



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:05 PM UTC

PDB ID : 6XAV / pdb_00006xav
EMDB ID : EMD-22115
Title : CryoEM Structure of E. coli Rho-dependent Transcription Pre-termination Complex bound with NusG
Authors : Hao, Z.T.; Kim, H.K.; Walz, T.; Nudler, E.
Deposited on : 2020-06-04
Resolution : 7.70 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

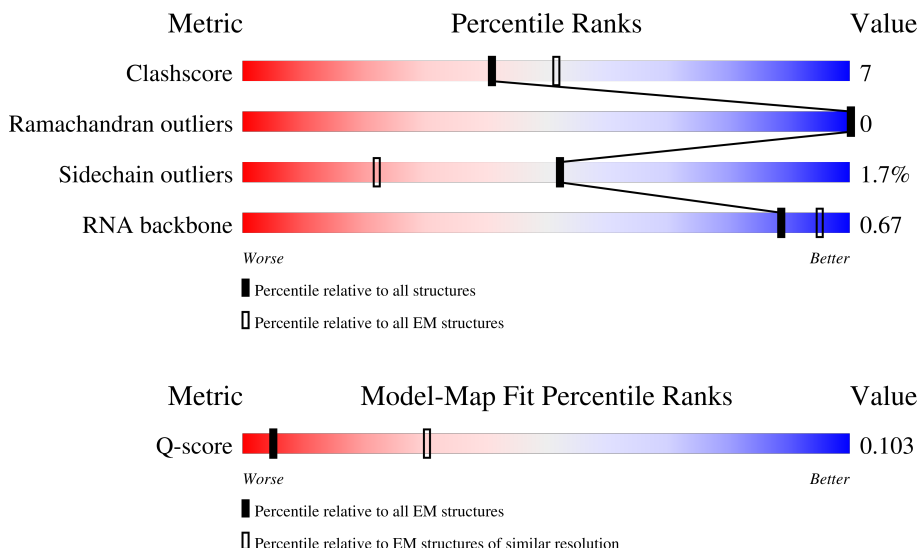
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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.



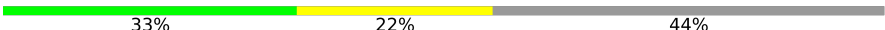
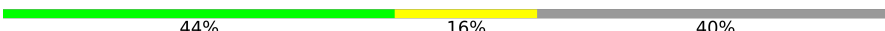
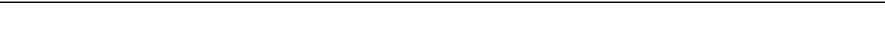
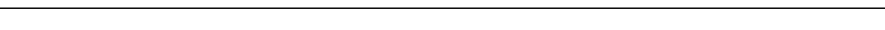
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	384 (7.20 - 8.20)

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	L	181	
2	N	31	
3	T	29	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	18	
5	W	91	
6	H	329	
6	K	329	
7	I	1342	
8	J	1416	
9	G	495	
10	A	419	
10	B	419	
10	C	419	
10	D	419	
10	E	419	
10	F	419	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 46728 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 Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	95	Total	C	N	O	S	0	0
			765	491	136	133	5		

- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	27	Total	C	N	O	P	0	0
			546	260	100	160	26		

- Molecule 3 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	29	Total	C	N	O	P	0	0
			583	279	99	177	28		

- Molecule 4 is a RNA chain called RNA (18-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	10	Total	C	N	O	P	0	0
			221	98	45	68	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	55	Total	C	N	O	S	0	0
			430	265	81	83	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	279	Total	C	N	O	S	0	0
			2003	1242	359	396	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	218	Total	C	N	O	S	0	0
			1679	1049	297	327	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	1304	Total	C	N	O	S	0	0
			10277	6445	1790	1998	44		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	1338	Total	C	N	O	S	0	0
			10392	6527	1856	1959	50		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	VAL	-	expression tag	UNP P0A8T7
J	1411	HIS	-	expression tag	UNP P0A8T7
J	1412	HIS	-	expression tag	UNP P0A8T7
J	1413	HIS	-	expression tag	UNP P0A8T7
J	1414	HIS	-	expression tag	UNP P0A8T7
J	1415	HIS	-	expression tag	UNP P0A8T7
J	1416	HIS	-	expression tag	UNP P0A8T7

- Molecule 9 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	166	Total	C	N	O	S	0	0
			1335	827	243	264	1		

