



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:39 PM UTC

PDB ID : 9GDQ / pdb_00009gdq
EMDB ID : EMD-51275
Title : Cryo-EM structure of Vibrio cholerae RNA polymerase Transcription Activation Complex with ToxR transcription factor and ompU promoter DNA
Authors : Alcaide-Jimenez, A.; Baudin, F.; Canals, A.; Machon, C.; Murciano, B.; Fabrega-Ferrer, M.; Bantysh, O.; Perez-Luque, R.; Krukons, E.S.; Muller, C.W.; Coll, M.
Deposited on : 2024-08-06
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

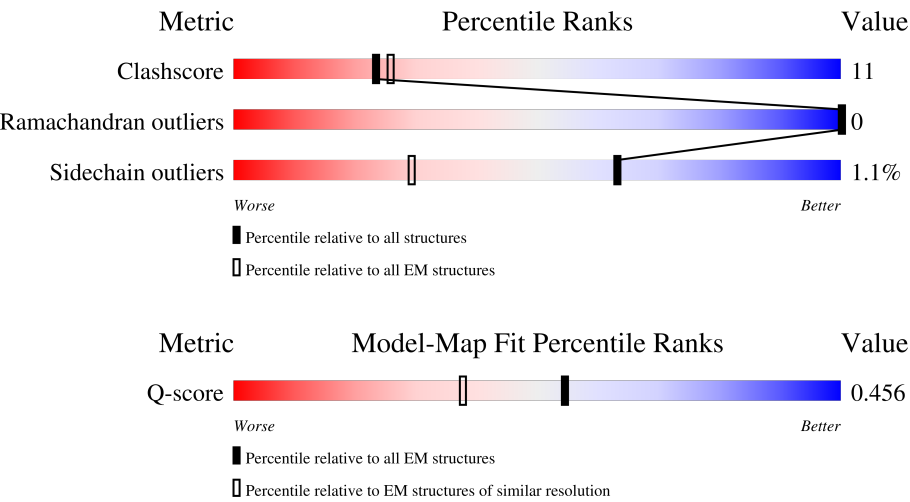
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	C	1341	5% 75% 22% ..
2	D	1401	5% 67% 19% 14%
3	E	90	58% 67% 10% 23%
4	A	330	52% 18% 30%

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Mol	Chain	Length	Quality of chain
4	B	330	
4	G	330	
5	F	621	
6	H	110	
6	K	110	
7	T	69	
8	N	69	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32619 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 DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1300	Total	C	N	O	S	0	0
			10187	6401	1769	1979	38		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	1202	Total	C	N	O	S	0	0
			9408	5912	1675	1774	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	69	Total	C	N	O	S	0	0
			545	332	102	110	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	231	Total	C	N	O	S	0	0
			1776	1111	312	348	5		
4	B	223	Total	C	N	O	S	0	0
			1704	1069	296	334	5		
4	G	71	Total	C	N	O	S	0	0
			557	353	98	104	2		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	468	Total	C	N	O	S	0	0
			3810	2384	690	719	17		

- Molecule 6 is a protein called Cholera toxin transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	110	Total	C	N	O	S	0	0
			902	571	155	174	2		
6	H	110	Total	C	N	O	S	0	0
			902	571	155	174	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	6	MET	-	initiating methionine	UNP P15795
H	6	MET	-	initiating methionine	UNP P15795

- Molecule 7 is a DNA chain called ompU promoter template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	69	Total	C	N	O	P	0	0
			1403	673	254	408	68		

- Molecule 8 is a DNA chain called ompU promoter non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	69	Total	C	N	O	P	0	0
			1422	680	262	412	68		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

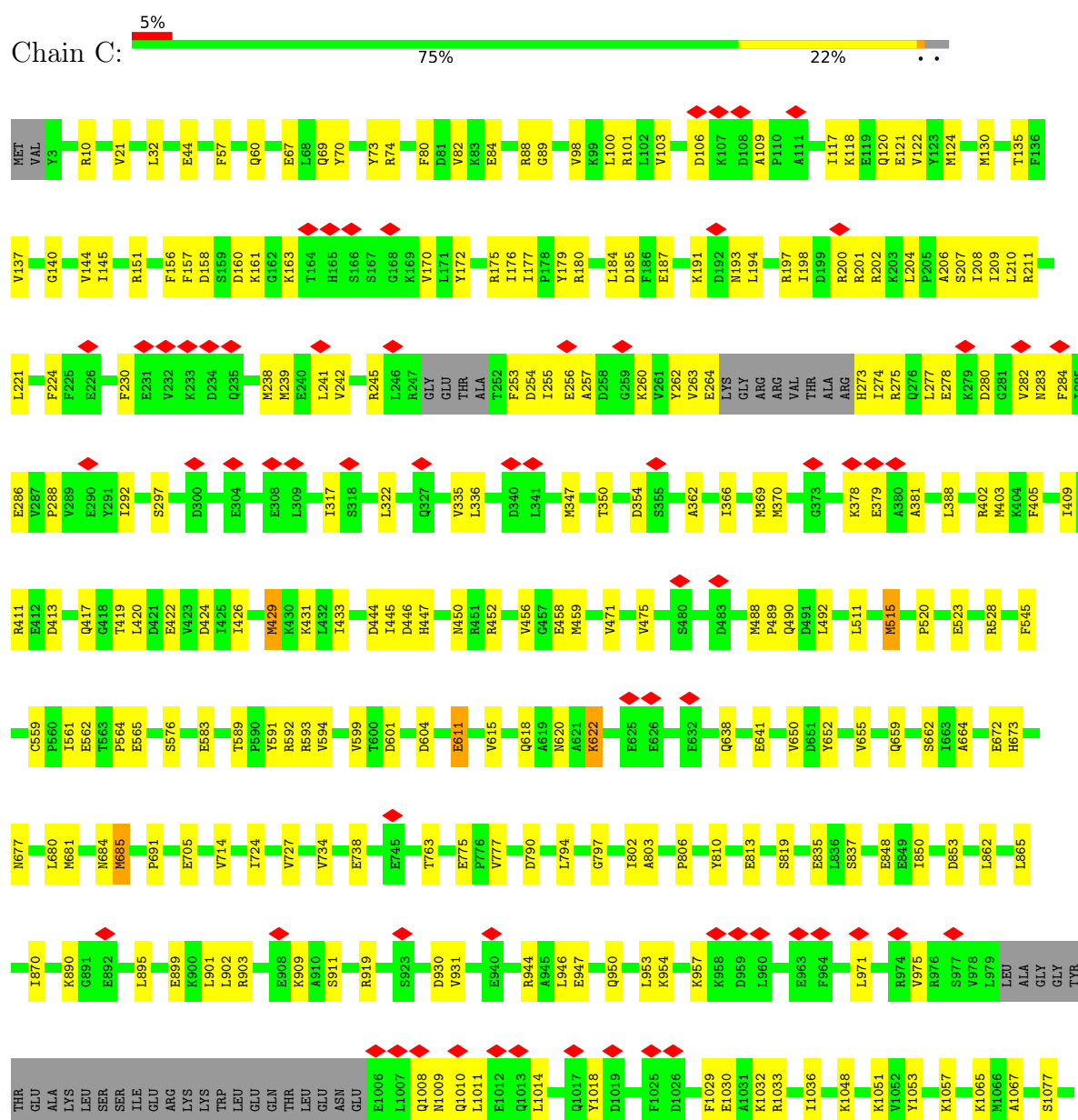
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

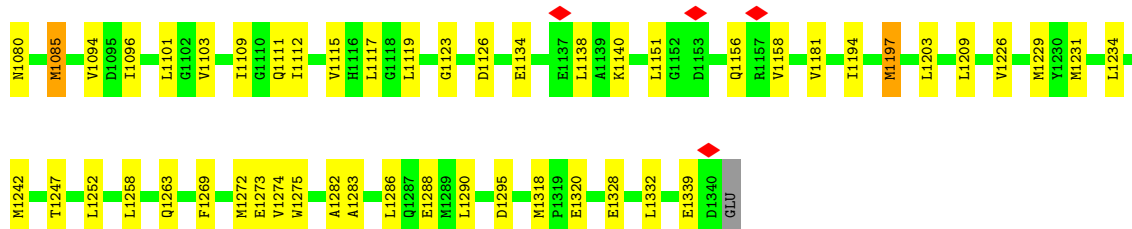
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

3 Residue-property plots

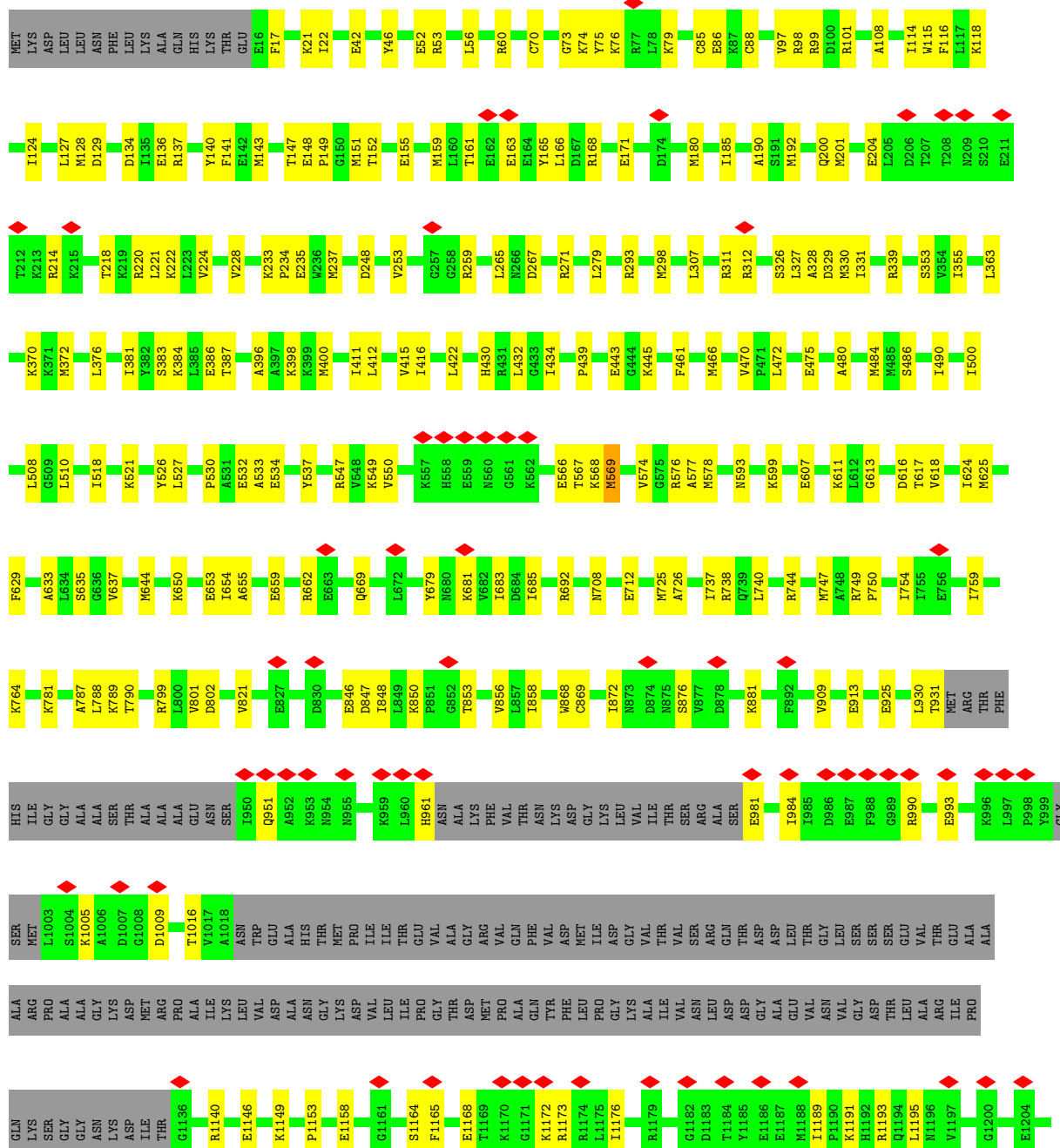
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

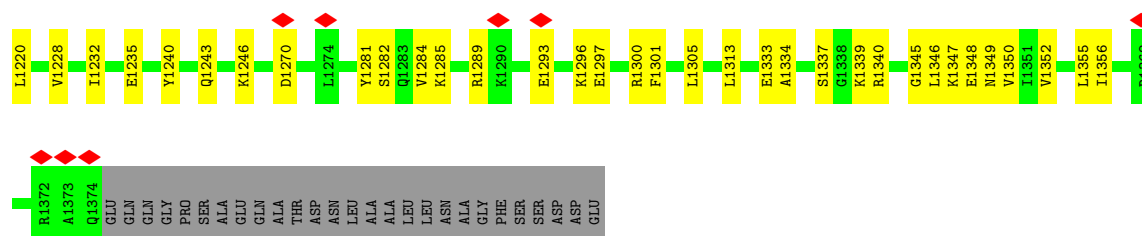
- Molecule 1: DNA-directed RNA polymerase subunit beta



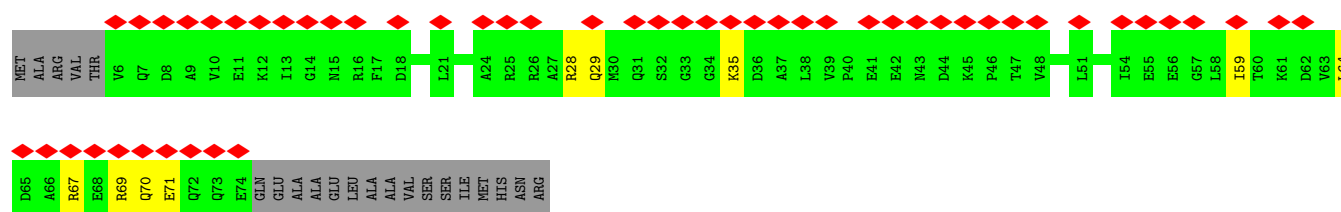


• Molecule 2: DNA-directed RNA polymerase subunit beta'

