22	0.46
3:B:82:ARG:NH2	3:B:147:TYR:OH	2.49	0.46
4:C:357:LYS:HB3	4:C:357:LYS:HE2	1.78	0.46
7:F:976:ASP:OD1	7:F:976:ASP:N	2.48	0.46
5:D:58:CYS:SG	5:D:60:LYS:N	2.89	0.46
7:F:472:ARG:NH2	7:F:967:GLU:OE2	2.48	0.46
3:A:45:SER:HB2	4:C:839:GLU:HG2	1.99	0.45
4:C:778:ASN:OD1	4:C:778:ASN:N	2.48	0.45
7:F:95:VAL:HG21	7:F:983:PHE:CD2	2.50	0.45
7:F:1097:GLU:CD	7:F:1100:ARG:HH21	2.23	0.45
8:G:359:THR:H	8:G:362:GLU:CD	2.24	0.45
9:R:184:LEU:HG	9:R:199:ILE:HD11	1.98	0.45
2:2:56:DA:H2''	2:2:57:DG:H8	1.81	0.45
3:A:69:GLY:HA3	3:A:133:ALA:HB2	1.97	0.45
5:D:573:GLU:HB3	5:D:586:THR:O	2.17	0.45
1:1:29:DT:H5''	9:S:204:ARG:CZ	2.46	0.45
3:B:103:PRO:HG3	3:B:131:GLU:HG2	1.98	0.45
4:C:663:TRP:HD1	4:C:666:TYR:CD2	2.35	0.45
4:C:742:LYS:H	4:C:773:SER:HB3	1.82	0.45
7:F:781:GLN:N	7:F:784:GLU:OE1	2.29	0.45
8:G:236:ARG:HH12	8:G:289:ALA:C	2.24	0.45
1:1:55:DA:H5''	5:D:47:ARG:HH12	1.81	0.45
3:A:90:SER:HB3	3:A:92:GLN:OE1	2.16	0.45
4:C:560:ARG:HG3	4:C:646:GLU:HB3	1.97	0.45
4:C:583:VAL:HG21	4:C:605:TYR:CE1	2.52	0.45
7:F:92:ILE:CG2	7:F:380:GLY:HA3	2.47	0.45
7:F:154:MET:HE3	7:F:154:MET:HB3	1.76	0.45
7:F:239:LEU:HB3	7:F:1115:GLN:OE1	2.17	0.45
7:F:497:THR:N	7:F:510:LEU:O	2.26	0.45
7:F:680:ASN:N	7:F:680:ASN:OD1	2.49	0.45
2:2:65:DG:H2''	2:2:66:DA:H8	1.81	0.45
3:A:22:PHE:CE2	3:A:206:GLN:HG3	2.51	0.45
4:C:1010:VAL:O	4:C:1018:ARG:HG2	2.17	0.45
4:C:1014:ASP:O	4:C:1018:ARG:HG3	2.17	0.45
5:D:373:GLY:HA3	5:D:454:GLN:HB2	1.98	0.45
5:D:520:THR:HG21	7:F:15:ILE:N	2.31	0.45
7:F:370:ALA:HB2	7:F:390:PHE:CD2	2.52	0.45
7:F:729:ALA:HA	7:F:741:LEU:O	2.16	0.45
7:F:776:GLN:HB3	7:F:795:LEU:HD11	1.98	0.45
2:2:70:DG:H2''	2:2:71:DA:N7	2.31	0.45
2:2:71:DA:H2''	2:2:72:DG:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:233:GLU:OE1	8:G:96:GLN:NE2	2.47	0.45
4:C:453:TRP:CZ3	4:C:462:LYS:HE3	2.52	0.45
5:D:251:ILE:HG12	5:D:252:PRO:HD2	1.99	0.45
5:D:355:TYR:HB3	5:D:476:VAL:HG13	1.99	0.45
5:D:411:ASP:HB3	5:D:414:ILE:HG12	1.98	0.45
6:E:37:ALA:HB1	6:E:56:PRO:HB2	1.98	0.45
7:F:94:GLU:OE2	7:F:97:ARG:NH2	2.46	0.45
7:F:441:ALA:HB3	7:F:983:PHE:HE1	1.81	0.45
1:1:37:DG:H2"	1:1:38:DG:C8	2.51	0.45
3:B:79:LEU:HD23	3:B:79:LEU:HA	1.76	0.45
4:C:644:ALA:O	4:C:651:ALA:N	2.43	0.45
4:C:694:ILE:CG2	4:C:806:VAL:HB	2.46	0.45
4:C:735:SER:OG	4:C:778:ASN:HA	2.16	0.45
4:C:820:ASP:O	4:C:832:ILE:HD12	2.17	0.45
4:C:988:GLY:N	4:C:991:GLU:OE1	2.47	0.45
5:D:432:ALA:HB3	5:D:433:PRO:HD3	1.98	0.45
7:F:941:ARG:HB3	7:F:949:GLN:HB3	1.99	0.45
9:S:221:LYS:NZ	9:S:231:GLU:OE1	2.33	0.45
3:B:76:ASP:O	3:B:80:ASN:ND2	2.50	0.45
4:C:959:LYS:HD3	5:D:471:GLN:HE21	1.81	0.45
5:D:550:ASP:OD1	5:D:551:LEU:N	2.48	0.45
7:F:207:LEU:O	7:F:210:VAL:HG12	2.16	0.45
9:S:30:ARG:HG3	9:S:45:LEU:HD13	1.99	0.45
9:S:101:ASP:OD2	9:S:115:ARG:NH1	2.43	0.45
9:S:219:TYR:CE1	9:S:233:PRO:HD3	2.51	0.45
4:C:171:TRP:CG	4:C:179:LYS:HD2	2.51	0.45
4:C:1019:ASN:OD1	4:C:1019:ASN:N	2.46	0.45
4:C:710:ILE:HD12	4:C:771:ASP:OD1	2.17	0.44
5:D:142:ASN:OD1	8:G:93:LEU:HD13	2.17	0.44
5:D:170:GLU:HA	5:D:173:ILE:HG22	1.99	0.44
5:D:356:SER:HA	5:D:474:VAL:O	2.18	0.44
7:F:150:MET:HG3	7:F:167:LYS:HA	1.99	0.44
2:2:52:DA:H2"	2:2:53:DA:C8	2.52	0.44
5:D:127:LEU:HD12	5:D:243:MET:HE1	1.99	0.44
7:F:1034:VAL:O	7:F:1041:GLN:HA	2.16	0.44
7:F:1073:PRO:HB2	7:F:1179:LEU:HD22	1.98	0.44
2:2:71:DA:H2"	2:2:72:DG:H8	1.82	0.44
3:A:147:TYR:CE1	3:A:166:ASP:HB3	2.52	0.44
4:C:294:LEU:HD21	4:C:303:VAL:HG12	1.97	0.44
7:F:454:ARG:HE	7:F:921:LEU:HD11	1.82	0.44
7:F:607:SER:HB3	7:F:630:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:340:PRO:O	8:G:343:ARG:HG2	2.16	0.44
9:S:119:LEU:HD23	9:S:122:ARG:HH11	1.83	0.44
9:S:219:TYR:HE1	9:S:233:PRO:HD3	1.83	0.44
1:1:15:DA:H1'	1:1:16:DG:H5'	1.98	0.44
4:C:18:VAL:HG21	4:C:388:LYS:HD3	1.99	0.44
4:C:499:VAL:HG23	4:C:506:THR:HG23	2.00	0.44
5:D:93:THR:OG1	5:D:94:GLU:N	2.50	0.44
5:D:520:THR:HG21	7:F:15:ILE:H	1.83	0.44
4:C:81:GLN:HG2	4:C:102:PHE:HE1	1.81	0.44
4:C:559:GLU:HA	4:C:646:GLU:OE1	2.18	0.44
7:F:337:LEU:HD22	7:F:1117:GLN:OE1	2.18	0.44
1:1:21:DA:H2''	1:1:22:DG:O5'	2.17	0.44
5:D:168:GLU:OE2	5:D:172:GLN:NE2	2.50	0.44
8:G:156:ARG:HA	8:G:159:ARG:HD2	1.99	0.44
8:G:183:MET:H	8:G:183:MET:HG2	1.65	0.44
5:D:331:LYS:HE2	5:D:336:ILE:HA	2.00	0.44
8:G:380:LYS:O	8:G:384:LYS:HG3	2.17	0.44
4:C:670:ASP:OD1	4:C:862:ARG:NH1	2.51	0.44
4:C:889:PHE:O	4:C:892:MET:HE2	2.17	0.44
7:F:510:LEU:HD11	7:F:876:CYS:HB2	2.00	0.44
7:F:1008:LYS:HG3	7:F:1009:GLU:N	2.32	0.44
7:F:1145:THR:HA	7:F:1165:MET:HE3	2.00	0.44
2:2:90:DC:H2'	2:2:91:DT:H71	1.99	0.44
4:C:579:ILE:HB	4:C:640:ALA:HB3	1.98	0.44
9:S:53:PHD:P	9:S:55:MET:H	2.41	0.44
2:2:95:DC:H2''	2:2:96:DA:C8	2.53	0.43
8:G:360:LEU:O	8:G:364:GLY:N	2.48	0.43
9:R:100:ASP:O	9:S:122:ARG:NH2	2.47	0.43
3:B:3:PHE:HA	3:B:26:PRO:HD2	2.00	0.43
3:B:161:ASP:HB3	3:B:162:PHE:H	1.68	0.43
4:C:112:ARG:NH2	4:C:121:GLU:OE1	2.50	0.43
4:C:722:ASP:HB3	4:C:728:ARG:HG2	1.99	0.43
5:D:69:GLU:HG3	5:D:76:LYS:HG2	1.99	0.43
7:F:211:SER:O	7:F:323:GLY:HA3	2.18	0.43