- Molecule 10 is a protein called Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	413	Total	C	N	O	S	0	0
			3253	2051	576	609	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	353	Total	C	N	O	S	0	0
			2803	1769	497	523	14		
10	B	407	Total	C	N	O	S	0	0
			3215	2028	570	600	17		
10	D	415	Total	C	N	O	S	0	0
			3263	2056	578	612	17		
10	E	415	Total	C	N	O	S	0	0
			3263	2056	578	612	17		
10	F	345	Total	C	N	O	S	0	0
			2697	1697	482	507	11		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	J	1	Total	Mg	0
			1	1	

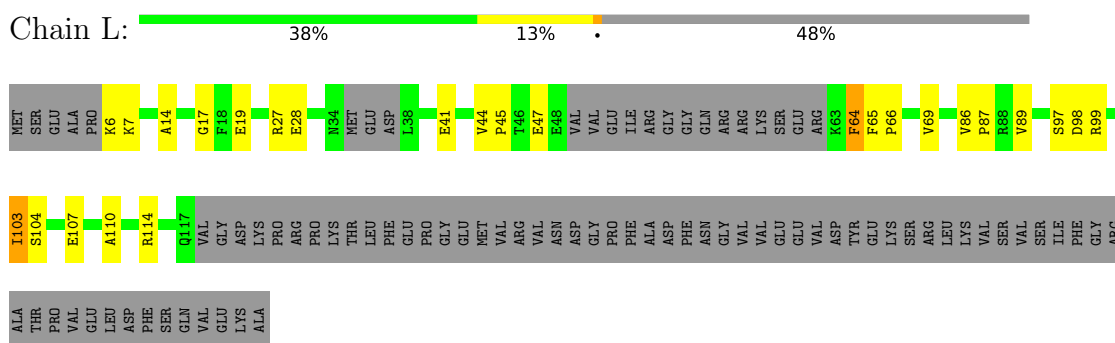
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	J	2	Total	Zn	0
			2	2	

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: Transcription termination/antitermination protein NusG



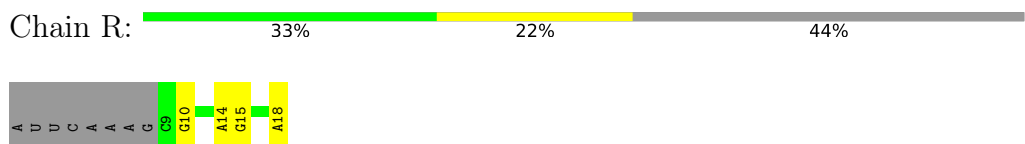
- Molecule 2: DNA (29-MER)



- Molecule 3: DNA (29-MER)

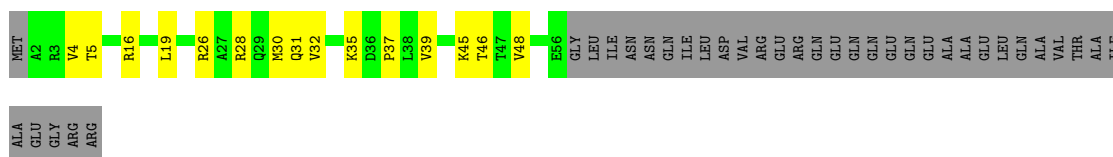


- Molecule 4: RNA (18-MER)



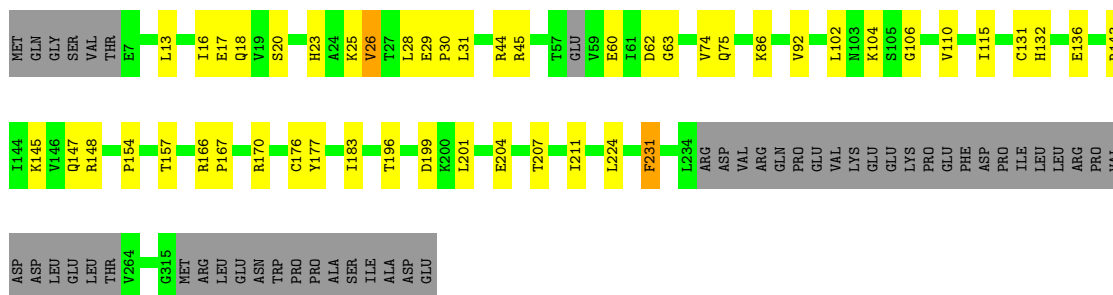
- Molecule 5: DNA-directed RNA polymerase subunit omega