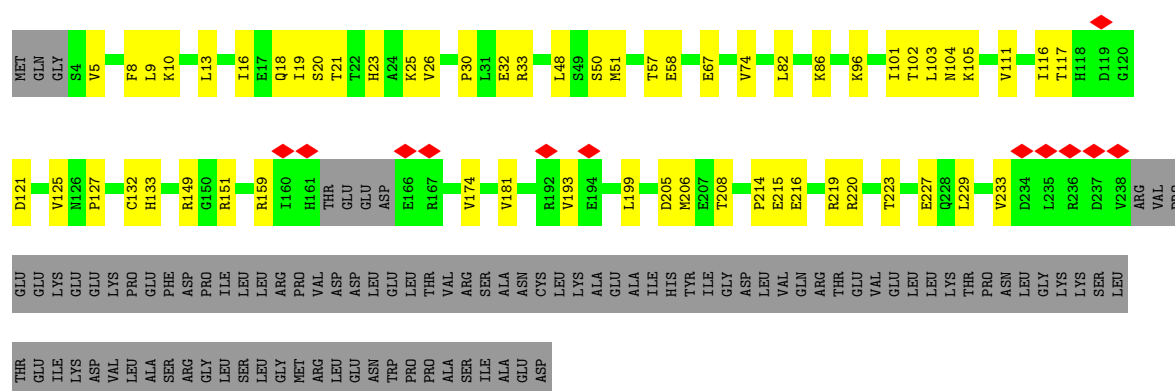




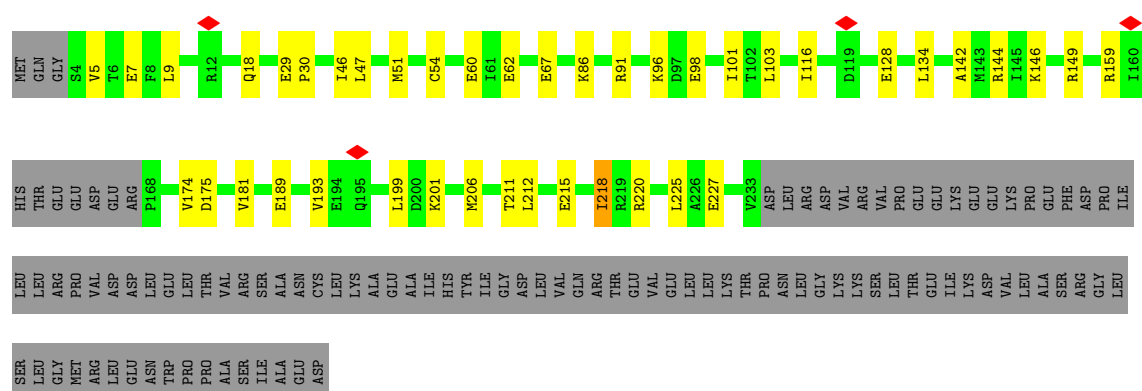
• Molecule 3: DNA-directed RNA polymerase subunit omega



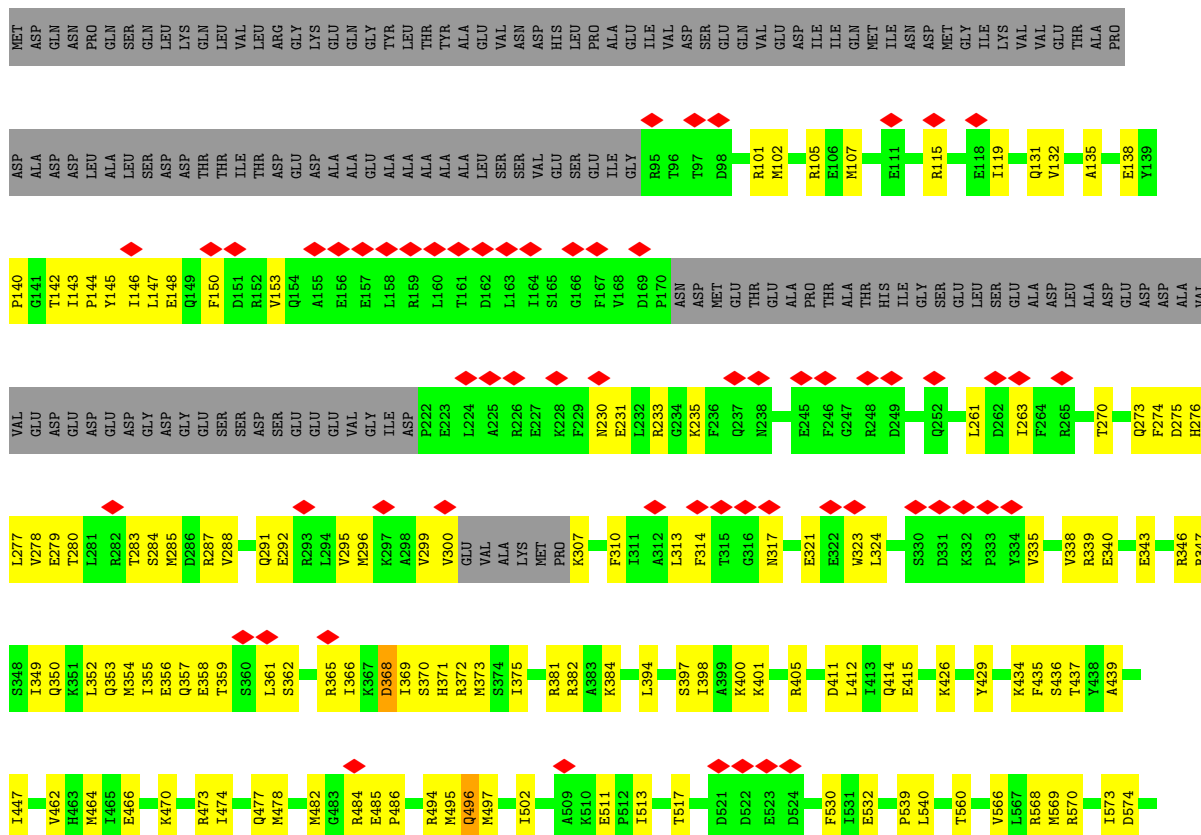
• Molecule 4: DNA-directed RNA polymerase subunit alpha



• Molecule 4: DNA-directed RNA polymerase subunit alpha

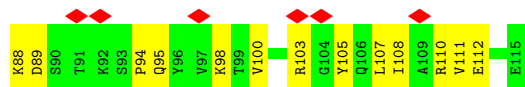
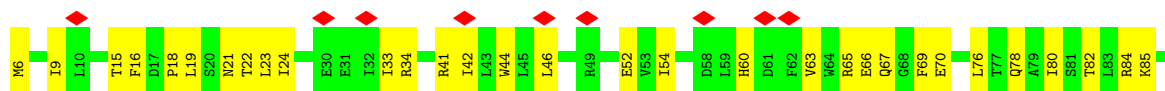


Chain G: 14% 8% 78%

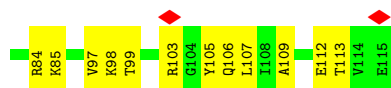




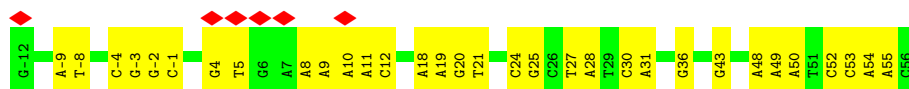
- Molecule 6: Cholera toxin transcriptional activator



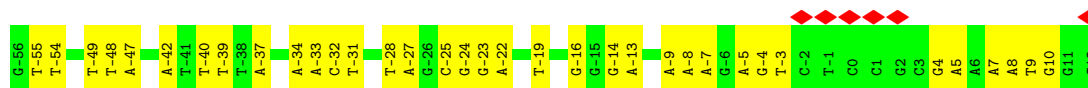
- Molecule 6: Cholera toxin transcriptional activator



- Molecule 7: ompU promoter template DNA strand



- Molecule 8: ompU promoter non-template DNA strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.24	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.001	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0996	Depositor
Map size (Å)	369.90002, 369.90002, 369.90002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.18	0/10347	0.37	0/13969
2	D	0.18	0/9552	0.36	0/12881
3	E	0.09	0/547	0.21	0/734
4	A	0.15	0/1798	0.32	0/2437
4	B	0.15	0/1725	0.31	0/2338
4	G	0.18	0/563	0.45	0/761
5	F	0.17	0/3861	0.46	0/5184
6	H	0.20	0/917	0.50	0/1237
6	K	0.16	0/917	0.42	0/1237
7	T	0.24	0/1573	0.42	0/2423
8	N	0.24	0/1597	0.42	0/2466
All	All	0.18	0/33397	0.38	0/45667