3:A:73:ASP:OD1	3:A:73:ASP:N	2.51	0.43
5:D:380:ILE:HD13	5:D:418:LEU:HD22	1.99	0.43
7:F:642:ASN:HD21	8:G:107:ASP:N	2.16	0.43
8:G:358:LYS:HB3	8:G:362:GLU:OE1	2.18	0.43
2:2:69:DC:H2'	2:2:70:DG:C8	2.54	0.43
4:C:233:GLU:CD	8:G:96:GLN:HE21	2.26	0.43
4:C:431:GLY:HA2	7:F:187:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:930:TYR:HA	4:C:937:PRO:HA	2.00	0.43
4:C:995:LEU:HD23	4:C:995:LEU:HA	1.84	0.43
5:D:342:GLY:O	5:D:346:GLN:HB2	2.19	0.43
7:F:34:ALA:O	7:F:38:VAL:HG23	2.18	0.43
8:G:126:ARG:HB2	8:G:142:TRP:CZ2	2.53	0.43
9:R:185:LYS:O	9:R:189:GLY:HA2	2.18	0.43
9:S:69:ARG:NH1	9:S:77:ILE:O	2.51	0.43
3:A:41:ARG:NH1	3:B:30:GLY:O	2.51	0.43
3:A:150:ILE:HG22	3:A:152:ARG:H	1.83	0.43
4:C:321:LEU:HD23	4:C:321:LEU:HA	1.88	0.43
4:C:879:LEU:HD23	4:C:879:LEU:HA	1.84	0.43
7:F:161:ILE:HD13	7:F:347:VAL:N	2.34	0.43
5:D:71:HIS:HB2	5:D:90:VAL:HG21	2.00	0.43
5:D:436:HIS:NE2	5:D:438:LEU:HB2	2.34	0.43
8:G:148:SER:OG	8:G:153:PHE:HB2	2.19	0.43
9:R:85:LEU:HD13	9:R:104:THR:OG1	2.19	0.43
3:B:100:VAL:HG13	3:B:129:LEU:HD22	2.01	0.43
4:C:197:TYR:CE1	4:C:203:PRO:HB2	2.53	0.43
4:C:880:LEU:HD21	4:C:908:GLU:HG2	2.01	0.43
7:F:488:TYR:HD1	7:F:847:THR:O	2.01	0.43
5:D:287:ARG:O	5:D:291:ILE:HG12	2.18	0.43
7:F:256:LEU:HD23	7:F:263:VAL:HA	2.01	0.43
8:G:122:LEU:HG	8:G:142:TRP:CZ2	2.53	0.43
4:C:279:LEU:HD23	4:C:279:LEU:HA	1.81	0.43
5:D:503:GLN:HE21	7:F:21:LYS:HE2	1.84	0.43
7:F:20:LEU:HD22	7:F:43:LEU:HD13	2.01	0.43
9:S:190:TYR:HB3	9:S:194:ASP:OD2	2.19	0.43
4:C:452:PHE:HB3	4:C:515:TYR:HB3	2.01	0.43
4:C:694:ILE:HG22	4:C:806:VAL:HB	2.01	0.43
1:1:29:DT:C3'	9:S:204:ARG:HH12	2.18	0.42
2:2:62:DA:H2'	2:2:63:DT:H71	2.01	0.42
3:B:50:THR:HG21	3:B:88:ALA:HB3	2.00	0.42
4:C:639:ILE:HD13	4:C:639:ILE:HA	1.81	0.42
4:C:804:MET:HE3	4:C:804:MET:HB2	1.72	0.42
5:D:106:LYS:HA	5:D:247:VAL:HG12	2.00	0.42
5:D:608:THR:HG22	5:D:610:GLY:N	2.33	0.42
7:F:771:ARG:NE	7:F:802:GLU:OE1	2.52	0.42
7:F:907:ASP:O	7:F:908:LEU:HD23	2.19	0.42
9:S:201:VAL:O	9:S:204:ARG:HB3	2.19	0.42
1:1:28:DC:H2'	1:1:29:DT:C7	2.49	0.42
3:B:19:TYR:OH	3:B:21:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:92:GLU:OE1	4:C:92:GLU:N	2.52	0.42
4:C:128:ILE:HG13	4:C:391:LEU:HB3	2.01	0.42
4:C:423:GLU:OE1	4:C:527:ALA:HB3	2.20	0.42
4:C:741:GLY:HA2	4:C:773:SER:HB3	2.01	0.42
7:F:246:LEU:HD22	7:F:271:ILE:HD13	2.00	0.42
7:F:564:ILE:HD11	7:F:574:LEU:HD13	2.01	0.42
7:F:674:VAL:HA	7:F:687:VAL:O	2.19	0.42
1:1:27:DT:H2''	1:1:28:DC:H6	1.84	0.42
2:2:80:DC:H2''	2:2:81:DC:C5	2.54	0.42
4:C:555:LEU:HD22	4:C:684:TYR:HA	1.99	0.42
5:D:42:GLU:HB3	5:D:52:GLU:HG3	2.01	0.42
7:F:1128:VAL:O	7:F:1132:GLN:HG2	2.19	0.42
9:S:218:ARG:NH2	9:S:241:HIS:HE1	2.17	0.42
1:1:24:DA:O5'	3:A:285:GLY:HA3	2.18	0.42
1:1:57:DC:OP1	8:G:239:ARG:NH2	2.52	0.42
4:C:167:ASN:HB2	4:C:169:LEU:HD23	2.00	0.42
4:C:201:ARG:HH11	4:C:298:LEU:HD21	1.84	0.42
4:C:245:GLU:HA	4:C:249:PHE:HB2	2.02	0.42
4:C:541:ARG:HD2	4:C:541:ARG:HA	1.77	0.42
4:C:879:LEU:HD13	4:C:918:VAL:HG11	2.01	0.42
5:D:284:ARG:NH1	5:D:301:GLU:OE2	2.52	0.42
5:D:584:THR:O	5:D:584:THR:OG1	2.33	0.42
9:R:101:ASP:OD2	9:R:115:ARG:HD3	2.18	0.42
2:2:59:DG:H2''	2:2:60:DA:C8	2.54	0.42
4:C:595:ILE:HD11	4:C:625:PRO:HB3	2.01	0.42
5:D:22:ARG:O	5:D:26:GLU:HB2	2.19	0.42
5:D:297:ILE:HD13	8:G:197:SER:HB3	2.01	0.42
7:F:539:ILE:O	7:F:833:ILE:HA	2.20	0.42
2:2:81:DC:H2'	2:2:82:DT:H71	2.01	0.42
3:B:103:PRO:HD3	3:B:131:GLU:HA	2.02	0.42
4:C:364:LYS:NZ	4:C:364:LYS:HB3	2.35	0.42
4:C:1044:MET:HE3	4:C:1044:MET:HB3	1.77	0.42
5:D:391:LEU:HB3	5:D:397:ILE:HG13	2.02	0.42
7:F:293:LEU:HD22	7:F:1103:GLN:CD	2.45	0.42
7:F:315:MET:HE3	7:F:315:MET:HB3	1.77	0.42
9:S:4:ARG:O	9:S:48:ASP:N	2.51	0.42
3:A:239:THR:HB	3:A:240:PRO:HD2	2.00	0.42
4:C:37:LEU:HD23	4:C:37:LEU:HA	1.92	0.42
4:C:699:THR:OG1	4:C:702:GLY:O	2.24	0.42
4:C:788:ARG:HG3	4:C:807:ARG:HB2	2.00	0.42
5:D:113:HIS:HB3	5:D:116:TYR:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:103:LEU:HD12	8:G:103:LEU:H	1.84	0.42
1:1:44:DT:H2'	1:1:45:DT:C7	2.50	0.42
1:1:69:DT:H6	1:1:69:DT:H2'	1.59	0.42
2:2:65:DG:H2''	2:2:66:DA:C8	2.55	0.42
4:C:99:GLN:HE22	4:C:351:ALA:HB2	1.85	0.42
5:D:622:LEU:HD23	5:D:622:LEU:HA	1.89	0.42
3:A:53:THR:HB	3:A:148:ARG:HH22	1.84	0.42
4:C:138:SER:HB2	4:C:148:HIS:CE1	2.54	0.42
4:C:800:PRO:HB2	8:G:290:GLN:NE2	2.35	0.42
5:D:359:SER:OG	5:D:451:ARG:O	2.36	0.42
5:D:481:GLU:OE2	6:E:38:LYS:HD2	2.20	0.42
7:F:508:ASP:O	7:F:875:GLN:HA	2.20	0.42
7:F:623:TYR:O	7:F:777:ARG:HA	2.20	0.42
7:F:995:LEU:HD12	7:F:995:LEU:HA	1.90	0.42
9:R:218:ARG:NH2	9:R:241:HIS:HE1	2.18	0.42
1:1:27:DT:H4'	9:S:224:TYR:CE1	2.55	0.42
4:C:406:PHE:HZ	7:F:188:LYS:HG2	1.85	0.42
9:R:53:PHD:OP3	9:R:55:MET:HB2	2.20	0.42
4:C:381:PRO:HD2	4:C:644:ALA:HB3	2.02	0.41
4:C:907:SER:O	4:C:911:GLU:HG2	2.20	0.41
4:C:975:PRO:HG2	5:D:352:ARG:O	2.20	0.41
7:F:1050:GLN:H	7:F:1050:GLN:CD	2.24	0.41
9:S:71:ASP:O	9:S:75:ALA:N	2.53	0.41
7:F:440:LYS:HA	7:F:984:GLU:HA	2.02	0.41
8:G:370:THR:OG1	8:G:371:ARG:N	2.51	0.41
9:S:69:ARG:NH2	9:S:100:ASP:OD2	2.53	0.41