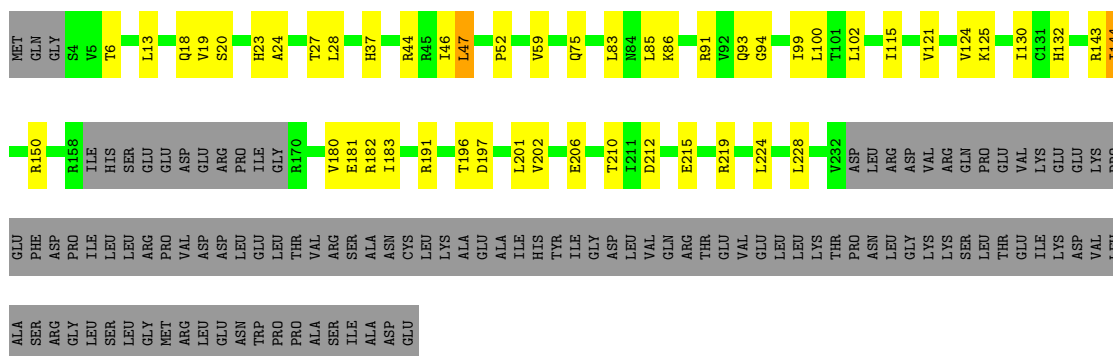
- Molecule 6: DNA-directed RNA polymerase subunit alpha

Chain K: 70% 14% 15%



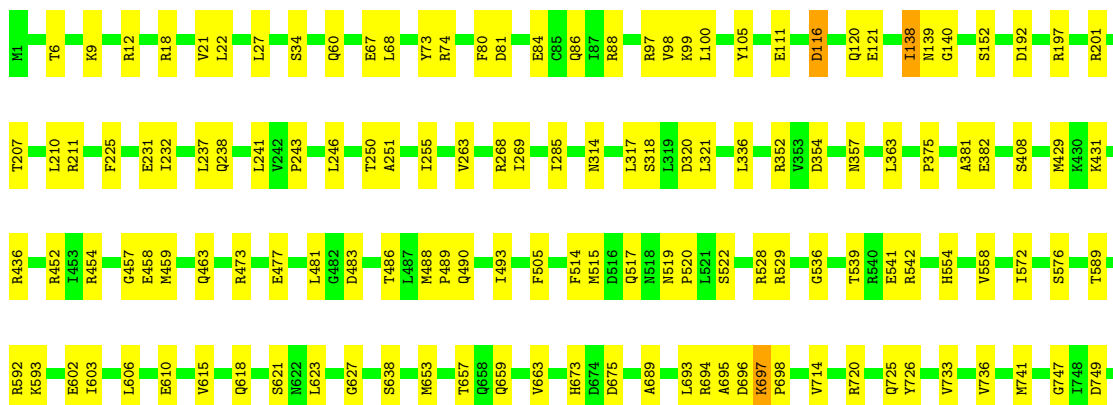
- Molecule 6: DNA-directed RNA polymerase subunit alpha