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	211	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	10187	0	10205	225	0
2	D	9408	0	9587	184	0
3	E	545	0	551	7	0
4	A	1776	0	1802	36	0
4	B	1704	0	1736	24	0
4	G	557	0	591	20	0
5	F	3810	0	3891	131	0
6	H	902	0	910	38	0
6	K	902	0	910	40	0
7	T	1403	0	780	27	0
8	N	1422	0	782	29	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	32619	0	31745	706	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 (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:SER:HB2	1:C:1085:MET:HE2	1.66	0.77
2:D:747:MET:HE3	2:D:759:ILE:HD12	1.66	0.76
5:F:283:THR:O	5:F:287:ARG:NE	2.17	0.76
6:K:9:ILE:HB	6:K:112:GLU:HB2	1.65	0.76
6:H:6:MET:HE1	6:H:113:THR:HG23	1.68	0.76
4:G:269:ASN:HA	4:G:272:LYS:HZ2	1.48	0.75
2:D:669:GLN:OE1	2:D:669:GLN:N	2.19	0.75
5:F:581:LEU:HB2	5:F:592:ARG:HH11	1.51	0.74
5:F:140:PRO:HD2	5:F:359:THR:HG22	1.70	0.73
2:D:265:LEU:HD11	2:D:330:MET:HE1	1.71	0.73
5:F:594:ARG:O	5:F:598:ILE:HG13	1.89	0.72
2:D:155:GLU:N	2:D:155:GLU:OE1	2.23	0.72
6:H:51:ASN:O	6:H:106:GLN:NE2	2.23	0.72
4:G:317:MET:SD	4:G:317:MET:N	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:GLU:OE1	1:C:662:SER:OG	2.08	0.71
5:F:362:SER:HA	5:F:365:ARG:HB2	1.70	0.71
1:C:207:SER:HA	1:C:210:LEU:HD12	1.70	0.71
5:F:276:HIS:ND1	5:F:279:GLU:OE2	2.24	0.71
2:D:52:GLU:N	2:D:52:GLU:OE1	2.24	0.71
5:F:566:VAL:HG23	5:F:584:VAL:HG11	1.73	0.71
1:C:475:VAL:HG22	1:C:492:LEU:HB3	1.73	0.70
1:C:1008:GLN:OE1	1:C:1008:GLN:N	2.25	0.70
1:C:902:LEU:HD11	5:F:615:LEU:HD22	1.74	0.70
1:C:69:GLN:OE1	1:C:101:ARG:NH2	2.26	0.69
1:C:565:GLU:N	1:C:565:GLU:OE2	2.25	0.69
1:C:444:ASP:HB3	1:C:447:HIS:HB2	1.75	0.69
6:H:24:ILE:HG12	6:H:32:ILE:HG12	1.74	0.69
2:D:381:ILE:HD11	2:D:412:LEU:HD13	1.76	0.68
5:F:482:MET:HE3	5:F:484:ARG:HB2	1.76	0.68
4:B:9:LEU:HD21	4:B:30:PRO:HG2	1.76	0.68
4:B:206:MET:HE1	4:B:218:ILE:HG12	1.74	0.68
1:C:187:GLU:N	1:C:187:GLU:OE1	2.27	0.68
2:D:534:GLU:HA	2:D:578:MET:HE2	1.76	0.67
1:C:1103:VAL:HG11	1:C:1112:ILE:HD11	1.76	0.67
1:C:204:LEU:HD21	1:C:369:MET:HG3	1.76	0.67
1:C:594:VAL:HG21	1:C:650:VAL:HG23	1.76	0.67
1:C:1032:LYS:O	1:C:1036:ILE:HD12	1.95	0.67
1:C:230:PHE:HA	1:C:238:MET:O	1.94	0.67
5:F:146:ILE:HG22	5:F:147:LEU:HD23	1.77	0.67
5:F:373:MET:HE3	5:F:373:MET:HA	1.77	0.67
1:C:641:GLU:OE1	2:D:749:ARG:NH1	2.28	0.67
1:C:1140:LYS:HB3	1:C:1140:LYS:HZ3	1.59	0.66
6:H:46:LEU:HB3	6:H:107:LEU:HB2	1.76	0.66
4:A:10:LYS:NZ	4:B:227:GLU:OE1	2.26	0.66
8:N:9:DT:H2'	8:N:10:DG:C8	2.31	0.66
2:D:1158:GLU:OE1	2:D:1158:GLU:N	2.25	0.66
6:H:37:SER:O	6:H:41:ARG:HG2	1.96	0.66
5:F:313:LEU:HB3	5:F:317:ASN:HB2	1.76	0.65
7:T:20:DG:N2	8:N:-19:DT:O2	2.29	0.65
6:H:34:ARG:HB2	6:H:34:ARG:NH1	2.11	0.65
1:C:444:ASP:O	1:C:450:ASN:ND2	2.30	0.65
2:D:799:ARG:NH1	2:D:1146:GLU:OE2	2.30	0.65
1:C:488:MET:HE3	1:C:489:PRO:HD2	1.79	0.64
2:D:259:ARG:NH1	5:F:511:GLU:O	2.31	0.64
5:F:362:SER:O	5:F:366:ILE:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:15:THR:HG22	6:K:24:ILE:HB	1.80	0.64
1:C:238:MET:HE1	1:C:284:PHE:HA	1.78	0.64
2:D:149:PRO:O	2:D:152:THR:OG1	2.14	0.64
2:D:510:LEU:HD11	2:D:624:ILE:HG23	1.80	0.64
1:C:103:VAL:HG12	1:C:117:ILE:HG22	1.79	0.64
5:F:296:MET:HE3	5:F:296:MET:HA	1.80	0.64
7:T:48:DA:OP2	6:H:85:LYS:NZ	2.27	0.63
2:D:124:ILE:HG22	2:D:128:MET:HE2	1.80	0.63
1:C:975:VAL:HG22	1:C:1014:LEU:HD13	1.80	0.63
5:F:496:GLN:NE2	5:F:496:GLN:O	2.32	0.63
1:C:946:LEU:O	1:C:950:GLN:HG2	1.98	0.63
3:E:67:ARG:NH1	3:E:71:GLU:OE2	2.32	0.63
4:A:216:GLU:OE2	4:A:220:ARG:NH2	2.31	0.63
5:F:368:ASP:HB2	5:F:372:ARG:HH12	1.63	0.63
6:K:46:LEU:HB3	6:K:107:LEU:HD13	1.81	0.63
5:F:405:ARG:NH2	7:T:10:DA:O5'	2.32	0.63
6:H:11:ALA:HB2	6:H:109:ALA:HB1	1.80	0.63
1:C:202:ARG:NH2	1:C:369:MET:SD	2.72	0.63
4:A:181:VAL:HA	4:A:208:THR:HG22	1.81	0.62
1:C:593:ARG:NH2	1:C:604:ASP:OD2	2.32	0.62
1:C:1290:LEU:HD11	2:D:1350:VAL:HG13	1.82	0.62
2:D:659:GLU:OE1	2:D:662:ARG:NH2	2.32	0.62
6:H:44:TRP:CD1	6:H:48:GLN:HE21	2.18	0.62
1:C:21:VAL:HG11	1:C:592:ARG:HD2	1.82	0.62
2:D:134:ASP:HB3	2:D:159:MET:HE2	1.81	0.62
2:D:1282:SER:HA	2:D:1285:LYS:HD3	1.81	0.62
4:A:101:ILE:HD12	4:A:116:ILE:HG21	1.81	0.62
5:F:593:GLU:OE1	5:F:593:GLU:N	2.29	0.62
1:C:120:GLN:NE2	1:C:490:GLN:HG2	2.15	0.62
1:C:724:ILE:HD13	1:C:734:VAL:HG22	1.79	0.62
1:C:1111:GLN:O	1:C:1115:VAL:HG23	1.99	0.62
4:B:18:GLN:NE2	4:B:215:GLU:OE2	2.32	0.62
4:B:128:GLU:OE1	4:B:128:GLU:N	2.33	0.62
1:C:160:ASP:O	1:C:163:LYS:NZ	2.32	0.61
1:C:802:ILE:HG13	1:C:1229:MET:HB3	1.83	0.61
2:D:396:ALA:O	2:D:400:MET:HG3	2.01	0.61
4:A:19:ILE:HD11	4:A:25:LYS:HG3	1.83	0.61
4:A:18:GLN:NE2	4:A:23:HIS:O	2.34	0.61
5:F:568:ARG:NH1	5:F:574:ASP:OD2	2.34	0.61
1:C:44:GLU:OE1	1:C:44:GLU:N	2.33	0.60
2:D:383:SER:O	2:D:387:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:86:LYS:HD3	4:B:175:ASP:HB2	1.83	0.60
4:A:223:THR:O	4:A:227:GLU:HG3	2.01	0.60
1:C:591:TYR:OH	1:C:611:GLU:OE2	2.17	0.60
5:F:585:GLY:HA2	5:F:590:VAL:HG13	1.84	0.60
5:F:343:GLU:O	5:F:347:ARG:NH2	2.35	0.60
5:F:513:ILE:HD11	5:F:517:THR:HG21	1.83	0.60
1:C:592:ARG:HG3	1:C:655:VAL:HG12	1.82	0.60
4:A:105:LYS:HG2	4:A:111:VAL:HG22	1.84	0.60
5:F:473:ARG:O	5:F:477:GLN:HG2	2.01	0.60
1:C:890:LYS:NZ	1:C:911:SER:O	2.30	0.60
1:C:1117:LEU:HD13	1:C:1194:ILE:HG12	1.84	0.60
5:F:474:ILE:HD11	5:F:494:ARG:HG2	1.84	0.60
1:C:135:THR:HG21	1:C:515:MET:HE2	1.82	0.59
1:C:257:ALA:HB3	1:C:260:LYS:HB2	1.84	0.59
1:C:583:GLU:H	1:C:583:GLU:CD	2.11	0.59
1:C:1030:GLU:OE1	1:C:1033:ARG:NH1	2.35	0.59
6:K:80:ILE:HG21	6:K:105:TYR:HE2	1.67	0.59
2:D:384:LYS:HB3	2:D:411:ILE:HD12	1.85	0.59
2:D:1172:LYS:HA	2:D:1191:LYS:HG2	1.84	0.59
2:D:850:LYS:HB3	2:D:853:THR:HB	1.85	0.59
5:F:284:SER:O	5:F:288:VAL:HG12	2.03	0.59
2:D:527:LEU:HD22	2:D:532:GLU:OE2	2.03	0.59
2:D:984:ILE:HB	2:D:993:GLU:HB2	1.83	0.59
4:A:57:THR:HG22	4:A:58:GLU:HG3	1.83	0.59
5:F:569:MET:HE2	5:F:584:VAL:HG22	1.83	0.59
1:C:837:SER:OG	1:C:1051:LYS:NZ	2.36	0.58
1:C:797:GLY:HA3	1:C:1231:MET:O	2.03	0.58
1:C:1109:ILE:HG21	2:D:644:MET:HE1	1.84	0.58
2:D:224:VAL:O	2:D:228:VAL:HG23	2.03	0.58
4:A:8:PHE:HD2	4:A:32:GLU:HG3	1.68	0.58
2:D:128:MET:HE1	2:D:185:ILE:HG23	1.85	0.58
1:C:84:GLU:O	1:C:88:ARG:HG3	2.04	0.58
2:D:527:LEU:HB2	2:D:550:VAL:HG22	1.86	0.58
2:D:201:MET:HE1	2:D:220:ARG:HE	1.69	0.58
5:F:143:ILE:O	5:F:147:LEU:HG	2.05	0.57
2:D:1345:GLY:O	2:D:1349:ASN:ND2	2.33	0.57
1:C:221:LEU:HD13	1:C:336:LEU:HD11	1.86	0.57
1:C:1101:LEU:HD23	2:D:725:MET:HG2	1.85	0.57
2:D:416:ILE:HG23	2:D:439:PRO:HG2	1.87	0.57
7:T:50:DA:C8	7:T:50:DA:H5'	2.40	0.57
8:N:-23:DG:H2''	8:N:-22:DA:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LYS:HZ2	1:C:282:VAL:HG13	1.70	0.57
1:C:1295:ASP:N	1:C:1295:ASP:OD1	2.37	0.57
1:C:528:ARG:NH2	1:C:576:SER:O	2.36	0.56
1:C:803:ALA:HB2	1:C:1094:VAL:HG11	1.85	0.56
2:D:1346:LEU:HD13	2:D:1356:ILE:HB	1.86	0.56
6:H:54:ILE:HD12	6:H:105:TYR:H	1.70	0.56
2:D:76:LYS:O	2:D:76:LYS:HG2	2.05	0.56
4:G:274:GLU:HB2	4:G:276:ILE:HD13	1.87	0.56
1:C:275:ARG:HA	1:C:278:GLU:HB2	1.88	0.56
2:D:190:ALA:HA	2:D:235:GLU:OE2	2.05	0.56
4:A:50:SER:O	4:A:51:MET:HE2	2.05	0.56
2:D:355:ILE:HG21	2:D:466:MET:HG3	1.87	0.56
2:D:566:GLU:OE1	2:D:568:LYS:HG2	2.03	0.56
5:F:231:GLU:O	5:F:235:LYS:HG2	2.06	0.56
2:D:140:TYR:HB3	5:F:102:MET:HE1	1.86	0.56
8:N:7:DA:H2''	8:N:8:DA:C8	2.40	0.56
5:F:142:THR:HG23	5:F:277:LEU:HD13	1.87	0.56
1:C:1111:GLN:HB2	1:C:1229:MET:HE1	1.88	0.56
6:K:41:ARG:HG3	6:K:63:VAL:HG22	1.88	0.56
6:H:9:ILE:HD12	6:H:112:GLU:OE2	2.06	0.56
5:F:274:PHE:O	5:F:278:VAL:HG23	2.05	0.56
4:B:46:ILE:HD11	4:B:225:LEU:HD13	1.87	0.56
8:N:-32:DC:H2''	8:N:-31:DT:H5'	1.88	0.56
1:C:260:LYS:HZ3	1:C:280:ASP:C	2.14	0.55
1:C:413:ASP:OD1	1:C:413:ASP:N	2.37	0.55
4:A:102:THR:OG1	4:A:117:THR:OG1	2.24	0.55
1:C:170:VAL:HB	1:C:172:TYR:HE1	1.71	0.55
7:T:4:DG:H2''	7:T:5:DT:H72	1.87	0.55
6:H:45:LEU:HD13	6:H:62:PHE:CD2	2.41	0.55
2:D:1153:PRO:O	2:D:1193:ARG:NH2	2.39	0.55
2:D:298:MET:HE1	5:F:414:GLN:HG3	1.88	0.55
1:C:362:ALA:O	1:C:366:ILE:HG23	2.06	0.55
1:C:954:LYS:O	1:C:957:LYS:HE3	2.07	0.55
5:F:436:SER:HG	8:N:-7:DA:H8	1.54	0.55
6:K:60:HIS:HB2	6:K:76:LEU:HD13	1.89	0.55
7:T:30:DC:H2''	7:T:31:DA:C8	2.42	0.55
4:A:18:GLN:NE2	4:A:20:SER:O	2.40	0.55
1:C:32:LEU:HA	1:C:130:MET:HE1	1.89	0.54
4:G:269:ASN:ND2	8:N:-39:DT:OP1	2.41	0.54
6:H:54:ILE:HD11	6:H:105:TYR:HB2	1.89	0.54
1:C:957:LYS:HB3	1:C:1029:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PHE:CE2	1:C:288:PRO:HD3	2.43	0.54
7:T:49:DA:H2"	7:T:50:DA:C8	2.42	0.54
1:C:208:ILE:HG23	1:C:362:ALA:HB1	1.89	0.54
1:C:411:ARG:NH1	1:C:424:ASP:OD1	2.40	0.54
1:C:1247:THR:HG21	5:F:539:PRO:HG2	1.89	0.54
1:C:370:MET:HE2	1:C:370:MET:HA	1.89	0.54
2:D:74:LYS:HE3	2:D:75:TYR:CE1	2.43	0.54
5:F:299:VAL:HG23	5:F:300:VAL:HG23	1.90	0.54
1:C:260:LYS:HA	1:C:277:LEU:HD13	1.89	0.54
5:F:285:MET:HE3	5:F:288:VAL:HG13	1.89	0.54
1:C:253:PHE:CZ	1:C:288:PRO:HD3	2.43	0.54
2:D:653:GLU:OE2	2:D:692:ARG:NE	2.41	0.54
4:A:132:CYS:SG	4:A:133:HIS:N	2.81	0.54
4:A:159:ARG:NH2	4:A:174:VAL:O	2.39	0.54
5:F:368:ASP:OD1	5:F:372:ARG:NH1	2.40	0.54
2:D:1164:SER:OG	2:D:1176:ILE:HG13	2.08	0.54
4:B:193:VAL:HG22	4:B:199:LEU:HD11	1.90	0.53
2:D:376:LEU:HD23	2:D:470:VAL:HG23	1.90	0.53
2:D:607:GLU:O	2:D:611:LYS:HG3	2.09	0.53
1:C:32:LEU:HD23	1:C:130:MET:HE3	1.90	0.53
1:C:1057:LYS:NZ	4:A:67:GLU:OE1	2.29	0.53
1:C:1282:ALA:HB2	2:D:484:MET:HE1	1.91	0.53
2:D:1333:GLU:O	2:D:1337:SER:OG	2.26	0.53
6:K:18:PRO:HB3	6:K:44:TRP:CD2	2.43	0.53
1:C:67:GLU:OE2	1:C:69:GLN:NE2	2.42	0.53
1:C:953:LEU:HD23	1:C:1036:ILE:HD13	1.89	0.53
2:D:97:VAL:HG22	2:D:101:ARG:HG3	1.91	0.53
2:D:930:LEU:HD11	2:D:1240:TYR:CE1	2.43	0.53
1:C:1065:LYS:HE2	1:C:1234:LEU:HD12	1.90	0.53
1:C:775:GLU:N	1:C:775:GLU:OE1	2.42	0.53
2:D:750:PRO:HA	2:D:781:LYS:HE3	1.91	0.53
2:D:961:HIS:O	2:D:981:GLU:N	2.42	0.53
5:F:279:GLU:O	5:F:283:THR:HG23	2.09	0.53
5:F:284:SER:O	5:F:287:ARG:HD2	2.09	0.53
1:C:681:MET:O	1:C:685:MET:HB2	2.10	0.52
1:C:1332:LEU:HD23	2:D:307:LEU:HD22	1.92	0.52
2:D:214:ARG:O	2:D:218:THR:HG22	2.10	0.52
5:F:532:GLU:N	5:F:532:GLU:OE1	2.42	0.52
7:T:30:DC:H2"	7:T:31:DA:H8	1.74	0.52
6:H:41:ARG:HH12	6:H:67:GLN:HE22	1.58	0.52
2:D:613:GLY:O	2:D:617:THR:OG1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLU:HB3	1:C:794:LEU:H	1.74	0.52
2:D:22:ILE:HG21	2:D:1334:ALA:HB1	1.90	0.52
4:A:206:MET:HE1	4:A:214:PRO:HA	1.90	0.52
6:H:67:GLN:HB2	6:H:69:PHE:CD1	2.45	0.52
2:D:443:GLU:OE1	2:D:443:GLU:N	2.38	0.52
4:A:5:VAL:HG21	4:B:149:ARG:HB3	1.92	0.52
5:F:435:PHE:HD1	5:F:435:PHE:O	1.92	0.52
2:D:99:ARG:HG2	2:D:248:ASP:HB2	1.91	0.52
1:C:175:ARG:HD3	1:C:177:ILE:HD11	1.91	0.52
2:D:1246:LYS:HB2	2:D:1246:LYS:NZ	2.25	0.52
1:C:565:GLU:OE2	1:C:684:ASN:ND2	2.43	0.52
8:N:-34:DA:H2"	8:N:-33:DA:H8	1.75	0.51
6:H:25:ASP:HB2	6:H:28:ASP:H	1.74	0.51
1:C:120:GLN:HG2	1:C:489:PRO:HG2	1.92	0.51
1:C:260:LYS:NZ	1:C:282:VAL:HG13	2.25	0.51
2:D:161:THR:O	2:D:165:TYR:N	2.38	0.51