1:1:41:DC:H1'	1:1:42:DA:C8	2.56	0.41
7:F:174:LEU:HB3	7:F:178:GLU:HB2	2.02	0.41
7:F:219:VAL:HG22	7:F:318:MET:HE1	2.01	0.41
7:F:770:ILE:HG12	7:F:801:LEU:HD11	2.00	0.41
9:R:147:ARG:NH1	9:R:149:GLU:OE1	2.54	0.41
1:1:69:DT:H4'	1:1:70:DT:OP1	2.20	0.41
4:C:271:ASN:OD1	4:C:271:ASN:N	2.53	0.41
7:F:562:TYR:HB2	7:F:574:LEU:HB3	2.01	0.41
7:F:968:ASP:OD1	7:F:969:LYS:HG3	2.21	0.41
7:F:1004:ALA:HB1	7:F:1074:HIS:NE2	2.35	0.41
9:S:71:ASP:HB3	9:S:74:THR:OG1	2.21	0.41
4:C:40:PHE:CD1	4:C:329:LEU:HD13	2.55	0.41
4:C:685:THR:HA	4:C:814:ARG:O	2.21	0.41
5:D:58:CYS:SG	5:D:61:ILE:N	2.93	0.41
5:D:395:HIS:NE2	5:D:413:LEU:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:126:LEU:HD23	7:F:126:LEU:HA	1.79	0.41
7:F:146:GLN:HB3	7:F:151:ARG:HD3	2.03	0.41
7:F:550:THR:OG1	7:F:565:GLU:O	2.33	0.41
8:G:299:ILE:HD13	8:G:299:ILE:HA	1.92	0.41
1:1:18:DT:OP2	9:R:204:ARG:HD2	2.20	0.41
3:A:182:ALA:HB3	3:A:190:ILE:HG22	2.01	0.41
7:F:385:LEU:HD12	7:F:409:SER:O	2.21	0.41
9:S:80:LEU:HD13	9:S:101:ASP:HB3	2.02	0.41
3:A:74:VAL:O	3:A:78:LEU:HG	2.21	0.41
4:C:30:GLU:O	4:C:34:ILE:HD12	2.20	0.41
4:C:112:ARG:HD2	4:C:575:SER:O	2.19	0.41
5:D:456:HIS:CD2	5:D:457:PRO:HD2	2.56	0.41
7:F:387:GLU:HA	7:F:408:GLY:H	1.85	0.41
7:F:819:ASP:OD2	7:F:822:ASP:N	2.49	0.41
9:R:100:ASP:HB3	9:S:122:ARG:NH2	2.31	0.41
2:2:92:DT:H2"	2:2:93:DT:H71	2.02	0.41
4:C:263:LYS:HB3	4:C:263:LYS:HE2	1.90	0.41
7:F:899:ARG:HE	7:F:899:ARG:HB2	1.75	0.41
3:A:52:VAL:HG22	3:A:141:VAL:HG12	2.03	0.41
3:A:147:TYR:HE1	3:A:166:ASP:HB3	1.86	0.41
3:B:221:GLU:HB3	3:B:222:PRO:HD3	2.03	0.41
4:C:208:LYS:HB2	4:C:208:LYS:HE3	1.77	0.41
4:C:399:LEU:CD1	4:C:408:VAL:HG11	2.50	0.41
4:C:891:GLU:OE2	4:C:898:SER:OG	2.21	0.41
4:C:1037:PRO:HD2	7:F:1226:ILE:O	2.21	0.41
5:D:149:PRO:O	5:D:183:ILE:HG22	2.21	0.41
5:D:328:ARG:HH21	8:G:294:SER:CB	2.34	0.41
7:F:95:VAL:HG11	7:F:983:PHE:CZ	2.53	0.41
7:F:151:ARG:NH2	7:F:182:SER:HB3	2.36	0.41
7:F:524:ARG:NE	7:F:540:ILE:HD11	2.36	0.41
7:F:1139:ILE:O	7:F:1149:PRO:HA	2.20	0.41
7:F:1229:LEU:HD23	7:F:1229:LEU:HA	1.96	0.41
8:G:165:ASP:O	8:G:169:GLN:HB2	2.21	0.41
9:R:4:ARG:O	9:R:48:ASP:N	2.50	0.41
9:R:148:PHE:CE2	9:S:226:ALA:HB2	2.55	0.41
9:R:157:VAL:HG11	9:R:209:LYS:HB3	2.03	0.41
1:1:38:DG:H2"	1:1:39:DC:C6	2.56	0.41
5:D:40:LYS:O	5:D:55:GLY:HA2	2.21	0.41
7:F:76:ALA:O	7:F:80:ILE:HG12	2.21	0.41
7:F:927:GLN:HE21	7:F:930:ASP:HA	1.85	0.41
7:F:963:VAL:HB	7:F:980:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:1137:VAL:HG23	7:F:1177:PRO:HA	2.02	0.41
9:R:142:THR:HB	9:R:151:ILE:HB	2.03	0.41
2:2:67:DG:H2"	2:2:68:DC:C6	2.56	0.40
4:C:154:PRO:HG3	4:C:254:TYR:CE1	2.56	0.40
4:C:162:PHE:CD1	4:C:172:VAL:HG22	2.55	0.40
4:C:691:LYS:HE3	4:C:691:LYS:HB3	1.82	0.40
5:D:359:SER:HB3	5:D:453:ILE:HG13	2.03	0.40
5:D:402:GLN:HG3	5:D:405:LYS:HE2	2.03	0.40
5:D:442:ALA:HB3	5:D:491:LEU:HA	2.03	0.40
7:F:771:ARG:HE	7:F:802:GLU:CD	2.29	0.40
7:F:1077:LEU:HD13	7:F:1102:VAL:HG21	2.03	0.40
1:1:37:DG:H2"	1:1:38:DG:H8	1.86	0.40
4:C:523:ILE:HG13	4:C:524:ILE:HG23	2.03	0.40
5:D:503:GLN:HB3	7:F:21:LYS:HE3	2.02	0.40
6:E:27:TYR:HB3	7:F:1234:THR:HA	2.02	0.40
7:F:206:ARG:HB3	7:F:1182:ILE:HG23	2.02	0.40
7:F:643:LYS:HB3	7:F:647:LEU:HD12	2.02	0.40
9:R:114:ALA:HB2	9:S:95:PHE:CE1	2.41	0.40
9:S:17:LEU:O	9:S:21:ASN:ND2	2.53	0.40
9:S:139:GLY:HA3	9:S:140:PRO:HD3	1.89	0.40
2:2:92:DT:C2'	2:2:93:DT:H71	2.51	0.40
3:B:72:GLU:OE2	3:B:125:TYR:OH	2.31	0.40
3:B:129:LEU:HD11	3:B:135:LEU:HB2	2.04	0.40
4:C:452:PHE:CD2	4:C:469:MET:HE2	2.57	0.40
5:D:80:HIS:HB3	5:D:83:ILE:HD12	2.04	0.40
5:D:370:HIS:HB3	5:D:493:SER:HB3	2.03	0.40
7:F:218:GLU:C	7:F:318:MET:HE1	2.47	0.40
7:F:472:ARG:CZ	7:F:967:GLU:HG2	2.51	0.40
7:F:575:LEU:HD11	7:F:590:GLU:HB2	2.03	0.40
7:F:963:VAL:O	7:F:979:VAL:HG23	2.21	0.40
7:F:1146:ILE:O	7:F:1146:ILE:HG22	2.21	0.40
9:R:9:ASP:OD2	9:R:53:PHD:HB3	2.21	0.40
1:1:33:DG:C2	1:1:34:DC:C2	3.09	0.40
7:F:1156:ARG:HG3	7:F:1156:ARG:HH11	1.86	0.40
8:G:330:ASP:N	8:G:330:ASP:OD1	2.53	0.40
9:R:60:ASP:OD1	9:R:63:THR:N	2.39	0.40
4:C:37:LEU:HD23	4:C:329:LEU:HD11	2.04	0.40
4:C:256:LEU:HD23	4:C:256:LEU:HA	1.98	0.40
4:C:329:LEU:HD23	4:C:329:LEU:HA	1.89	0.40
5:D:38:VAL:HG11	5:D:56:LEU:HD23	2.04	0.40
7:F:1096:LEU:HD23	7:F:1096:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:340:PRO:HA	8:G:343:ARG:HE	1.87	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	
3	A	270/309 (87%)	265 (98%)	5 (2%)	0	100	100
3	B	209/309 (68%)	202 (97%)	7 (3%)	0	100	100
4	C	1036/1100 (94%)	988 (95%)	48 (5%)	0	100	100
5	D	613/624 (98%)	602 (98%)	10 (2%)	1 (0%)	44	72
6	E	51/76 (67%)	50 (98%)	1 (2%)	0	100	100
7	F	1199/1318 (91%)	1143 (95%)	56 (5%)	0	100	100
8	G	304/399 (76%)	294 (97%)	10 (3%)	0	100	100
9	R	231/249 (93%)	224 (97%)	5 (2%)	2 (1%)	14	47
9	S	227/249 (91%)	218 (96%)	5 (2%)	4 (2%)	7	35
All	All	4140/4633 (89%)	3986 (96%)	147 (4%)	7 (0%)	45	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	R	85	LEU
9	S	85	LEU
5	D	79	ARG
9	S	139	GLY
9	S	140	PRO
9	R	86	GLY
9	S	86	GLY