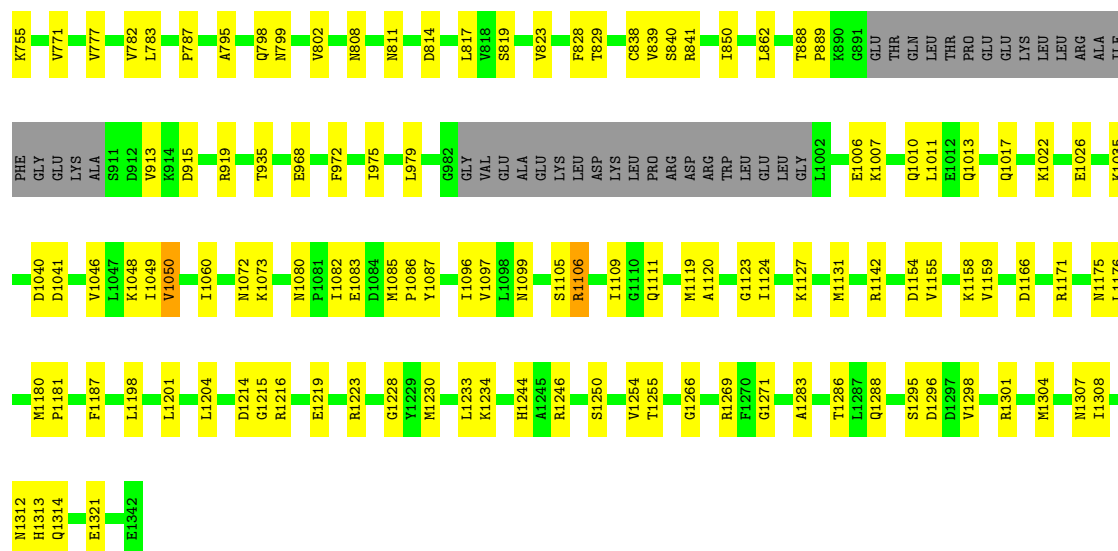
Chain H: 51% 15% 34%



- Molecule 7: DNA-directed RNA polymerase subunit beta

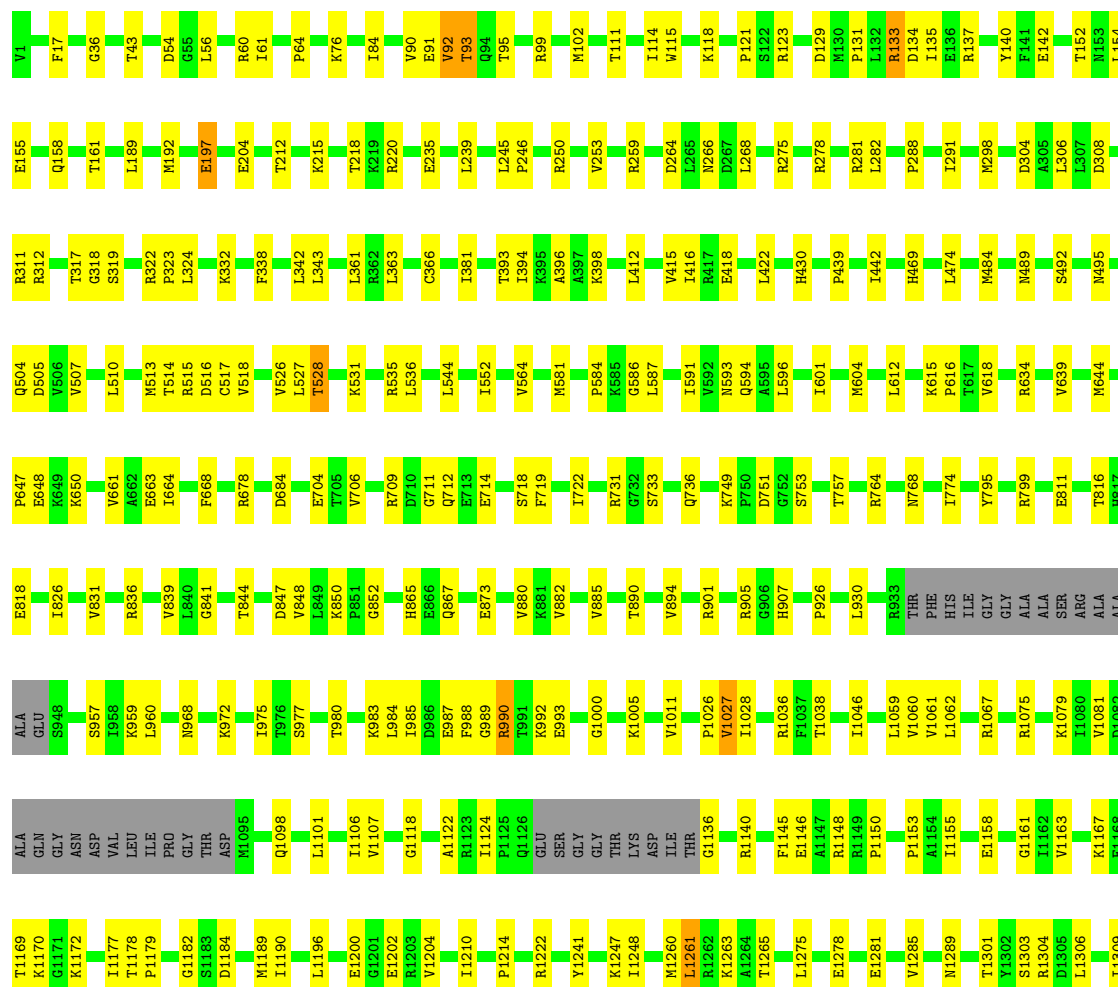
Chain I: 78% 18% 4%