5:F:429:TYR:HD1	5:F:429:TYR:H	1.58	0.51
1:C:459:MET:HE2	1:C:511:LEU:HD13	1.92	0.51
1:C:1151:LEU:HD22	1:C:1197:MET:HG3	1.93	0.51
2:D:326:SER:OG	2:D:329:ASP:OD2	2.27	0.51
1:C:297:SER:HB2	1:C:317:ILE:HD11	1.93	0.51
1:C:60:GLN:HE22	1:C:67:GLU:HB3	1.75	0.51
4:A:215:GLU:O	4:A:219:ARG:HG3	2.10	0.51
4:B:96:LYS:O	4:B:149:ARG:NH2	2.42	0.51
6:H:98:LYS:HB3	6:H:106:GLN:HB3	1.93	0.51
1:C:1080:ASN:HD22	1:C:1085:MET:HG2	1.76	0.51
2:D:430:HIS:CE1	2:D:432:LEU:HB2	2.45	0.51
2:D:141:PHE:C	2:D:180:MET:HE3	2.36	0.51
2:D:846:GLU:HA	2:D:846:GLU:OE1	2.11	0.51
6:K:16:PHE:HB2	6:K:23:LEU:HD12	1.93	0.51
6:K:42:ILE:HG21	6:K:80:ILE:HD11	1.93	0.51
6:K:46:LEU:HD22	6:K:107:LEU:HD22	1.92	0.51
2:D:574:VAL:HG12	2:D:578:MET:HE3	1.92	0.51
4:A:103:LEU:C	4:A:104:ASN:HD22	2.20	0.51
5:F:310:PHE:O	5:F:314:PHE:N	2.44	0.51
5:F:570:ARG:NH1	5:F:599:GLU:OE1	2.44	0.51
6:H:39:GLU:OE2	6:H:39:GLU:N	2.33	0.51
2:D:168:ARG:HA	2:D:171:GLU:OE2	2.10	0.50
6:H:106:GLN:OE1	6:H:106:GLN:HA	2.11	0.50
2:D:298:MET:CE	5:F:414:GLN:HG3	2.42	0.50
2:D:679:TYR:OH	2:D:754:ILE:O	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:435:PHE:CE1	5:F:439:ALA:HB2	2.46	0.50
4:G:298:LYS:O	4:G:302:THR:HG23	2.11	0.50
1:C:230:PHE:CE2	1:C:292:ILE:HD11	2.46	0.50
1:C:559:CYS:HB2	1:C:662:SER:HB3	1.92	0.50
3:E:29:GLN:OE1	3:E:67:ARG:NH2	2.45	0.50
4:B:159:ARG:NH2	4:B:174:VAL:O	2.43	0.50
2:D:533:ALA:HB1	2:D:574:VAL:HG13	1.94	0.50
5:F:470:LYS:NZ	5:F:470:LYS:HB2	2.26	0.50
5:F:353:GLN:HA	5:F:356:GLU:HG2	1.93	0.50
4:G:264:THR:HG22	4:G:266:ARG:H	1.76	0.50
1:C:242:VAL:HB	1:C:245:ARG:HD2	1.94	0.50
1:C:901:LEU:HD22	5:F:573:ILE:HD11	1.94	0.50
1:C:615:VAL:HG12	1:C:638:GLN:HG3	1.92	0.50
1:C:1085:MET:HE3	1:C:1094:VAL:HG23	1.93	0.50
4:A:121:ASP:OD1	4:A:121:ASP:N	2.35	0.50
5:F:145:TYR:HA	5:F:148:GLU:HG2	1.94	0.50
1:C:971:LEU:O	1:C:975:VAL:HG23	2.12	0.49
1:C:1339:GLU:OE1	2:D:21:LYS:HB2	2.12	0.49
7:T:18:DA:H2"	7:T:19:DA:C8	2.47	0.49
2:D:136:GLU:OE2	2:D:312:ARG:NH1	2.44	0.49
2:D:1281:TYR:CE2	2:D:1285:LYS:HD2	2.47	0.49
4:A:20:SER:OG	4:A:21:THR:N	2.45	0.49
2:D:789:LYS:HD3	2:D:930:LEU:O	2.12	0.49
5:F:277:LEU:O	5:F:280:THR:OG1	2.30	0.49
6:K:22:THR:HG22	6:K:34:ARG:HH12	1.77	0.49
2:D:802:ASP:OD2	2:D:1347:LYS:NZ	2.46	0.49
2:D:1189:ILE:HD13	2:D:1195:LEU:HD11	1.94	0.49
5:F:275:ASP:O	5:F:279:GLU:HG3	2.12	0.49
2:D:518:ILE:HG12	2:D:547:ARG:NH1	2.28	0.49
2:D:1173:ARG:HB2	2:D:1191:LYS:HD2	1.95	0.49
5:F:397:SER:O	5:F:401:LYS:NZ	2.45	0.49
6:H:10:LEU:HD11	6:H:43:LEU:HD11	1.94	0.49
1:C:144:VAL:HG23	1:C:515:MET:HG2	1.95	0.49
2:D:526:TYR:CD2	2:D:569:MET:HE1	2.47	0.49
2:D:537:TYR:CD2	2:D:578:MET:HE1	2.48	0.49
2:D:1140:ARG:NH2	2:D:1235:GLU:OE1	2.42	0.49
6:H:23:LEU:HB3	6:H:33:ILE:HG22	1.94	0.49
2:D:46:TYR:OH	8:N:-16:DG:OP2	2.31	0.49
2:D:574:VAL:O	2:D:578:MET:HG3	2.13	0.49
5:F:107:MET:HE1	8:N:-5:DA:C8	2.47	0.49
1:C:238:MET:HE3	1:C:239:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:495:MET:HG2	5:F:497:MET:HB3	1.95	0.48
4:G:308:LEU:HD13	4:G:313:LEU:O	2.13	0.48
1:C:738:GLU:H	1:C:738:GLU:CD	2.20	0.48
1:C:1258:LEU:HD13	1:C:1263:GLN:HB3	1.95	0.48
4:A:16:ILE:HD12	4:A:26:VAL:HG22	1.94	0.48
2:D:475:GLU:CD	3:E:28:ARG:HH12	2.22	0.48
1:C:445:ILE:HG23	1:C:446:ASP:OD1	2.14	0.48
5:F:349:ILE:HG13	5:F:350:GLN:OE1	2.13	0.48
1:C:57:PHE:HD2	1:C:70:TYR:HB2	1.78	0.48
1:C:1134:GLU:N	1:C:1134:GLU:OE1	2.47	0.48
4:B:101:ILE:HD12	4:B:116:ILE:HG21	1.94	0.48
5:F:434:LYS:HD3	8:N:-8:DA:H5"	1.96	0.48
7:T:52:DC:H2"	7:T:53:DC:C5	2.48	0.48
2:D:129:ASP:N	2:D:220:ARG:HH12	2.11	0.48
1:C:80:PHE:HB3	1:C:84:GLU:HG2	1.95	0.48
6:H:56:ARG:HH21	6:H:76:LEU:HB3	1.77	0.48
1:C:263:VAL:HG23	1:C:263:VAL:O	2.13	0.48
1:C:957:LYS:C	1:C:957:LYS:HD2	2.39	0.48
4:G:308:LEU:O	4:G:312:GLY:N	2.47	0.48
6:H:13:LYS:HG2	6:H:14:PHE:CD1	2.49	0.48
6:H:84:ARG:NH2	6:H:97:VAL:O	2.46	0.48
2:D:1289:ARG:O	2:D:1293:GLU:HG2	2.14	0.48
5:F:335:VAL:HA	5:F:338:VAL:CG1	2.44	0.48
6:K:44:TRP:CD1	6:K:44:TRP:C	2.92	0.48
1:C:1119:LEU:HG	1:C:1203:LEU:HD13	1.95	0.48
4:A:149:ARG:HG2	4:B:5:VAL:HG11	1.94	0.48
5:F:307:LYS:N	5:F:310:PHE:HB3	2.29	0.48
6:K:22:THR:HG22	6:K:34:ARG:NH1	2.29	0.48
6:K:80:ILE:HG12	6:K:105:TYR:CE2	2.49	0.48
1:C:60:GLN:HA	1:C:60:GLN:NE2	2.28	0.47
2:D:137:ARG:HB3	2:D:143:MET:HG3	1.96	0.47
5:F:497:MET:HG2	5:F:502:ILE:CD1	2.44	0.47
8:N:-14:DG:H2"	8:N:-13:DA:H8	1.79	0.47
1:C:274:ILE:HG22	1:C:278:GLU:HG2	1.96	0.47
2:D:576:ARG:HD3	2:D:593:ASN:HA	1.96	0.47
2:D:744:ARG:NE	2:D:747:MET:HE1	2.30	0.47
5:F:270:THR:HB	5:F:273:GLN:HG2	1.96	0.47
5:F:582:GLU:HG2	5:F:592:ARG:NH2	2.29	0.47
1:C:862:LEU:HD13	1:C:865:LEU:HD22	1.95	0.47
5:F:412:LEU:HD22	5:F:447:ILE:HG23	1.96	0.47
7:T:54:DA:H2"	7:T:55:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ASP:HB2	1:C:197:ARG:HB3	1.94	0.47
1:C:1318:MET:HE1	2:D:17:PHE:CE1	2.49	0.47
2:D:821:VAL:HG12	2:D:881:LYS:HG3	1.95	0.47
3:E:69:ARG:HH22	3:E:70:GLN:HE21	1.62	0.47
4:A:193:VAL:HG21	4:A:199:LEU:HD12	1.95	0.47
5:F:400:LYS:HA	5:F:400:LYS:HE2	1.96	0.47
4:G:307:VAL:O	4:G:310:SER:OG	2.21	0.47
7:T:8:DA:H2''	7:T:9:DA:C8	2.50	0.47
1:C:1269:PHE:CZ	1:C:1273:GLU:HB3	2.49	0.47
2:D:931:THR:OG1	2:D:1243:GLN:NE2	2.48	0.47
2:D:1220:LEU:HD22	2:D:1305:LEU:HB2	1.97	0.47
5:F:292:GLU:HA	5:F:295:VAL:HG12	1.96	0.47
4:B:103:LEU:HB2	4:B:116:ILE:HG12	1.96	0.47
2:D:876:SER:OG	2:D:990:ARG:NH2	2.48	0.47
5:F:350:GLN:OE1	5:F:350:GLN:N	2.48	0.47
5:F:401:LYS:HE2	5:F:401:LYS:HB2	1.75	0.47
5:F:426:LYS:NZ	5:F:426:LYS:HB3	2.30	0.47
5:F:437:THR:HB	8:N:-8:DA:C8	2.49	0.47
6:K:23:LEU:HB3	6:K:33:ILE:HB	1.96	0.47
2:D:566:GLU:OE1	2:D:567:THR:N	2.48	0.47
5:F:353:GLN:HA	5:F:356:GLU:CG	2.44	0.47
6:K:67:GLN:HB3	6:K:69:PHE:CZ	2.50	0.47
1:C:594:VAL:HG12	1:C:599:VAL:HG22	1.97	0.47
1:C:919:ARG:HH11	1:C:919:ARG:HG2	1.80	0.47
2:D:163:GLU:HA	2:D:166:LEU:HG	1.96	0.47
2:D:530:PRO:HB3	2:D:577:ALA:O	2.15	0.47
4:A:30:PRO:HB2	4:A:199:LEU:HD13	1.97	0.47
4:G:322:TRP:HD1	4:G:323:PRO:HA	1.80	0.47
1:C:1252:LEU:HD21	2:D:253:VAL:HG11	1.97	0.46
2:D:86:GLU:H	2:D:86:GLU:CD	2.22	0.46
4:G:293:THR:HB	4:G:296:LEU:HB3	1.97	0.46
4:G:298:LYS:NZ	4:G:298:LYS:HB3	2.30	0.46
2:D:1300:ARG:HE	2:D:1301:PHE:H	1.63	0.46
2:D:1334:ALA:HA	2:D:1339:LYS:HD3	1.97	0.46
4:B:47:LEU:HB3	4:B:181:VAL:HG21	1.97	0.46
4:B:212:LEU:HD11	4:B:220:ARG:NH2	2.30	0.46
1:C:429:MET:O	1:C:433:ILE:HG12	2.16	0.46
4:B:54:CYS:SG	4:B:149:ARG:NH1	2.88	0.46
5:F:135:ALA:O	5:F:369:ILE:HD11	2.16	0.46
6:K:60:HIS:CD2	6:K:60:HIS:C	2.94	0.46
1:C:176:ILE:CG2	1:C:184:LEU:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:ASP:HB3	2:D:271:ARG:HH12	1.79	0.46
5:F:400:LYS:HE3	8:N:-4:DG:H4'	1.97	0.46
1:C:74:ARG:NH1	1:C:121:GLU:OE2	2.47	0.46
2:D:233:LYS:HE2	2:D:235:GLU:HG2	1.96	0.46
2:D:1165:PHE:HZ	2:D:1168:GLU:HG3	1.80	0.46
2:D:1270:ASP:HB3	2:D:1296:LYS:HE2	1.98	0.46
5:F:590:VAL:HG11	5:F:595:ILE:HD11	1.98	0.46
1:C:89:GLY:HA2	1:C:140:GLY:HA3	1.97	0.46
1:C:564:PRO:HA	1:C:684:ASN:HD21	1.81	0.46
2:D:363:LEU:HD12	2:D:618:VAL:HB	1.97	0.46
1:C:224:PHE:HE1	1:C:429:MET:HB3	1.80	0.46
2:D:118:LYS:HD3	2:D:312:ARG:NH1	2.30	0.46
2:D:635:SER:OG	2:D:637:VAL:HG23	2.15	0.46
5:F:346:ARG:NH1	5:F:347:ARG:HH12	2.14	0.46
4:G:279:ILE:HG12	4:G:280:GLY:H	1.80	0.46
1:C:145:ILE:HB	1:C:456:VAL:HG22	1.97	0.46
1:C:151:ARG:HD3	1:C:445:ILE:HD11	1.97	0.46
2:D:328:ALA:HA	2:D:331:ILE:HG12	1.98	0.46
2:D:422:LEU:HD13	2:D:434:ILE:HD11	1.97	0.46
2:D:847:ASP:HB3	2:D:856:VAL:HG13	1.95	0.46
4:B:67:GLU:N	4:B:67:GLU:OE1	2.47	0.46
5:F:368:ASP:CB	5:F:372:ARG:HH12	2.29	0.46
6:K:21:ASN:O	6:K:21:ASN:ND2	2.48	0.46
1:C:84:GLU:OE1	1:C:84:GLU:N	2.32	0.46
2:D:370:LYS:HZ1	2:D:443:GLU:HG3	1.81	0.46
1:C:224:PHE:CG	1:C:347:MET:HG2	2.50	0.46
1:C:724:ILE:HG21	1:C:727:VAL:HG22	1.96	0.46
5:F:335:VAL:HA	5:F:338:VAL:HG12	1.98	0.46
6:K:107:LEU:HD23	6:K:107:LEU:H	1.80	0.46
1:C:850:ILE:HD12	1:C:1048:LYS:HD2	1.98	0.45
2:D:108:ALA:HB3	2:D:279:LEU:HD23	1.98	0.45
4:B:98:GLU:OE2	4:B:146:LYS:HD2	2.16	0.45
6:H:20:SER:O	6:H:22:THR:HG23	2.16	0.45
1:C:515:MET:HE1	1:C:523:GLU:OE2	2.16	0.45
1:C:1123:GLY:HA2	1:C:1126:ASP:OD2	2.16	0.45
8:N:-24:DG:H2''	8:N:-23:DG:H8	1.80	0.45
1:C:21:VAL:HG23	1:C:601:ASP:OD1	2.17	0.45
2:D:327:LEU:HA	2:D:330:MET:HE2	1.98	0.45
6:K:67:GLN:HE22	6:H:103:ARG:HD2	1.81	0.45
6:H:99:THR:HG23	6:H:105:TYR:CE1	2.51	0.45
1:C:256:GLU:HG2	1:C:286:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:ASN:HB2	1:C:1010:GLN:NE2	2.32	0.45
1:C:1288:GLU:OE2	2:D:472:LEU:HB2	2.16	0.45
2:D:549:LYS:HE3	2:D:569:MET:HE3	1.97	0.45
5:F:354:MET:SD	5:F:355:ILE:HG12	2.57	0.45
6:K:6:MET:HE3	6:K:6:MET:HB3	1.83	0.45
7:T:27:DT:H2''	7:T:28:DA:C8	2.51	0.45
8:N:-48:DT:H2''	8:N:-47:DA:H5'	1.99	0.45
1:C:82:VAL:HG13	1:C:137:VAL:HG21	1.97	0.45
1:C:895:LEU:HD22	1:C:899:GLU:HG2	1.98	0.45
2:D:930:LEU:HD11	2:D:1240:TYR:HE1	1.79	0.45
5:F:362:SER:HB3	5:F:366:ILE:HG13	1.99	0.45
4:G:290:LEU:HD23	4:G:290:LEU:HA	1.82	0.45
6:K:18:PRO:HB3	6:K:44:TRP:CE3	2.52	0.45
1:C:253:PHE:HZ	1:C:286:GLU:O	2.00	0.45
1:C:622:LYS:H	1:C:622:LYS:HG2	1.58	0.45
1:C:1328:GLU:OE1	2:D:330:MET:HG3	2.17	0.45
8:N:-55:DT:H2''	8:N:-54:DT:C5	2.52	0.45
1:C:677:ASN:O	1:C:681:MET:HE3	2.16	0.45
1:C:1242:MET:HE3	2:D:372:MET:HG2	1.98	0.45
2:D:430:HIS:CD2	2:D:925:GLU:HG3	2.51	0.45
2:D:625:MET:HE3	2:D:629:PHE:CE2	2.52	0.45
2:D:650:LYS:O	2:D:654:ILE:HG12	2.17	0.45
6:K:78:GLN:HG2	8:N:-40:DT:H71	1.97	0.45
1:C:297:SER:HA	1:C:335:VAL:HG12	1.98	0.45
1:C:724:ILE:HD11	1:C:777:VAL:HG11	1.98	0.45
2:D:114:ILE:HD11	2:D:311:ARG:HB3	1.97	0.45
2:D:147:THR:HG22	2:D:148:GLU:HG3	1.98	0.45
4:A:74:VAL:HG13	4:A:132:CYS:SG	2.57	0.45
5:F:131:GLN:HE22	5:F:372:ARG:HB3	1.81	0.45
1:C:405:PHE:O	1:C:409:ILE:HG12	2.17	0.45
1:C:422:GLU:O	1:C:426:ILE:HG12	2.16	0.45
5:F:355:ILE:O	5:F:358:GLU:HB2	2.17	0.45
1:C:1181:VAL:HG11	1:C:1197:MET:HE1	1.98	0.45
2:D:53:ARG:NH2	2:D:60:ARG:HH11	2.15	0.45
7:T:-4:DC:H2'	7:T:-3:DG:C8	2.52	0.45
1:C:176:ILE:HD13	1:C:420:LEU:HD11	1.98	0.44
1:C:1272:MET:HE3	7:T:-1:DC:H4'	1.99	0.44
2:D:201:MET:HG2	2:D:221:LEU:HB2	1.99	0.44
5:F:381:ARG:NH2	5:F:382:ARG:HH22	2.15	0.44
1:C:191:LYS:HG3	1:C:193:ASN:OD1	2.17	0.44
2:D:681:LYS:O	2:D:685:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:869:CYS:HA	2:D:872:ILE:HG22	1.99	0.44
5:F:353:GLN:O	5:F:357:GLN:HG3	2.17	0.44
5:F:464:MET:HE2	5:F:464:MET:HB2	1.80	0.44
1:C:545:PHE:CZ	2:D:788:LEU:HD12	2.52	0.44
1:C:813:GLU:HB2	2:D:461:PHE:HD1	1.82	0.44
1:C:1283:ALA:HB1	2:D:1355:LEU:HD22	1.98	0.44
1:C:1318:MET:HE1	2:D:17:PHE:HE1	1.82	0.44
5:F:287:ARG:O	5:F:291:GLN:HG2	2.17	0.44
7:T:-2:DG:H2'	7:T:-1:DC:H6	1.81	0.44
7:T:24:DC:H2''	7:T:25:DG:C8	2.52	0.44
1:C:347:MET:HE3	1:C:350:THR:HB	1.99	0.44
1:C:971:LEU:HD22	1:C:1018:TYR:HD2	1.82	0.44
2:D:116:PHE:O	2:D:124:ILE:HG13	2.16	0.44
2:D:599:LYS:NZ	2:D:599:LYS:HB3	2.33	0.44
2:D:858:ILE:HG12	2:D:868:TRP:CE3	2.53	0.44
2:D:1284:VAL:HG11	2:D:1301:PHE:CD2	2.52	0.44
4:G:280:GLY:O	4:G:283:VAL:HG12	2.16	0.44