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	
3	A	234/262 (89%)	221 (94%)	13 (6%)	17	45
3	B	178/262 (68%)	173 (97%)	5 (3%)	38	60
4	C	887/938 (95%)	847 (96%)	40 (4%)	23	50
5	D	532/539 (99%)	522 (98%)	10 (2%)	52	70
6	E	50/68 (74%)	49 (98%)	1 (2%)	50	68
7	F	1001/1093 (92%)	941 (94%)	60 (6%)	16	43
8	G	263/344 (76%)	256 (97%)	7 (3%)	40	61
9	R	207/217 (95%)	201 (97%)	6 (3%)	37	59
9	S	204/217 (94%)	199 (98%)	5 (2%)	42	62
All	All	3556/3940 (90%)	3409 (96%)	147 (4%)	28	52

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	5	VAL
3	A	55	VAL
3	A	73	ASP
3	A	84	LEU
3	A	85	VAL
3	A	86	VAL
3	A	179	VAL
3	A	190	ILE
3	A	206	GLN
3	A	242	SER
3	A	270	LEU
3	A	291	GLU
3	A	299	ILE
3	B	4	GLN
3	B	5	VAL
3	B	62	HIS
3	B	81	VAL
3	B	226	VAL

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Mol	Chain	Res	Type
4	C	18	VAL
4	C	40	PHE
4	C	52	LEU
4	C	57	LYS
4	C	164	THR
4	C	196	ILE
4	C	223	MET
4	C	237	VAL
4	C	264	LEU
4	C	321	LEU
4	C	322	GLN
4	C	354	VAL
4	C	376	MET
4	C	463	ASP
4	C	477	LEU
4	C	506	THR
4	C	518	LEU
4	C	587	ILE
4	C	597	VAL
4	C	620	CYS
4	C	633	VAL
4	C	686	SER
4	C	700	LYS
4	C	704	GLU
4	C	727	ILE
4	C	734	GLU
4	C	780	GLU
4	C	839	GLU
4	C	863	MET
4	C	864	ASN
4	C	929	VAL
4	C	944	VAL
4	C	950	LEU
4	C	953	VAL
4	C	954	HIS
4	C	972	THR
4	C	1010	VAL
4	C	1019	ASN
4	C	1029	LYS
4	C	1039	SER
5	D	15	LEU
5	D	26	GLU

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Mol	Chain	Res	Type
5	D	58	CYS
5	D	192	LEU
5	D	228	ARG
5	D	421	VAL
5	D	427	VAL
5	D	476	VAL
5	D	545	GLU
5	D	613	LEU
6	E	12	LEU
7	F	14	VAL
7	F	36	THR
7	F	58	ILE
7	F	102	ILE
7	F	120	PHE
7	F	122	GLU
7	F	131	MET
7	F	169	ASN
7	F	199	ASP
7	F	212	GLN
7	F	219	VAL
7	F	238	ILE
7	F	255	VAL
7	F	260	THR
7	F	272	ASN
7	F	274	ASP
7	F	286	LYS
7	F	295	CYS
7	F	300	SER
7	F	301	VAL
7	F	316	VAL
7	F	318	MET
7	F	320	GLU
7	F	347	VAL
7	F	402	THR
7	F	409	SER
7	F	447	THR
7	F	448	ASP
7	F	517	THR
7	F	546	LEU
7	F	580	THR
7	F	581	LYS
7	F	600	THR

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Mol	Chain	Res	Type
7	F	609	VAL
7	F	625	VAL
7	F	649	ASN
7	F	660	THR
7	F	673	ILE
7	F	680	ASN
7	F	681	ASP
7	F	683	LEU
7	F	686	ILE
7	F	689	LYS
7	F	697	ASP
7	F	700	ASP
7	F	721	LEU
7	F	756	VAL
7	F	770	ILE
7	F	832	ILE
7	F	833	ILE
7	F	857	VAL
7	F	907	ASP
7	F	957	ARG
7	F	966	VAL
7	F	976	ASP
7	F	1035	ILE
7	F	1067	THR
7	F	1112	SER
7	F	1137	VAL
7	F	1182	ILE
8	G	170	SER
8	G	183	MET
8	G	244	LEU
8	G	322	VAL
8	G	363	ILE
8	G	367	PHE
8	G	394	LEU
9	R	15	LEU
9	R	54	LEU
9	R	85	LEU
9	R	133	SER
9	R	174	HIS
9	R	236	THR
9	S	15	LEU
9	S	54	LEU