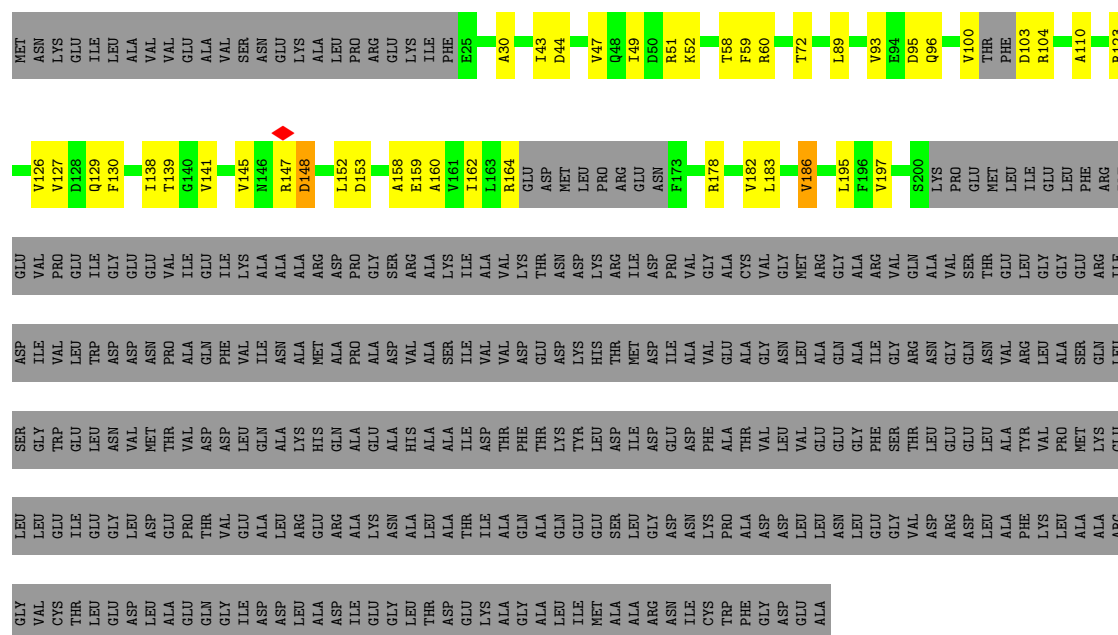
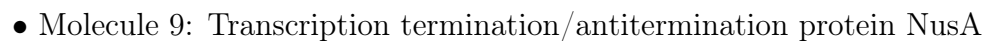




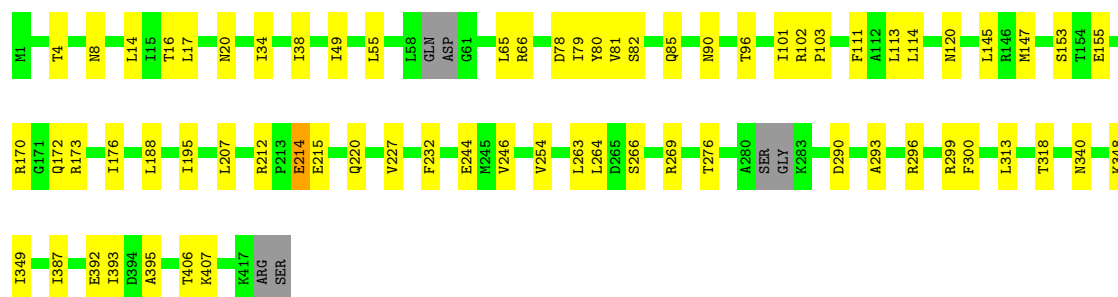
• Molecule 8: DNA-directed RNA polymerase subunit beta'