7:T:24:DC:H2''	7:T:25:DG:H8	1.81	0.44
8:N:-4:DG:H2''	8:N:-3:DT:H5''	2.00	0.44
6:H:66:GLU:HB2	6:H:67:GLN:NE2	2.32	0.44
1:C:379:GLU:CD	1:C:379:GLU:H	2.26	0.44
6:K:19:LEU:HB3	6:H:51:ASN:OD1	2.18	0.44
2:D:480:ALA:HA	2:D:484:MET:HB2	2.00	0.44
2:D:490:ILE:HB	2:D:500:ILE:HD13	1.98	0.44
4:A:9:LEU:N	4:A:32:GLU:OE2	2.40	0.44
5:F:600:ALA:O	5:F:604:ARG:HD3	2.18	0.44
1:C:106:ASP:HB3	1:C:109:ALA:HB3	1.99	0.44
1:C:810:TYR:O	1:C:1077:SER:OG	2.28	0.44
2:D:151:MET:SD	2:D:151:MET:N	2.90	0.44
2:D:353:SER:OG	2:D:445:LYS:O	2.33	0.44
3:E:35:LYS:HE2	3:E:35:LYS:HB3	1.78	0.44
4:B:91:ARG:NH1	4:B:211:THR:O	2.51	0.44
5:F:478:MET:HE2	5:F:486:PRO:HB3	1.99	0.44
8:N:-28:DT:H2''	8:N:-27:DA:C8	2.53	0.44
1:C:118:LYS:HB3	1:C:488:MET:SD	2.57	0.44
1:C:157:PHE:CZ	1:C:431:LYS:HG2	2.52	0.44
2:D:85:CYS:HB2	2:D:88:CYS:SG	2.58	0.44
5:F:594:ARG:HD2	5:F:597:GLN:HE21	1.82	0.44
1:C:57:PHE:CD2	1:C:70:TYR:HB2	2.52	0.43
1:C:520:PRO:HG3	1:C:714:VAL:HG21	1.99	0.43
1:C:615:VAL:HG12	1:C:638:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:60:GLU:HB2	4:B:144:ARG:HB3	2.00	0.43
4:G:279:ILE:HG12	4:G:280:GLY:N	2.33	0.43
6:K:94:PRO:HB3	6:K:98:LYS:HD3	2.00	0.43
1:C:73:TYR:CD1	1:C:73:TYR:C	2.96	0.43
1:C:206:ALA:O	1:C:209:ILE:HG22	2.17	0.43
2:D:848:ILE:HD12	2:D:858:ILE:HD12	2.00	0.43
2:D:1168:GLU:HG2	2:D:1173:ARG:HG3	2.00	0.43
5:F:371:HIS:O	5:F:375:ILE:HG13	2.18	0.43
5:F:581:LEU:HD12	5:F:581:LEU:H	1.83	0.43
6:K:100:VAL:HG13	6:K:103:ARG:HB2	1.99	0.43
1:C:895:LEU:HB3	1:C:899:GLU:HG3	1.99	0.43
5:F:585:GLY:HA2	5:F:590:VAL:CG1	2.48	0.43
1:C:402:ARG:HD2	1:C:402:ARG:HA	1.74	0.43
1:C:520:PRO:O	1:C:523:GLU:HB2	2.18	0.43
2:D:70:CYS:SG	2:D:73:GLY:N	2.91	0.43
2:D:222:LYS:HD3	2:D:222:LYS:HA	1.76	0.43
4:B:62:GLU:HG2	4:B:142:ALA:HB3	2.01	0.43
5:F:132:VAL:HG13	5:F:274:PHE:HZ	1.84	0.43
5:F:231:GLU:O	5:F:235:LYS:NZ	2.46	0.43
6:K:34:ARG:HA	6:K:34:ARG:HD2	1.71	0.43
6:K:41:ARG:NH2	6:K:66:GLU:HG2	2.33	0.43
7:T:9:DA:H4'	7:T:10:DA:N7	2.32	0.43
8:N:4:DG:H2''	8:N:5:DA:C8	2.53	0.43
1:C:10:ARG:NH1	1:C:790:ASP:OD2	2.44	0.43
1:C:255:ILE:HD13	1:C:262:TYR:HB2	2.00	0.43
1:C:292:ILE:HG21	1:C:322:LEU:HD21	2.00	0.43
1:C:1138:LEU:HD12	1:C:1138:LEU:HA	1.87	0.43
5:F:613:GLU:H	5:F:613:GLU:CD	2.21	0.43
6:K:103:ARG:HD2	6:K:103:ARG:HA	1.85	0.43
7:T:43:DG:C2	8:N:-42:DA:C2	3.07	0.43
1:C:561:ILE:O	1:C:680:LEU:HD13	2.18	0.43
1:C:901:LEU:HD22	5:F:573:ILE:CD1	2.48	0.43
1:C:1274:VAL:HG13	1:C:1286:LEU:HD11	2.00	0.43
2:D:951:GLN:OE1	2:D:1016:THR:OG1	2.36	0.43
5:F:570:ARG:HD3	5:F:599:GLU:OE1	2.19	0.43
6:K:110:ARG:HG2	6:K:112:GLU:OE2	2.18	0.43
6:H:55:SER:HA	6:H:103:ARG:O	2.18	0.43
1:C:254:ASP:HA	1:C:264:GLU:OE2	2.18	0.43
1:C:870:ILE:HG21	1:C:931:VAL:HG11	2.01	0.43
2:D:115:TRP:HH2	2:D:331:ILE:HD11	1.83	0.43
5:F:284:SER:HA	5:F:287:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:291:GLN:HG3	5:F:352:LEU:HD22	2.01	0.43
5:F:394:LEU:O	5:F:398:ILE:HG13	2.19	0.43
6:H:67:GLN:CD	6:H:67:GLN:N	2.77	0.43
2:D:234:PRO:O	2:D:237:MET:HB2	2.19	0.43
2:D:1270:ASP:OD2	2:D:1297:GLU:HG2	2.18	0.43
5:F:339:ARG:NH2	5:F:340:GLU:HA	2.34	0.43
5:F:473:ARG:NH2	7:T:12:DC:OP2	2.52	0.43
6:K:67:GLN:HB3	6:K:69:PHE:CE2	2.54	0.43
6:K:84:ARG:NH2	7:T:36:DG:OP1	2.45	0.43
6:K:89:ASP:OD1	6:K:95:GLN:HB2	2.18	0.43
1:C:156:PHE:CE2	1:C:450:ASN:HB3	2.53	0.43
2:D:398:LYS:HD3	5:F:540:LEU:HD21	2.00	0.43
5:F:370:SER:HA	5:F:373:MET:HG2	2.00	0.43
6:H:61:ASP:HA	6:H:65:ARG:HG2	2.01	0.43
5:F:115:ARG:O	5:F:119:ILE:HG12	2.18	0.43
5:F:144:PRO:O	5:F:148:GLU:HG2	2.19	0.43
4:G:253:ILE:HG23	4:G:254:LEU:HD22	2.01	0.43
8:N:-25:DC:H2"	8:N:-24:DG:H8	1.84	0.43
1:C:260:LYS:HG2	1:C:277:LEU:HB3	2.01	0.42
1:C:899:GLU:CD	1:C:903:ARG:HH21	2.27	0.42
1:C:1209:LEU:HD12	1:C:1226:VAL:HB	2.01	0.42
5:F:313:LEU:HD13	5:F:317:ASN:HD22	1.83	0.42
6:K:110:ARG:HG3	6:K:111:VAL:N	2.34	0.42
1:C:901:LEU:HD12	1:C:901:LEU:HA	1.84	0.42
2:D:876:SER:HG	2:D:990:ARG:HH21	1.67	0.42
2:D:1164:SER:HG	2:D:1176:ILE:HG13	1.83	0.42
5:F:313:LEU:HD12	5:F:323:TRP:CE3	2.54	0.42
6:H:54:ILE:HD13	6:H:59:LEU:HD21	2.01	0.42
2:D:127:LEU:HG	2:D:192:MET:HE1	2.02	0.42
2:D:1189:ILE:HG21	2:D:1195:LEU:HD21	2.01	0.42
5:F:346:ARG:HB2	5:F:347:ARG:NH2	2.34	0.42
6:K:41:ARG:HH22	6:K:66:GLU:HG2	1.83	0.42
1:C:70:TYR:HA	1:C:100:LEU:HD23	2.02	0.42
1:C:1320:GLU:CD	2:D:99:ARG:HH21	2.27	0.42
7:T:11:DA:H2"	7:T:12:DC:H5"	2.01	0.42
1:C:369:MET:HE3	1:C:369:MET:O	2.20	0.42
2:D:200:GLN:O	2:D:204:GLU:HB2	2.19	0.42
2:D:443:GLU:N	2:D:443:GLU:CD	2.78	0.42
4:A:151:ARG:NH2	4:B:7:GLU:O	2.52	0.42
5:F:346:ARG:CZ	5:F:347:ARG:HH22	2.32	0.42
5:F:462:VAL:O	5:F:466:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:85:LYS:O	6:K:88:LYS:HD3	2.19	0.42
2:D:411:ILE:O	2:D:415:VAL:HG23	2.19	0.42
2:D:1284:VAL:HG11	2:D:1301:PHE:HD2	1.84	0.42
1:C:158:ASP:OD1	1:C:158:ASP:N	2.52	0.42
1:C:835:GLU:OE1	1:C:1051:LYS:HB3	2.20	0.42
1:C:909:LYS:HA	1:C:909:LYS:HD3	1.84	0.42
2:D:787:ALA:O	2:D:790:THR:OG1	2.30	0.42
5:F:581:LEU:HD23	5:F:595:ILE:HG22	2.00	0.42
1:C:253:PHE:CG	1:C:254:ASP:N	2.87	0.42
1:C:403:MET:HE3	1:C:403:MET:HA	2.02	0.42
2:D:708:ASN:OD1	2:D:712:GLU:N	2.53	0.42
4:A:82:LEU:O	4:A:86:LYS:HG3	2.19	0.42
1:C:160:ASP:O	1:C:161:LYS:HB3	2.20	0.42
1:C:179:TYR:HD1	1:C:180:ARG:HG3	1.84	0.42
2:D:508:LEU:HD21	2:D:637:VAL:HG11	2.02	0.42
2:D:1340:ARG:NH1	2:D:1340:ARG:HB3	2.35	0.42
5:F:131:GLN:NE2	5:F:372:ARG:HB3	2.35	0.42
5:F:147:LEU:HD12	5:F:233:ARG:HH11	1.85	0.42
5:F:352:LEU:HD23	5:F:352:LEU:H	1.84	0.42
8:N:-9:DA:H2'	8:N:-8:DA:C8	2.55	0.42
1:C:98:VAL:HG11	1:C:124:MET:SD	2.59	0.42
2:D:1349:ASN:HA	2:D:1352:VAL:HG22	2.02	0.42
4:B:29:GLU:OE1	4:B:201:LYS:NZ	2.47	0.42
6:H:44:TRP:NE1	6:H:48:GLN:HE21	2.17	0.42
1:C:417:GLN:NE2	1:C:419:THR:O	2.50	0.41
1:C:853:ASP:OD1	1:C:853:ASP:N	2.52	0.41
1:C:1275:TRP:CE2	2:D:801:VAL:HG11	2.55	0.41
2:D:79:LYS:H	2:D:79:LYS:HG2	1.63	0.41
1:C:452:ARG:NH2	1:C:458:GLU:OE1	2.49	0.41
1:C:691:PRO:HD2	1:C:763:THR:HG21	2.02	0.41
1:C:806:PRO:O	2:D:633:ALA:HA	2.19	0.41
2:D:327:LEU:HD23	2:D:330:MET:HE2	2.02	0.41
4:A:96:LYS:HE3	4:A:96:LYS:HB3	1.89	0.41
5:F:434:LYS:HE2	5:F:434:LYS:HB3	1.83	0.41
6:K:65:ARG:NH1	6:K:70:GLU:HG2	2.35	0.41
1:C:120:GLN:NE2	1:C:488:MET:HB3	2.36	0.41
1:C:161:LYS:O	1:C:161:LYS:HG2	2.19	0.41
1:C:1258:LEU:HD11	5:F:532:GLU:HG3	2.01	0.41
6:H:54:ILE:HD12	6:H:54:ILE:O	2.18	0.41
1:C:802:ILE:HD13	1:C:1096:ILE:HB	2.01	0.41
1:C:944:ARG:HA	1:C:947:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1005:LYS:HD3	2:D:1009:ASP:HB3	2.02	0.41
5:F:321:GLU:OE2	5:F:324:LEU:HD23	2.21	0.41
5:F:594:ARG:HH21	8:N:-37:DA:H3'	1.85	0.41
1:C:378:LYS:O	1:C:381:ALA:HB3	2.21	0.41
1:C:618:GLN:HG3	1:C:620:ASN:OD1	2.20	0.41
2:D:363:LEU:O	2:D:486:SER:OG	2.34	0.41
4:A:19:ILE:HD12	4:A:19:ILE:H	1.85	0.41
5:F:138:GLU:OE2	5:F:261:LEU:HD11	2.20	0.41
5:F:485:GLU:OE1	5:F:485:GLU:HA	2.21	0.41
5:F:532:GLU:N	5:F:532:GLU:CD	2.79	0.41
1:C:185:ASP:OD2	1:C:200:ARG:NH1	2.51	0.41
1:C:1109:ILE:HD11	2:D:740:LEU:HD21	2.03	0.41
2:D:1149:LYS:HE2	2:D:1149:LYS:HB2	1.72	0.41
4:A:229:LEU:O	4:A:233:VAL:HG23	2.19	0.41
5:F:381:ARG:HA	5:F:384:LYS:CD	2.51	0.41
6:K:95:GLN:HE21	6:K:95:GLN:HB3	1.63	0.41
7:T:53:DC:H2''	7:T:54:DA:C8	2.55	0.41
6:H:55:SER:O	6:H:59:LEU:HD23	2.20	0.41
1:C:194:LEU:HG	1:C:206:ALA:HB2	2.03	0.41
1:C:201:ARG:HB3	1:C:369:MET:HE2	2.02	0.41
1:C:685:MET:HE3	1:C:1067:ALA:HB1	2.03	0.41
2:D:521:LYS:HB3	2:D:521:LYS:HE3	1.78	0.41
2:D:909:VAL:HG23	2:D:913:GLU:OE2	2.21	0.41
5:F:231:GLU:OE1	5:F:263:ILE:HG21	2.20	0.41
5:F:437:THR:HA	8:N:-7:DA:N7	2.36	0.41
6:H:45:LEU:HD13	6:H:62:PHE:CE2	2.56	0.41
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.93	0.41
1:C:1036:ILE:HD12	1:C:1036:ILE:H	1.86	0.41
4:A:205:ASP:OD1	4:A:205:ASP:C	2.63	0.41
4:G:290:LEU:O	4:G:293:THR:OG1	2.22	0.41
6:K:108:ILE:N	6:K:108:ILE:HD12	2.36	0.41
8:N:-24:DG:H2''	8:N:-23:DG:C8	2.55	0.41
1:C:206:ALA:HB1	1:C:429:MET:HE2	2.03	0.41
1:C:230:PHE:CZ	1:C:292:ILE:HD11	2.56	0.41
1:C:241:LEU:HD13	1:C:283:ASN:OD1	2.21	0.41
1:C:1156:GLN:HG2	1:C:1158:VAL:HG23	2.02	0.41
2:D:141:PHE:HB3	2:D:293:ARG:HD2	2.03	0.41
2:D:616:ASP:OD1	2:D:616:ASP:N	2.53	0.41
2:D:625:MET:HE3	2:D:629:PHE:HE2	1.86	0.41
2:D:644:MET:HE2	2:D:764:LYS:HG3	2.03	0.41
3:E:59:ILE:HD13	3:E:59:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:530:PHE:CD1	5:F:530:PHE:N	2.88	0.41
5:F:530:PHE:N	5:F:530:PHE:HD1	2.19	0.41
7:T:-9:DA:H4'	7:T:-8:DT:OP1	2.20	0.41
7:T:20:DG:C8	7:T:21:DT:H72	2.56	0.41
1:C:98:VAL:HG13	1:C:122:VAL:HG13	2.03	0.41
1:C:562:GLU:OE1	1:C:664:ALA:HB3	2.20	0.41
1:C:672:GLU:HG2	1:C:673:HIS:CD2	2.56	0.41
2:D:372:MET:HE2	2:D:372:MET:HB3	1.88	0.41
5:F:150:PHE:HA	5:F:153:VAL:HG12	2.03	0.41
4:G:322:TRP:HA	4:G:323:PRO:HA	1.92	0.41
2:D:1281:TYR:O	2:D:1285:LYS:HG3	2.21	0.40
4:A:48:LEU:HD23	4:A:181:VAL:HG12	2.03	0.40
5:F:411:ASP:O	5:F:415:GLU:HG2	2.21	0.40
6:K:21:ASN:O	6:K:21:ASN:CG	2.64	0.40
1:C:156:PHE:CZ	1:C:450:ASN:HB3	2.56	0.40
2:D:56:LEU:HD23	2:D:56:LEU:HA	1.95	0.40
2:D:655:ALA:O	2:D:659:GLU:HG2	2.21	0.40
3:E:59:ILE:HD12	3:E:64:LEU:HD21	2.03	0.40
5:F:335:VAL:O	5:F:339:ARG:HB2	2.21	0.40
8:N:-49:DT:H2'	8:N:-48:DT:H71	2.03	0.40
1:C:589:THR:OG1	1:C:659:GLN:NE2	2.54	0.40
1:C:591:TYR:HB3	1:C:652:TYR:HB3	2.02	0.40
1:C:1011:LEU:HD23	1:C:1011:LEU:HA	1.92	0.40
2:D:98:ARG:HB3	2:D:248:ASP:OD1	2.21	0.40
4:A:125:VAL:O	4:A:127:PRO:HD3	2.21	0.40
5:F:230:ASN:HA	5:F:233:ARG:HB2	2.03	0.40
1:C:919:ARG:HG2	1:C:919:ARG:NH1	2.36	0.40
1:C:930:ASP:HB3	1:C:1053:TYR:CD2	2.57	0.40
4:G:254:LEU:HD22	4:G:254:LEU:H	1.86	0.40
7:T:-9:DA:OP2	7:T:-9:DA:H3'	2.22	0.40
8:N:-34:DA:H2''	8:N:-33:DA:C8	2.54	0.40
1:C:184:LEU:HD13	1:C:198:ILE:HG12	2.03	0.40
2:D:726:ALA:HB2	2:D:737:ILE:HD11	2.03	0.40
2:D:1228:VAL:O	2:D:1232:ILE:HG13	2.21	0.40
5:F:101:ARG:O	5:F:105:ARG:HG3	2.22	0.40
6:H:34:ARG:HB2	6:H:34:ARG:HH11	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1292/1341 (96%)	1256 (97%)	36 (3%)	0	100	100
2	D	1192/1401 (85%)	1166 (98%)	26 (2%)	0	100	100
3	E	67/90 (74%)	67 (100%)	0	0	100	100
4	A	227/330 (69%)	222 (98%)	5 (2%)	0	100	100
4	B	219/330 (66%)	218 (100%)	1 (0%)	0	100	100
4	G	69/330 (21%)	62 (90%)	7 (10%)	0	100	100
5	F	462/621 (74%)	455 (98%)	7 (2%)	0	100	100
6	H	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
6	K	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
All	All	3744/4663 (80%)	3653 (98%)	91 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1111/1144 (97%)	1100 (99%)	11 (1%)	68	79
2	D	1012/1168 (87%)	1004 (99%)	8 (1%)	73	81
3	E	58/74 (78%)	58 (100%)	0	100	100
4	A	195/283 (69%)	193 (99%)	2 (1%)	68	79
4	B	187/283 (66%)	183 (98%)	4 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	63/283 (22%)	61 (97%)	2 (3%)	34	64
5	F	417/544 (77%)	413 (99%)	4 (1%)	68	79
6	H	103/103 (100%)	100 (97%)	3 (3%)	37	66
6	K	103/103 (100%)	100 (97%)	3 (3%)	37	66
All	All	3249/3985 (82%)	3212 (99%)	37 (1%)	63	78