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Mol	Chain	Res	Type
9	S	85	LEU
9	S	174	HIS
9	S	236	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	37	ASN
3	A	94	GLN
3	A	164	GLN
3	A	206	GLN
3	A	257	ASN
3	B	46	ASN
3	B	62	HIS
3	B	80	ASN
3	B	123	ASN
3	B	124	HIS
4	C	149	ASN
4	C	207	GLN
4	C	308	HIS
4	C	439	HIS
4	C	536	HIS
4	C	613	GLN
4	C	794	GLN
4	C	817	GLN
4	C	973	GLN
5	D	100	HIS
5	D	156	GLN
5	D	193	GLN
5	D	194	GLN
5	D	425	HIS
5	D	475	HIS
5	D	483	GLN
5	D	503	GLN
5	D	546	GLN
6	E	28	HIS
7	F	109	ASN
7	F	269	GLN
7	F	277	ASN
7	F	303	GLN
7	F	314	GLN

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Mol	Chain	Res	Type
7	F	389	ASN
7	F	586	HIS
7	F	642	ASN
7	F	654	GLN
7	F	927	GLN
7	F	973	GLN
7	F	1153	HIS
7	F	1199	GLN
8	G	171	ASN
8	G	190	GLN
8	G	209	HIS
9	R	44	GLN
9	R	174	HIS
9	R	244	GLN
9	S	174	HIS
9	S	239	HIS
9	S	241	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	PHD	R	53	9	9,11,12	4.09	1 (11%)	9,15,17	1.85	3 (33%)
9	PHD	S	53	9	9,11,12	4.03	1 (11%)	9,15,17	1.76	2 (22%)

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
9	PHD	R	53	9	-	4/8/11/13	-
9	PHD	S	53	9	-	4/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	53	PHD	P-OD1	12.10	1.81	1.59
9	S	53	PHD	P-OD1	11.94	1.81	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	53	PHD	OD1-P-OP1	-3.71	97.61	109.47
9	R	53	PHD	OD1-P-OP1	-3.68	97.70	109.47
9	S	53	PHD	OP3-P-OP2	2.35	116.60	107.80
9	R	53	PHD	OP3-P-OP2	2.22	116.14	107.80
9	R	53	PHD	CA-CB-CG	2.02	117.11	112.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	S	53	PHD	CG-OD1-P-OP1
9	R	53	PHD	C-CA-CB-CG
9	R	53	PHD	CA-CB-CG-OD1
9	S	53	PHD	CA-CB-CG-OD1
9	S	53	PHD	CA-CB-CG-OD2
9	R	53	PHD	CA-CB-CG-OD2
9	R	53	PHD	CG-OD1-P-OP2
9	S	53	PHD	CG-OD1-P-OP2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	53	PHD	4	0
9	S	53	PHD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

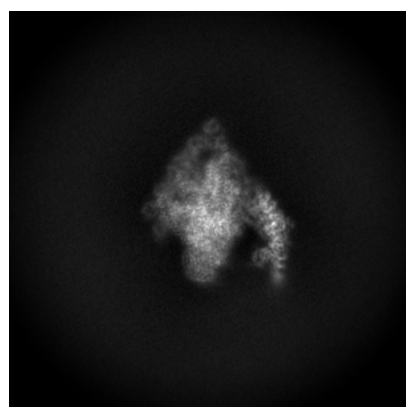
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47223. These allow visual inspection of the internal detail of the map and identification of artifacts.

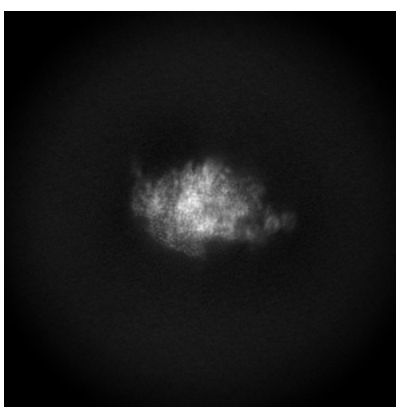
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

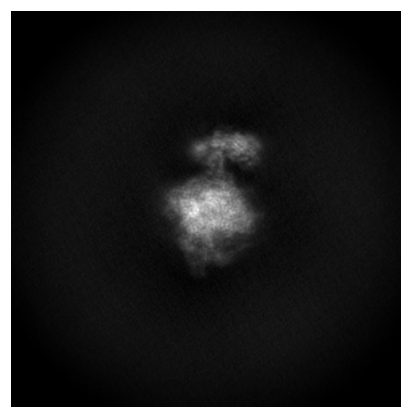
6.1.1 Primary map



X



Y

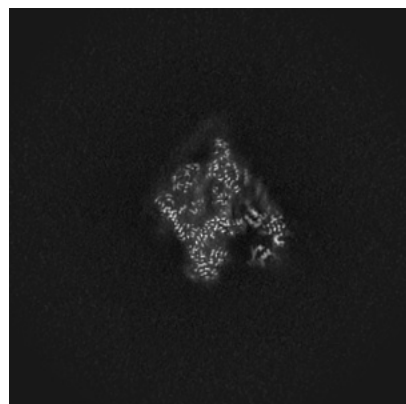


Z

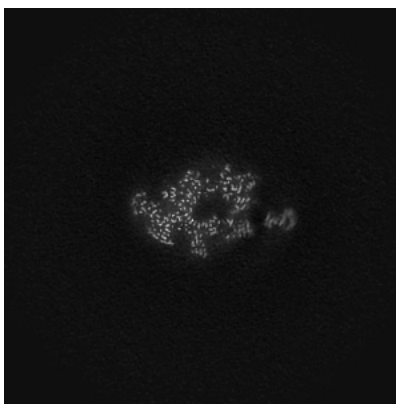
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

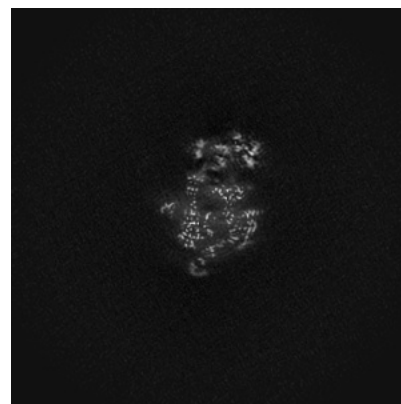
6.2.1 Primary map



X Index: 200



Y Index: 200

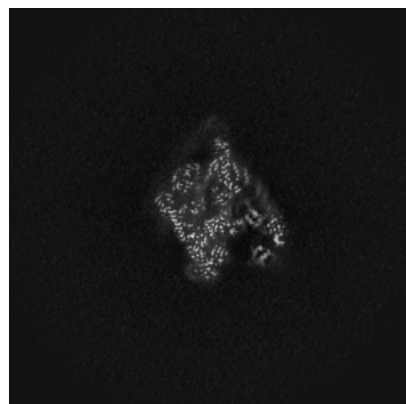


Z Index: 200

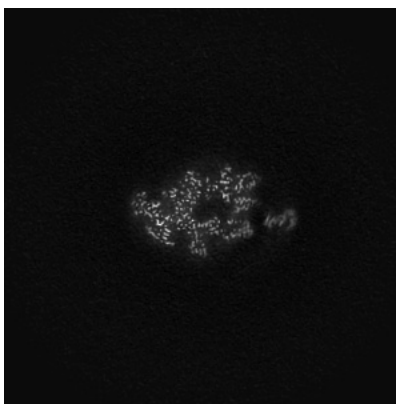
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