Chain J: 74% 20% 6%

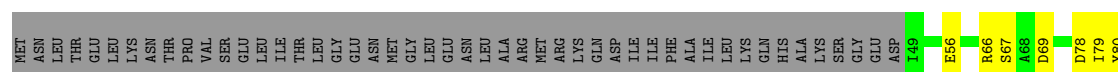




Chain C: 82% 16%



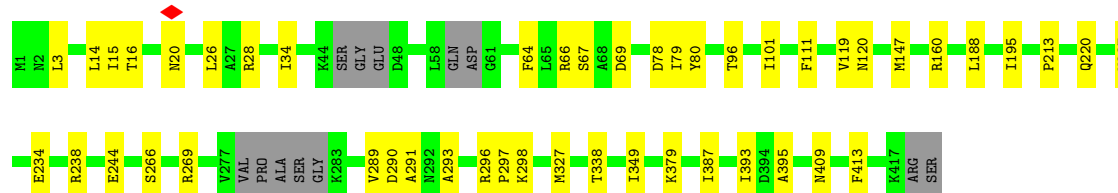
Chain A: 73% 11% 16%





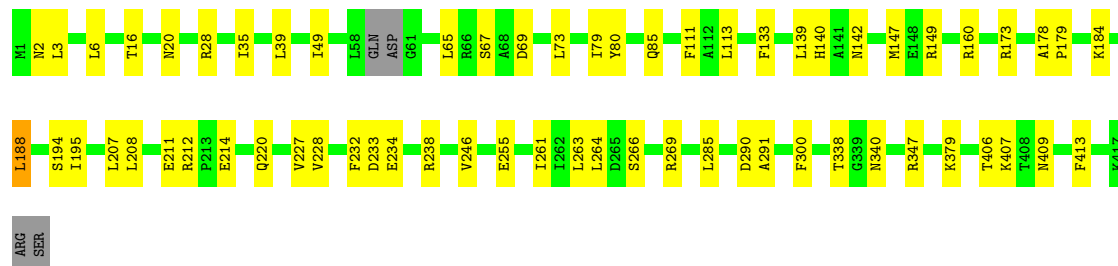
- Molecule 10: Transcription termination factor Rho

Chain B: 86% 11% .



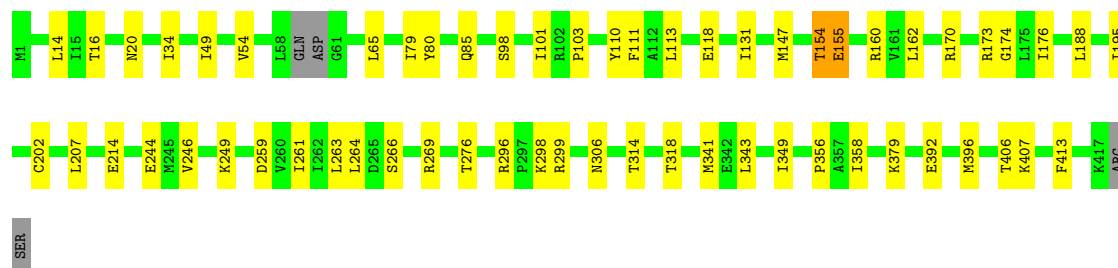
- Molecule 10: Transcription termination factor Rho

Chain D: 84% 15% .



- Molecule 10: Transcription termination factor Rho

Chain E: 85% 14% .



- Molecule 10: Transcription termination factor Rho

Chain F: 68% 14% 18%



V206	L207	L208	E211	R212	P213	E214	V227	F232	D233	R238	E244	M245	V246	L253	V254	E255	K258	I262	L263	L264	A260	SER	GLY	K283	R296	F300	L313	T314	I315	T318	G339	N340	M341	L345	S346	R347	R353	VAL	PHE	PRO	ALA	ILE	ASP		
TYR	ASN	ARG	SER	GLY	THR	ARG	LYS	GLU	GLU	LEU	LEU	THR	THR	GLN	GLU	GLU	LEU	GLN	LYS	MET	TRP	ILE	LEU	ARG	LYS	ILE	ILE	HIS	PRO	MET	GLY	GLY	ILE	ASP	ALA	MET	GLU	PHE	ASP	ASP	ASP	ASP	ASP	ASP	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size ($\text{\AA}$)	366.8, 366.8, 366.8	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	L	0.27	0/782	0.39	0/1052
2	N	0.16	0/610	0.28	0/936
3	T	0.19	0/650	0.34	0/1000
4	R	0.04	0/248	0.05	0/386
5	W	0.34	0/432	0.51	0/582
6	H	0.12	0/1698	0.33	0/2301
6	K	0.18	0/2023	0.36	0/2749
7	I	0.12	0/10439	0.34	0/14082
8	J	0.16	0/10547	0.36	0/14238
9	G	0.21	0/1347	0.34	0/1814
10	A	0.11	0/2847	0.26	0/3832
10	B	0.09	0/3260	0.24	0/4384
10	C	0.09	0/3300	0.25	0/4441
10	D	0.09	0/3311	0.25	0/4457
10	E	0.09	0/3311	0.25	0/4457
10	F	0.09	0/2734	0.24	0/3683
All	All	0.14	0/47539	0.31	0/64394

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	765	0	763	30	0
2	N	546	0	305	11	0
3	T	583	0	329	10	0
4	R	221	0	109	2	0
5	W	430	0	445	13	0
6	H	1679	0	1715	35	0
6	K	2003	0	1880	29	0
7	I	10277	0	10284	162	0
8	J	10392	0	10590	185	0
9	G	1335	0	1337	22	0
10	A	2803	0	2860	28	0
10	B	3215	0	3301	28	0
10	C	3253	0	3337	42	0
10	D	3263	0	3346	34	0
10	E	3263	0	3346	40	0
10	F	2697	0	2771	37	0
11	J	1	0	0	0	0
12	J	2	0	0	0	0
All	All	46728	0	46718	645	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 7.