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	273	HIS
1	C	354	ASP
1	C	429	MET
1	C	471	VAL
1	C	515	MET
1	C	611	GLU
1	C	622	LYS
1	C	685	MET
1	C	848	GLU
1	C	1085	MET
1	C	1197	MET
2	D	42	GLU
2	D	339	ARG
2	D	386	GLU
2	D	569	MET
2	D	683	ILE
2	D	738	ARG
2	D	1313	LEU
2	D	1348	GLU
4	A	13	LEU
4	A	33	ARG
4	B	51	MET
4	B	134	LEU
4	B	189	GLU
4	B	218	ILE
5	F	361	LEU
5	F	368	ASP
5	F	496	GLN
5	F	560	THR
4	G	263	LEU
4	G	318	ARG
6	K	52	GLU

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Mol	Chain	Res	Type
6	K	54	ILE
6	K	82	THR
6	H	7	LYS
6	H	23	LEU
6	H	61	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	C	60	GLN
1	C	65	ASN
1	C	120	GLN
1	C	324	ASN
1	C	645	HIS
1	C	673	HIS
1	C	684	ASN
1	C	1010	GLN
1	C	1013	GLN
1	C	1061	GLN
1	C	1263	GLN
1	C	1287	GLN
1	C	1335	ASN
2	D	364	HIS
2	D	430	HIS
2	D	680	ASN
2	D	812	HIS
2	D	825	HIS
2	D	861	ASN
2	D	897	GLN
2	D	954	ASN
2	D	1226	HIS
2	D	1243	GLN
2	D	1251	HIS
4	A	18	GLN
4	A	37	HIS
4	A	66	HIS
4	A	104	ASN
4	B	104	ASN
4	B	118	HIS
5	F	317	ASN
5	F	357	GLN