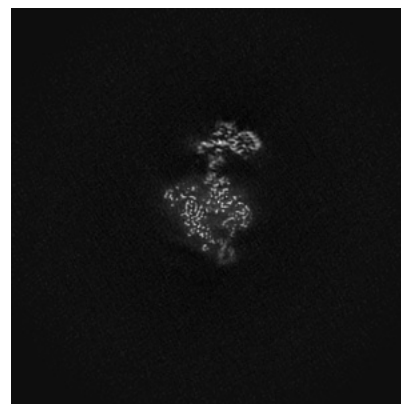
6.3.1 Primary map



X Index: 199



Y Index: 201

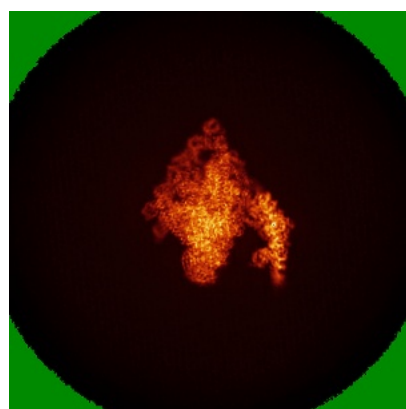


Z Index: 185

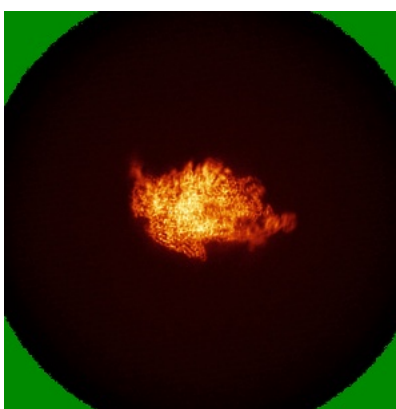
The images above show the largest variance slices of the map in three orthogonal directions.

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

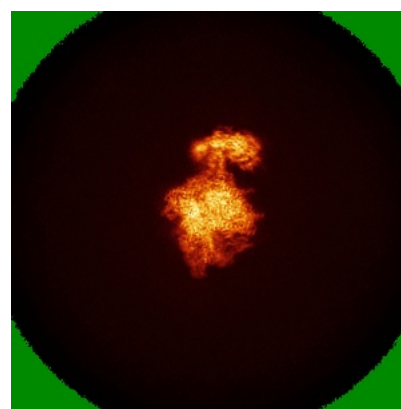
6.4.1 Primary map



X



Y

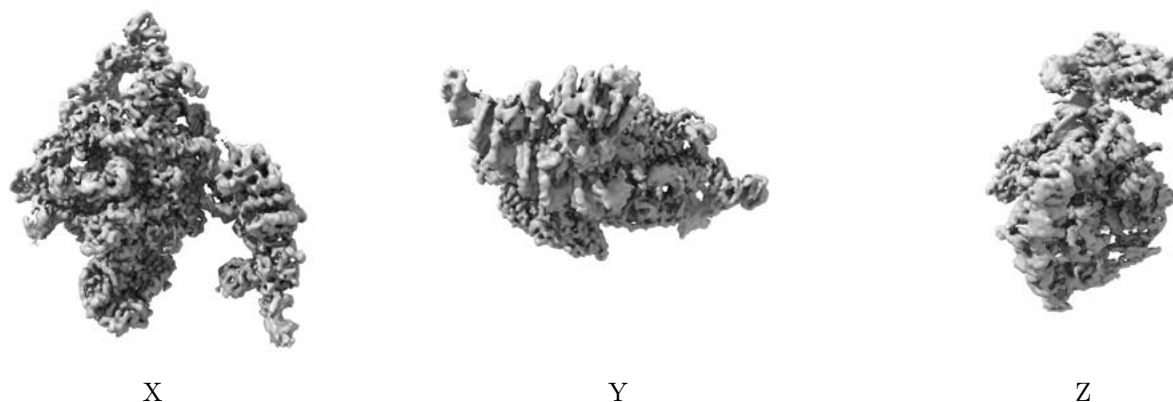


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

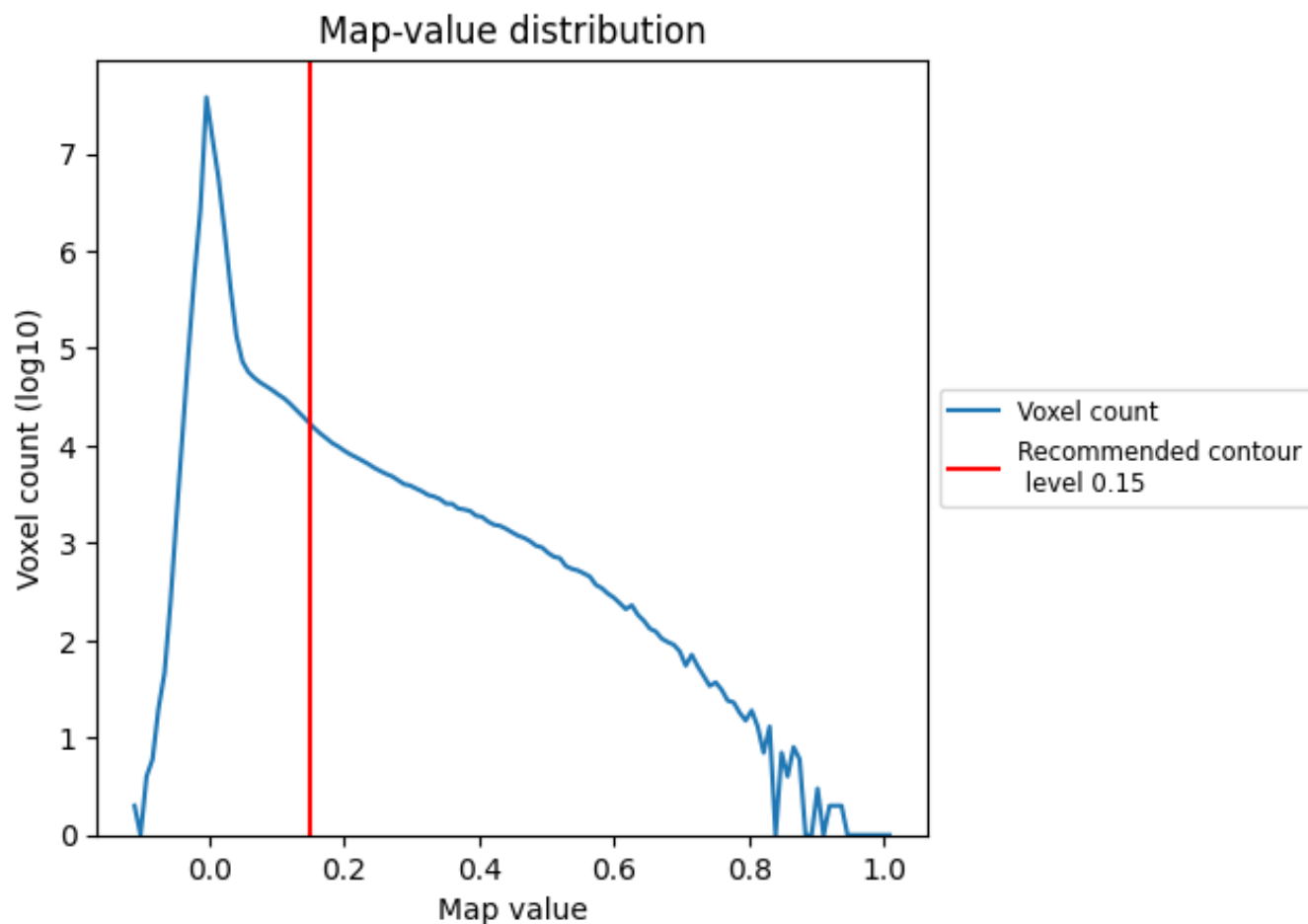
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