All (645) 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)
8:J:826:ILE:HG21	8:J:992:LYS:O	1.65	0.95
1:L:45:PRO:HB2	1:L:64:PHE:CE2	2.11	0.86
1:L:64:PHE:HB3	8:J:281:ARG:HH12	1.42	0.83
6:K:29:GLU:HG3	6:K:30:PRO:HA	1.63	0.81
8:J:155:GLU:HB3	8:J:158:GLN:HB2	1.65	0.78
8:J:1327:GLU:O	8:J:1331:VAL:HG23	1.85	0.77
6:K:29:GLU:CG	6:K:30:PRO:HA	2.14	0.77
1:L:64:PHE:HA	8:J:281:ARG:HH22	1.51	0.76
8:J:826:ILE:CG2	8:J:992:LYS:O	2.38	0.71
10:E:299:ARG:HH21	10:F:233:ASP:HB3	1.56	0.70
8:J:749:LYS:HG2	8:J:753:SER:H	1.57	0.70
8:J:985:ILE:HG23	8:J:989:GLY:HA2	1.73	0.70
1:L:64:PHE:HA	8:J:281:ARG:NH2	2.06	0.69
7:I:241:LEU:HD22	7:I:285:ILE:HD13	1.73	0.69
8:J:275:ARG:HH11	8:J:298:MET:HB3	1.58	0.69
7:I:1022:LYS:HA	7:I:1026:GLU:HB2	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:589:THR:OG1	7:I:659:GLN:NE2	2.25	0.68
8:J:749:LYS:HG3	8:J:751:ASP:H	1.59	0.68
8:J:343:LEU:HD11	8:J:1324:SER:HB2	1.75	0.68
8:J:749:LYS:HE3	8:J:751:ASP:HB3	1.76	0.68
10:C:102:ARG:HG3	10:C:114:LEU:HB2	1.75	0.68
7:I:1013:GLN:O	7:I:1017:GLN:N	2.25	0.67
8:J:1346:GLY:O	8:J:1350:ASN:ND2	2.26	0.67
1:L:47:GLU:HG3	1:L:64:PHE:HE1	1.61	0.66
6:K:145:LYS:HE2	6:K:147:GLN:HE21	1.61	0.66
8:J:1075:ARG:NH2	8:J:1169:THR:OG1	2.28	0.66
6:K:16:ILE:HG12	6:K:26:VAL:HG13	1.78	0.65
7:I:819:SER:HB2	7:I:1085:MET:HE3	1.77	0.65
7:I:528:ARG:NH2	7:I:576:SER:O	2.30	0.65
10:D:285:LEU:HD21	10:E:276:THR:HG23	1.78	0.65
10:F:208:LEU:HB3	10:F:211:GLU:HG3	1.78	0.65
1:L:65:PHE:HZ	8:J:288:PRO:HD2	1.62	0.65
9:G:162:ILE:HG12	9:G:197:VAL:HB	1.78	0.65
7:I:12:ARG:HG3	7:I:1181:PRO:HB2	1.79	0.65
1:L:104:SER:HB2	1:L:107:GLU:HB2	1.79	0.64
7:I:463:GLN:HG2	7:I:505:PHE:HB2	1.79	0.64
8:J:268:LEU:HB3	8:J:306:LEU:HD23	1.78	0.64
7:I:1022:LYS:HE3	10:C:82:SER:HB2	1.78	0.64
8:J:647:PRO:HG2	8:J:650:LYS:HB2	1.78	0.64
8:J:1161:GLY:HA3	8:J:1179:PRO:HA	1.79	0.64
6:H:28:LEU:HD12	6:H:201:LEU:HD23	1.79	0.64
7:I:840:SER:HG	7:I:1048:LYS:H	1.43	0.64
8:J:36:GLY:HA3	8:J:61:ILE:HD12	1.79	0.63
7:I:231:GLU:N	7:I:238:GLN:O	2.30	0.63
1:L:98:ASP:HA	7:I:375:PRO:HD3	1.80	0.63
8:J:121:PRO:HG2	8:J:123:ARG:HH12	1.64	0.63
6:K:60:GLU:HG2	6:K:170:ARG:HA	1.79	0.63
8:J:1285:VAL:O	8:J:1289:ASN:ND2	2.30	0.63
7:I:210:LEU:HD21	7:I:429:MET:HE1	1.79	0.63