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Mol	Chain	Res	Type
5	F	463	HIS
5	F	477	GLN
5	F	496	GLN
5	F	597	GLN
6	K	51	ASN
6	K	60	HIS
6	K	95	GLN
6	H	67	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

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 ⓘ

There are no chain breaks in this entry.

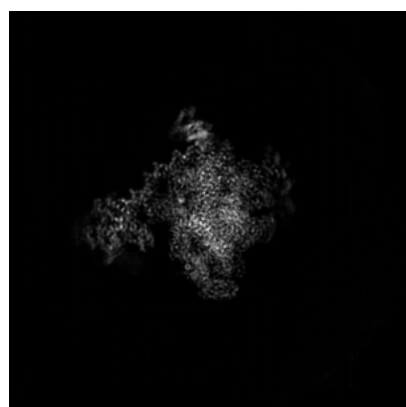
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51275. These allow visual inspection of the internal detail of the map and identification of artifacts.

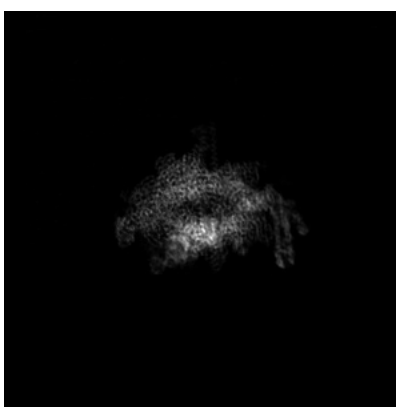
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 225



Y Index: 225

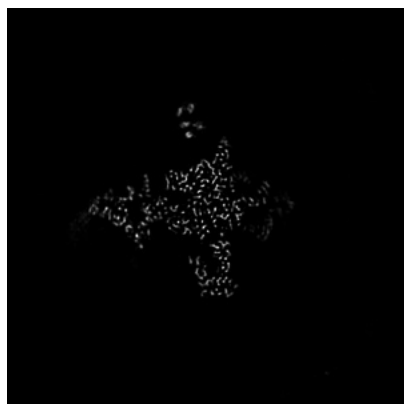


Z Index: 225

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: 204



Y Index: 219

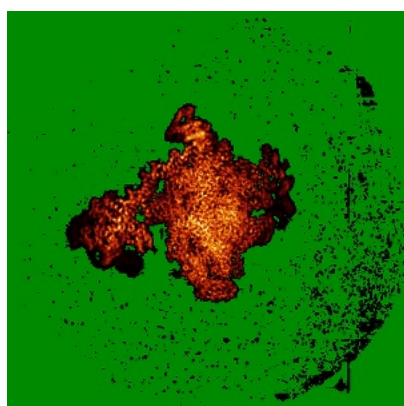


Z Index: 215

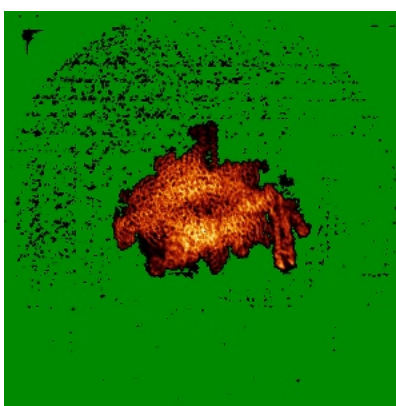
The images above show the largest variance slices of the map in three orthogonal directions.

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

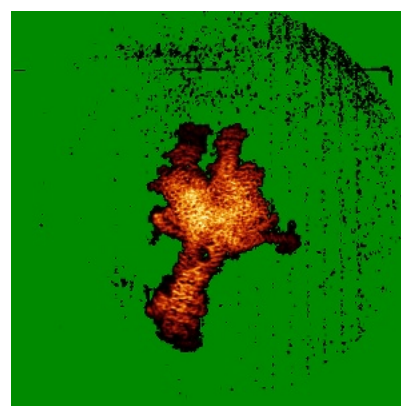
6.4.1 Primary map



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 0.0996. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

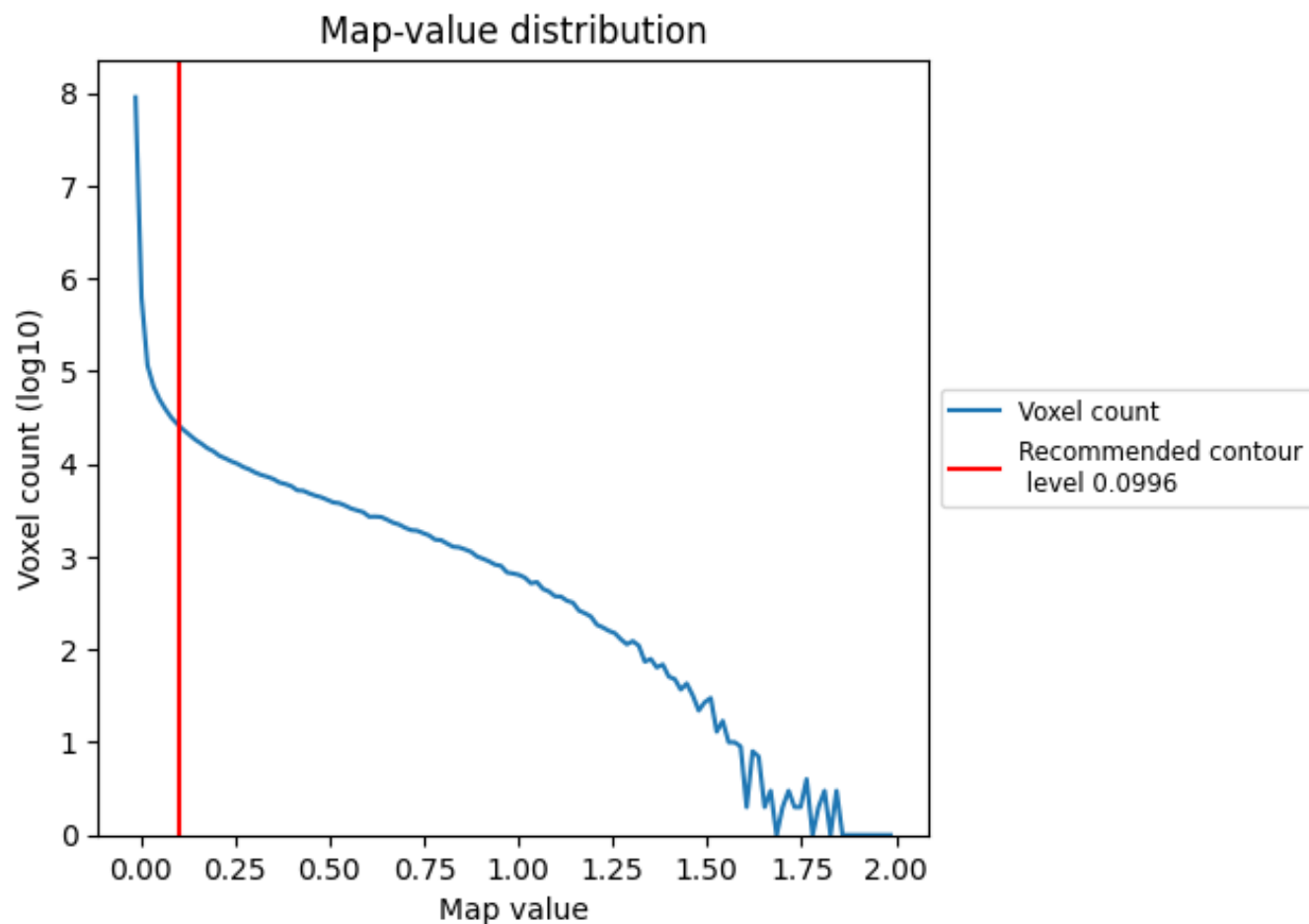
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

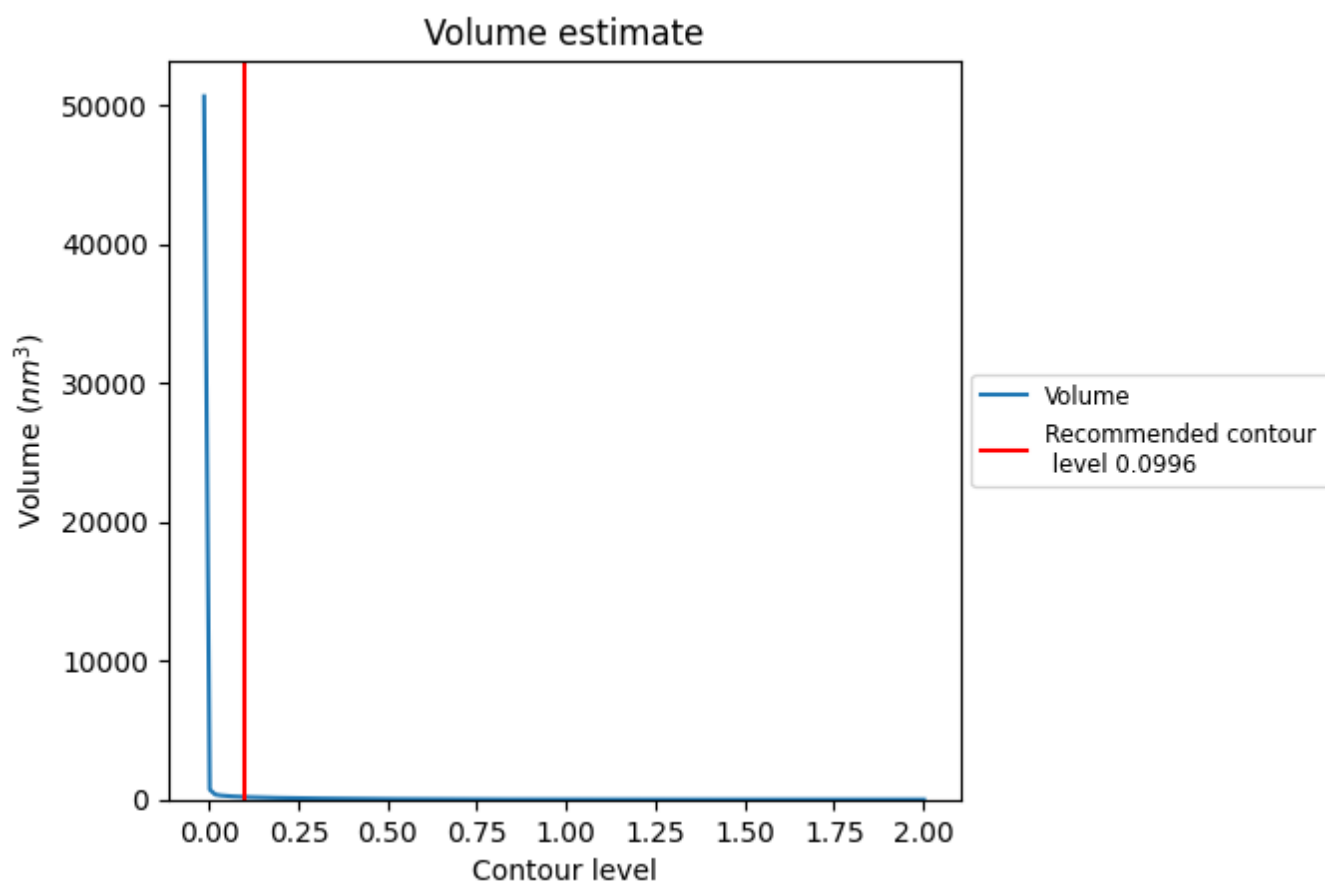
This section contains the results of statistical analysis of the map.

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.

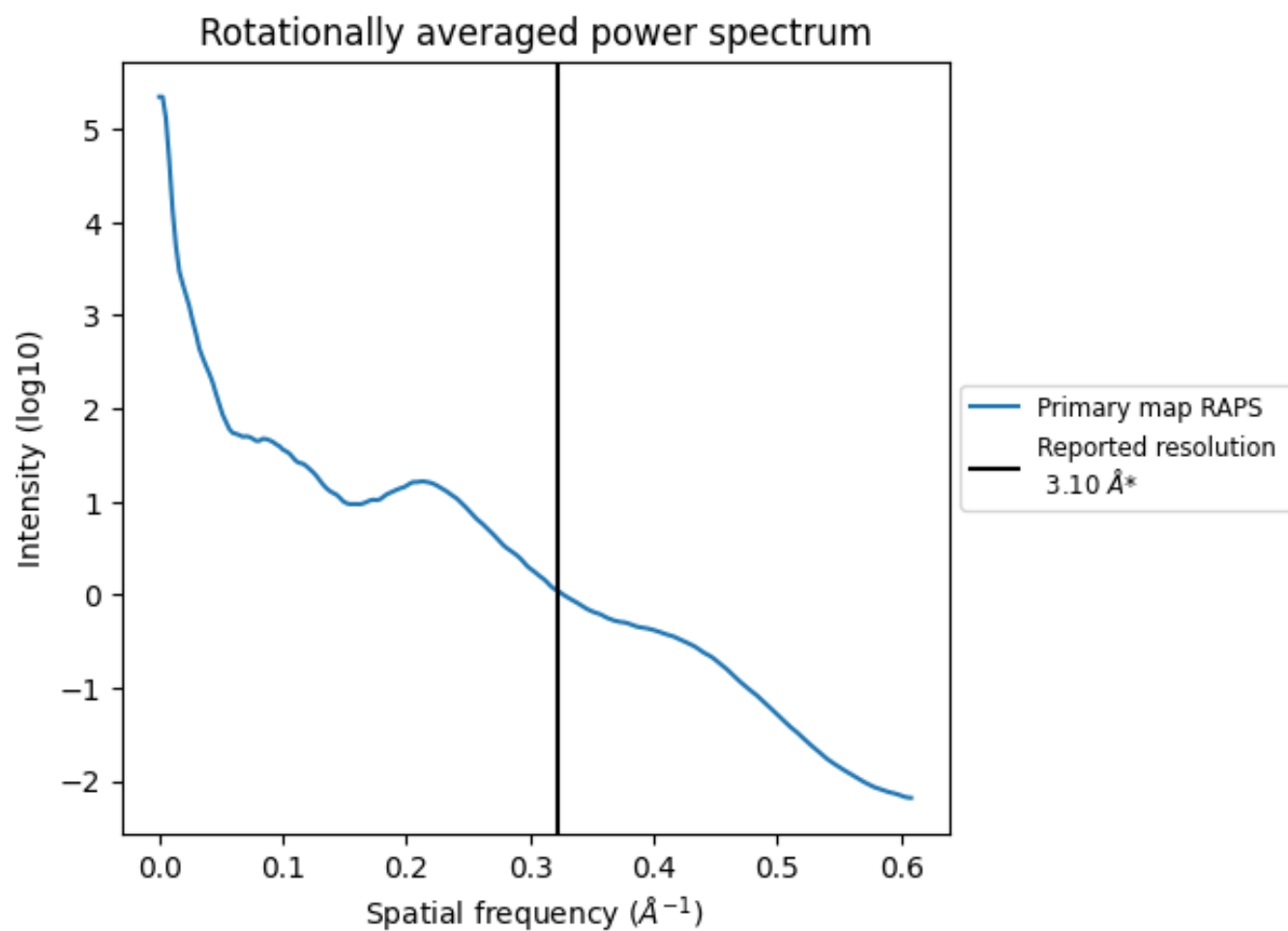
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 169 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 ⓘ