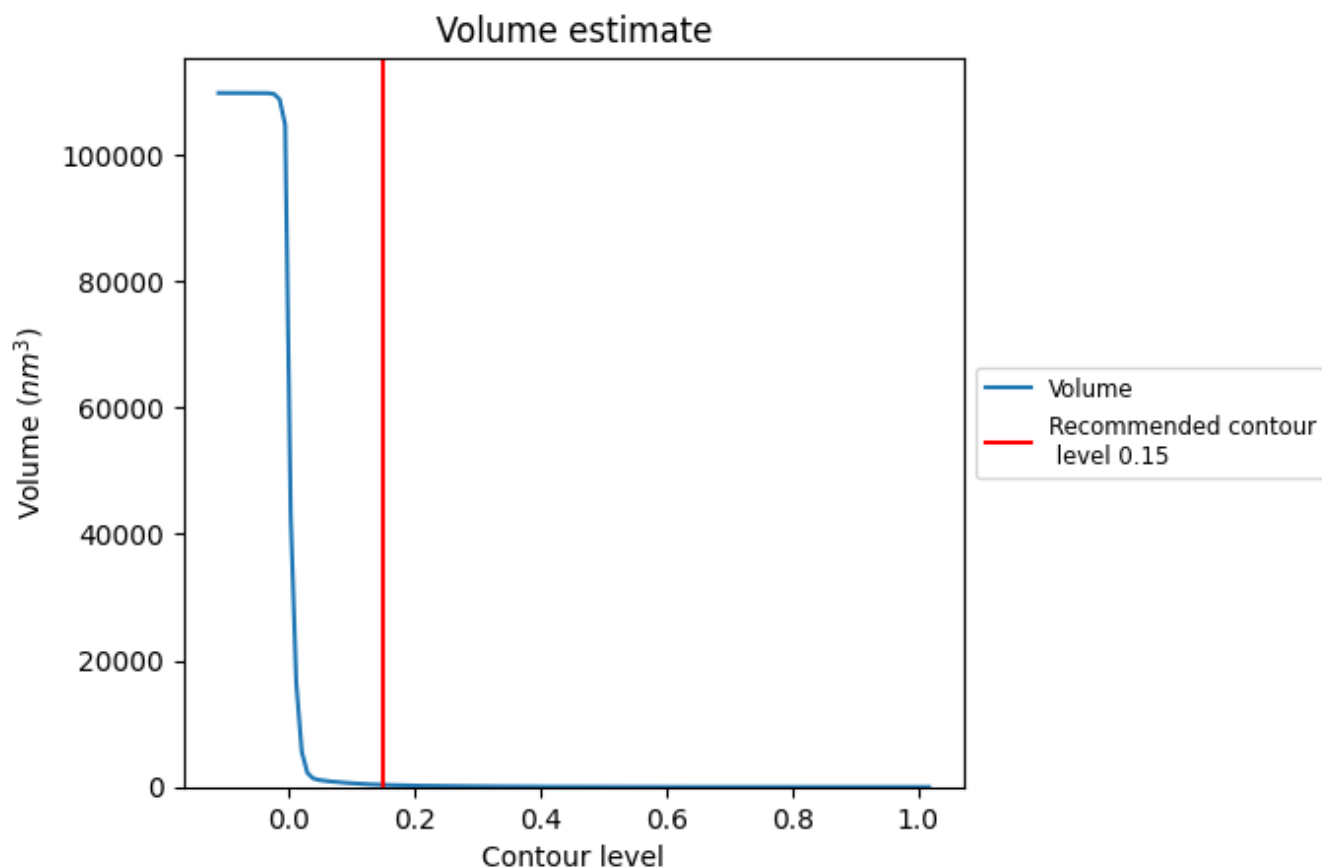
This section contains the results of statistical analysis of the map.

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.

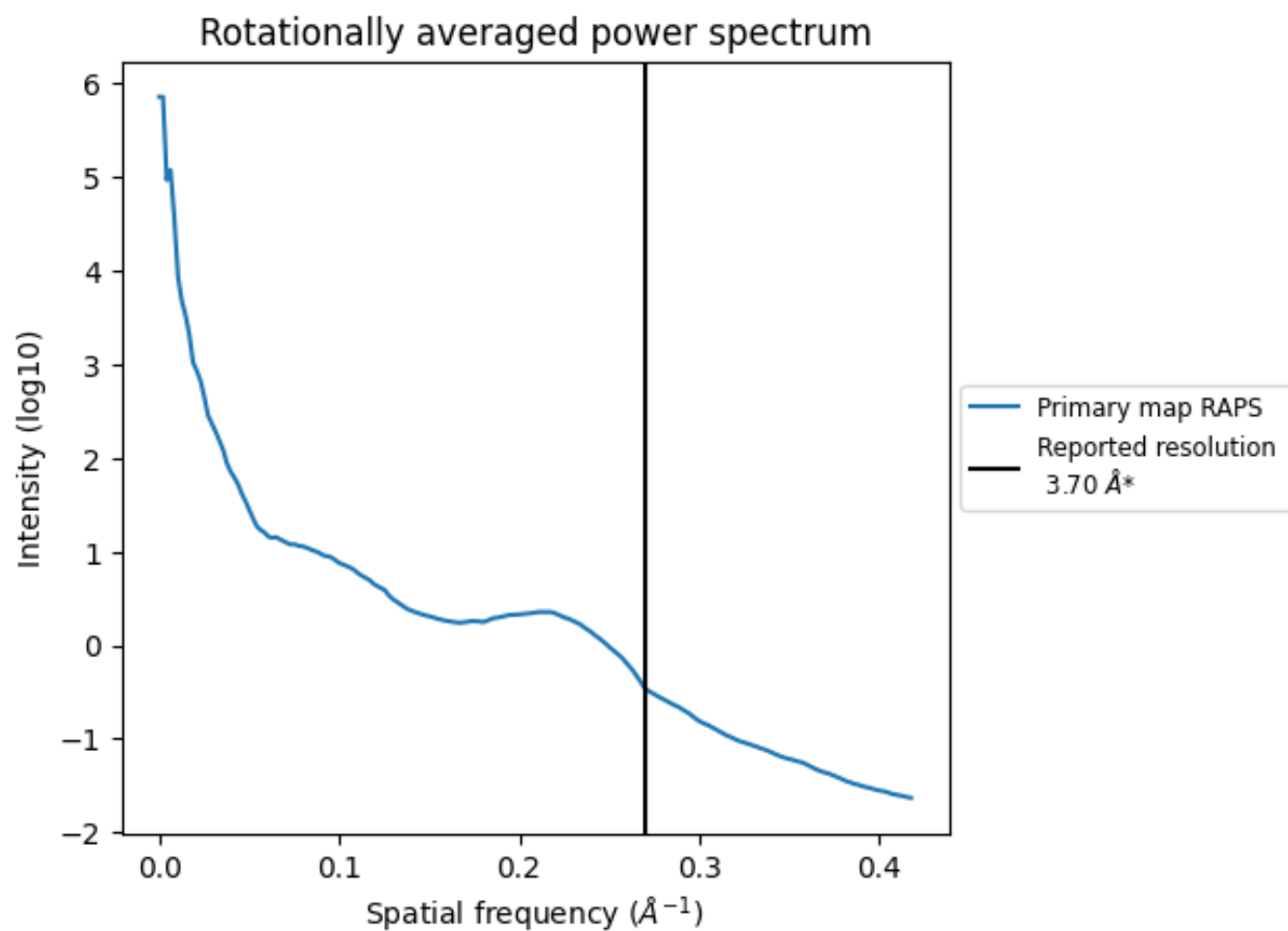
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 335 nm^3 ; this corresponds to an approximate mass of 302 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 0.270 Å⁻¹

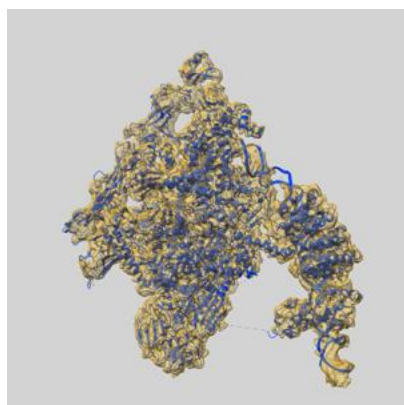
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

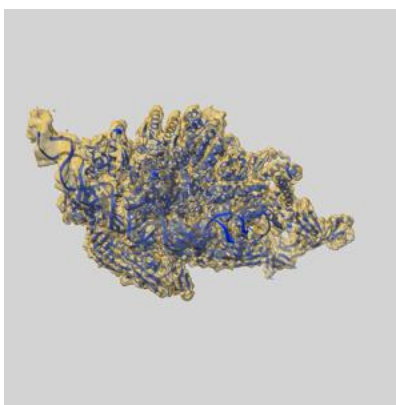
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47223 and PDB model 9DVU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

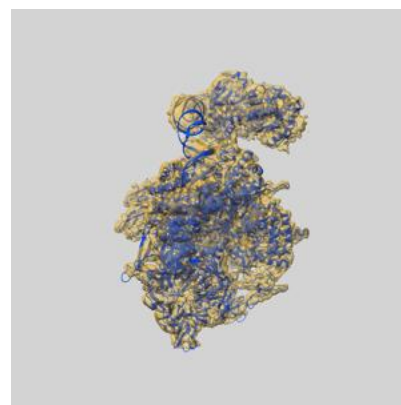
9.1 Map-model overlay [i](#)



X



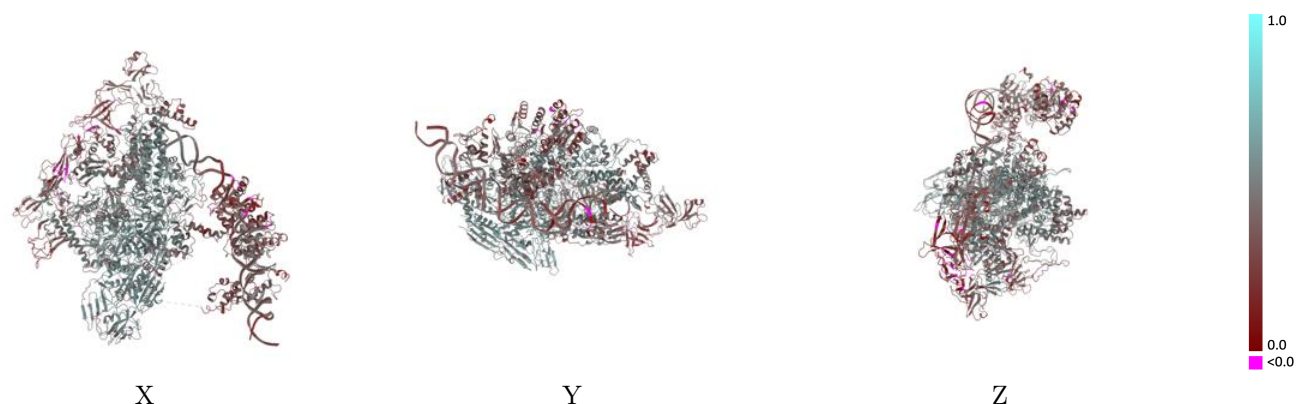
Y



Z

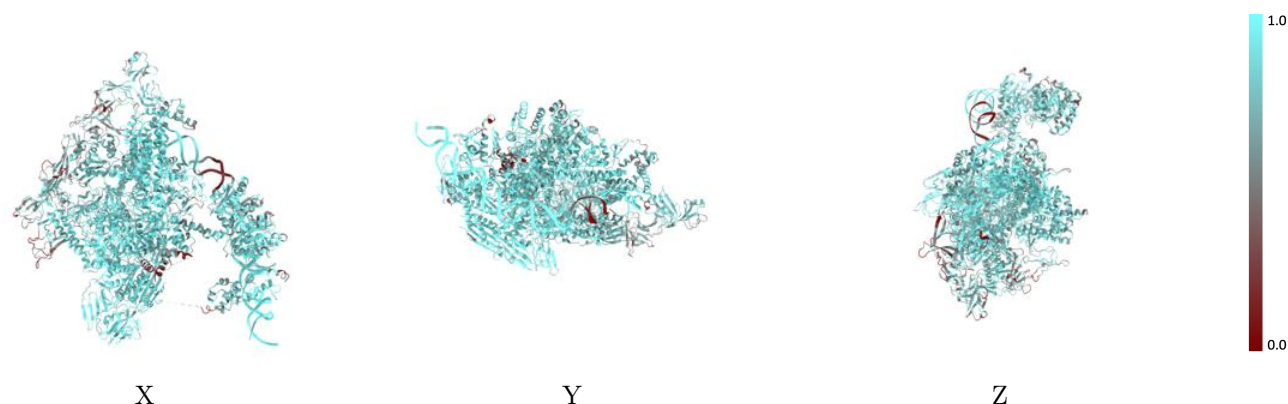
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



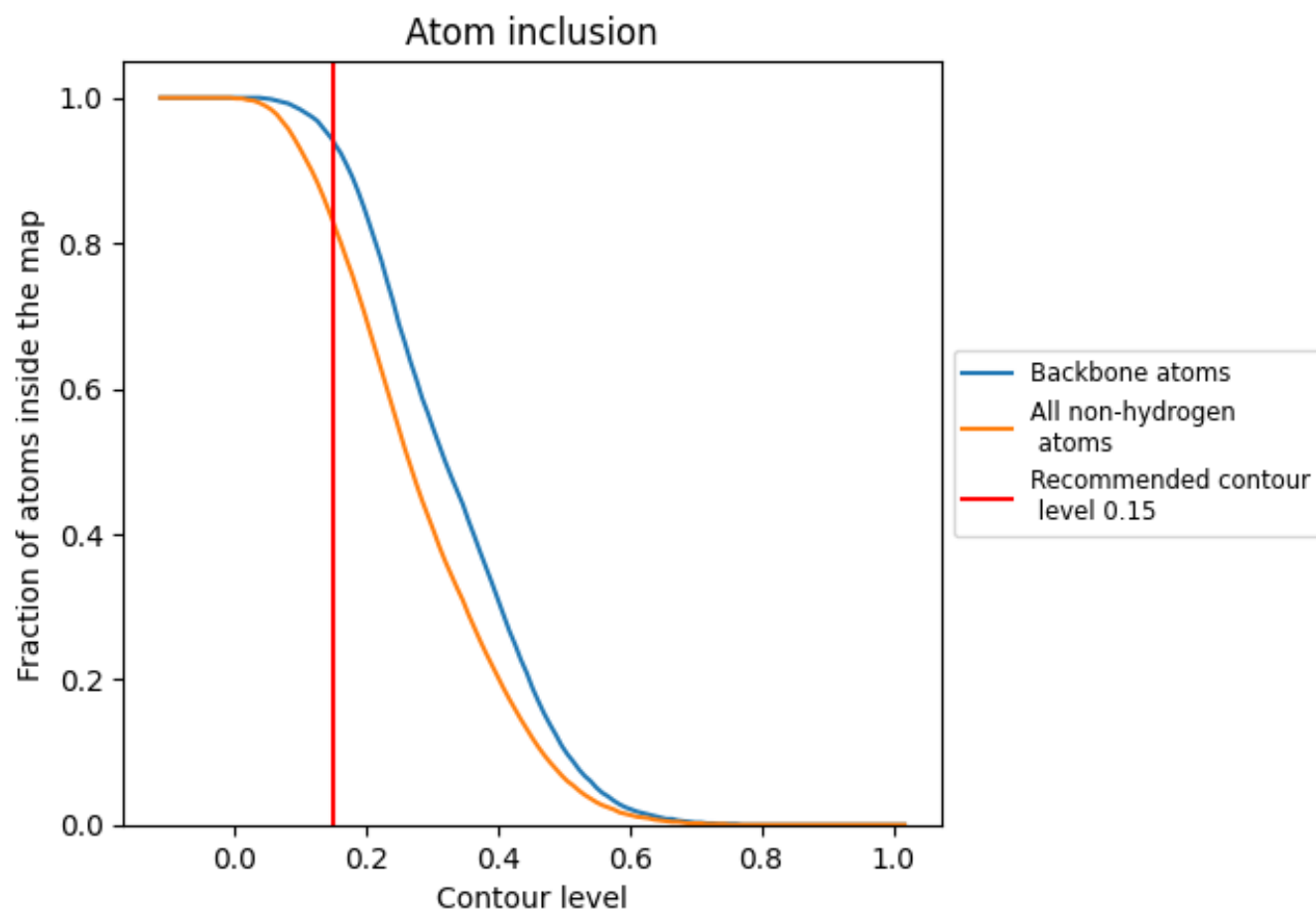
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8310	<div></div> 0.4350
1	<div></div> 0.8720	<div></div> 0.3630
2	<div></div> 0.8140	<div></div> 0.3200
A	<div></div> 0.8780	<div></div> 0.4770
B	<div></div> 0.9210	<div></div> 0.5210
C	<div></div> 0.8900	<div></div> 0.5000
D	<div></div> 0.9170	<div></div> 0.5200
E	<div></div> 0.3550	<div></div> 0.4210
F	<div></div> 0.7380	<div></div> 0.3790
G	<div></div> 0.8290	<div></div> 0.4090
R	<div></div> 0.8100	<div></div> 0.3450
S	<div></div> 0.8020	<div></div> 0.3160

1.0

0.0

<0.0