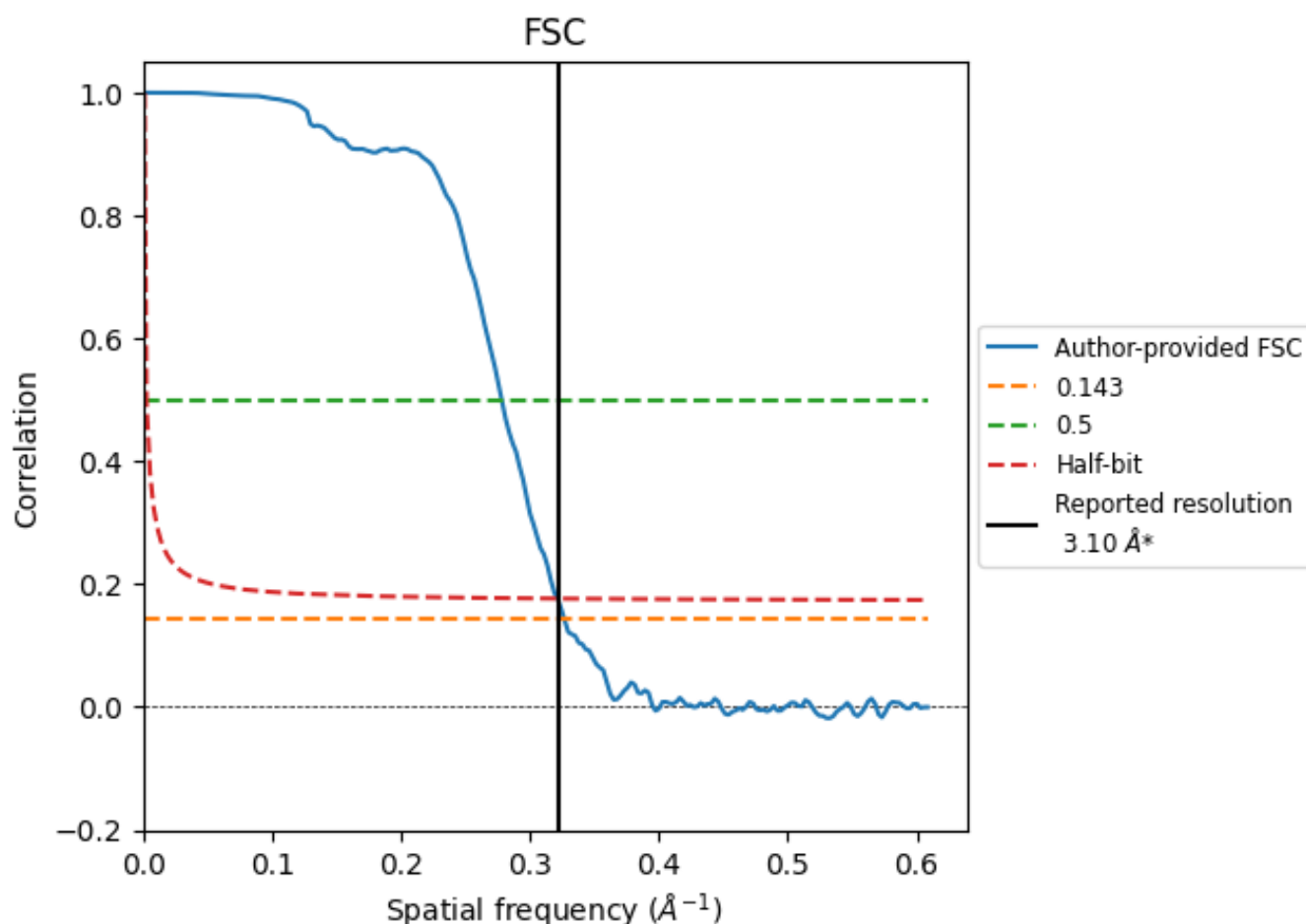


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

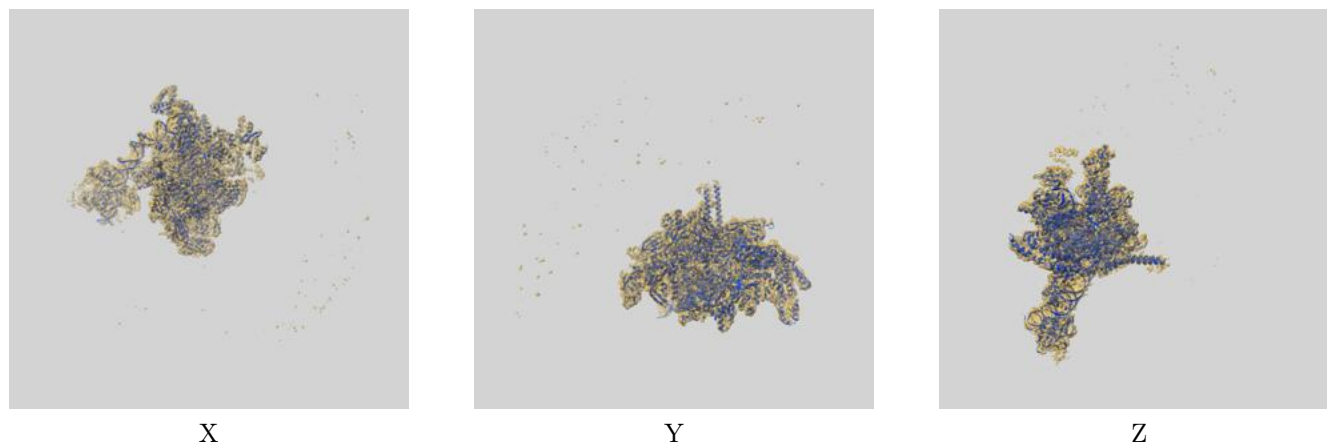
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.60	3.11
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

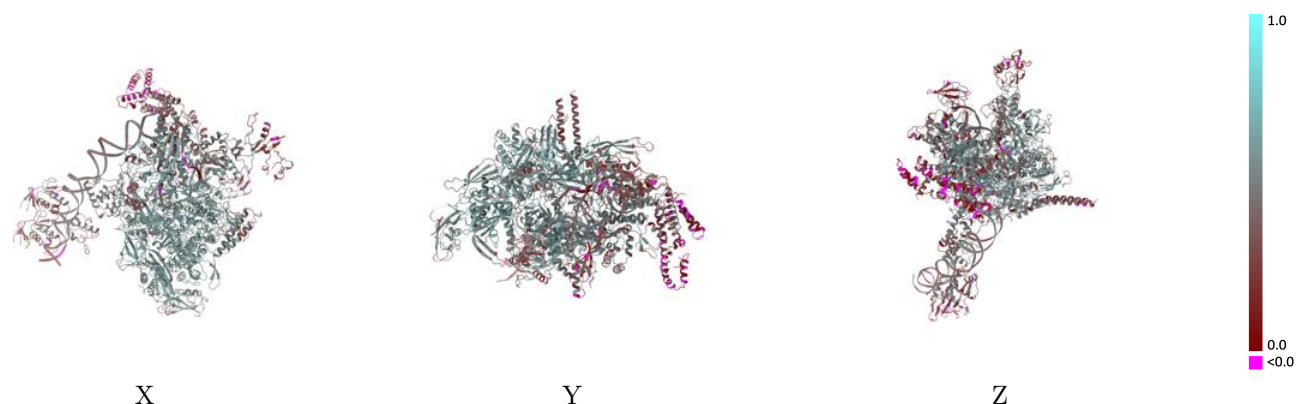
This section contains information regarding the fit between EMDB map EMD-51275 and PDB model 9GDQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



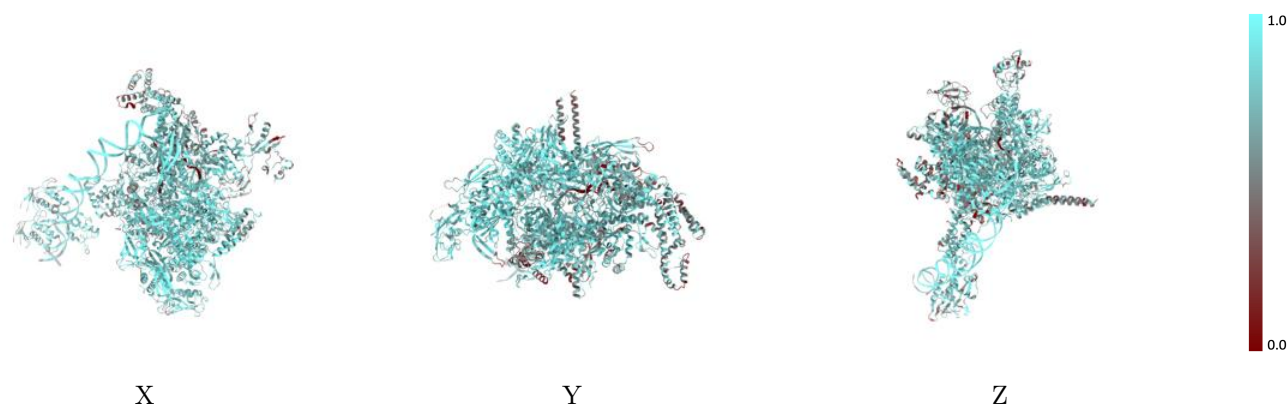
The images above show the 3D surface view of the map at the recommended contour level 0.0996 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



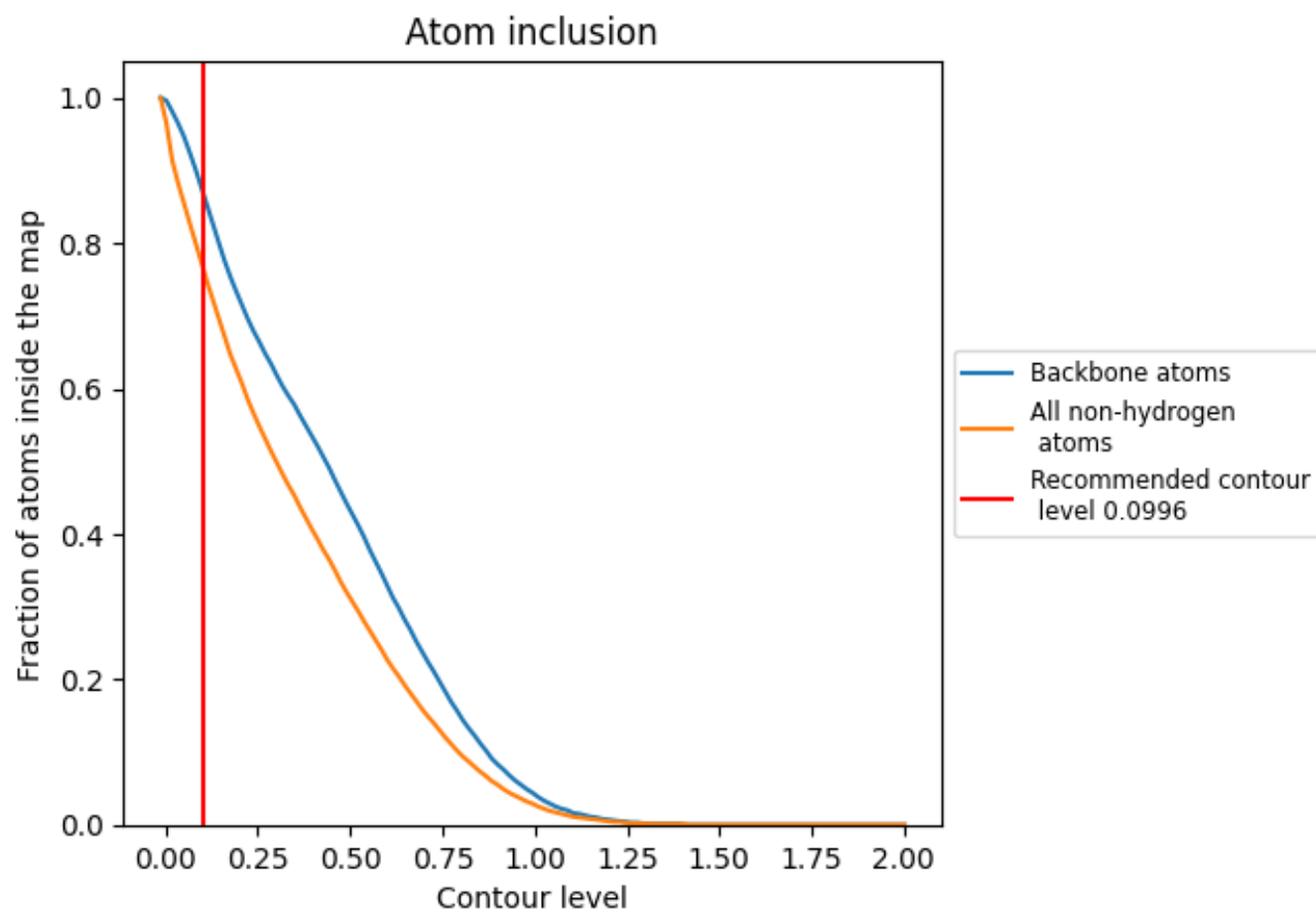
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0996).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (0.0996) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.4560
A	0.8160	0.5290
B	0.8070	0.5160
C	0.7950	0.4980
D	0.8030	0.5070
E	0.2580	0.3690
F	0.6800	0.3180
G	0.7940	0.3580
H	0.6850	0.2720
K	0.7090	0.3300
N	0.7760	0.3670
T	0.7900	0.3800

1.0

0.0

<0.0