6:K:44:ARG:HG3	6:K:183:ILE:HB	1.81	0.62
7:I:657:THR:HB	7:I:1187:PHE:HB2	1.81	0.62
8:J:612:LEU:HB3	8:J:616:PRO:HG2	1.81	0.62
10:C:16:THR:O	10:C:20:ASN:ND2	2.33	0.62
8:J:43:THR:HG22	8:J:56:LEU:HD12	1.80	0.62
6:K:31:LEU:HB2	6:K:199:ASP:O	2.00	0.61
10:C:173:ARG:NH2	10:D:214:GLU:OE2	2.31	0.61
8:J:140:TYR:HE2	8:J:312:ARG:HE	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:16:THR:O	10:D:20:ASN:ND2	2.33	0.61
8:J:968:ASN:HD21	8:J:972:LYS:HB2	1.66	0.61
10:E:170:ARG:NH1	10:E:202:CYS:SG	2.74	0.61
10:F:16:THR:O	10:F:20:ASN:ND2	2.32	0.61
6:K:92:VAL:O	6:K:148:ARG:NH2	2.32	0.60
7:I:720:ARG:HE	7:I:736:VAL:HG11	1.65	0.60
10:F:206:VAL:HB	10:F:227:VAL:HG13	1.84	0.60
7:I:1254:VAL:O	8:J:99:ARG:NH2	2.34	0.60
8:J:1163:VAL:HG23	8:J:1177:ILE:HG12	1.83	0.60
7:I:1072:ASN:ND2	7:I:1111:GLN:OE1	2.35	0.59
8:J:885:VAL:HG23	8:J:894:VAL:HG11	1.84	0.59
8:J:977:SER:OG	8:J:980:THR:OG1	2.20	0.59
3:T:12:DG:OP1	8:J:1326:GLN:HG2	2.03	0.59
7:I:1072:ASN:HD21	7:I:1230:MET:HE1	1.67	0.59
10:F:73:LEU:HB2	10:F:238:ARG:HH21	1.68	0.59
10:F:262:ILE:HB	10:F:315:ILE:HG12	1.84	0.59
8:J:984:LEU:HB3	8:J:993:GLU:HB2	1.82	0.59
6:H:47:LEU:HD22	6:H:183:ILE:HD12	1.85	0.59
10:E:80:TYR:N	10:E:111:PHE:O	2.35	0.59
1:L:27:ARG:NH2	1:L:41:GLU:OE1	2.29	0.59
7:I:828:PHE:HB3	7:I:1234:LYS:HD2	1.83	0.59
7:I:841:ARG:HD3	7:I:1046:VAL:HG12	1.84	0.59
8:J:54:ASP:OD1	8:J:60:ARG:NH2	2.35	0.59
1:L:19:GLU:HG3	1:L:69:VAL:HG22	1.85	0.59
7:I:363:LEU:HB3	7:I:381:ALA:HB1	1.84	0.58
10:B:16:THR:O	10:B:20:ASN:ND2	2.35	0.58
10:E:349:ILE:HG21	10:E:396:MET:HG3	1.83	0.58
8:J:507:VAL:HG12	8:J:601:ILE:HD12	1.85	0.58
10:A:66:ARG:NH1	10:A:78:ASP:OD2	2.36	0.58
6:K:131:CYS:SG	6:K:132:HIS:N	2.76	0.58
6:H:59:VAL:HG22	6:H:144:ILE:HA	1.83	0.58
8:J:1179:PRO:HB2	8:J:1182:GLY:H	1.68	0.58
8:J:1260:MET:HE2	8:J:1306:LEU:HD11	1.86	0.58
10:F:66:ARG:NH1	10:F:78:ASP:OD2	2.35	0.58
1:L:99:ARG:NH2	8:J:161:THR:OG1	2.32	0.58
8:J:114:ILE:HD12	8:J:304:ASP:HB3	1.85	0.58
8:J:584:PRO:HG2	8:J:587:LEU:HD13	1.84	0.58
10:D:6:LEU:HD23	10:D:35:ILE:HG23	1.84	0.58
10:E:16:THR:O	10:E:20:ASN:ND2	2.35	0.58
7:I:241:LEU:HD11	7:I:246:LEU:HD21	1.84	0.58
7:I:197:ARG:NH1	7:I:201:ARG:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:158:THR:HA	10:A:356:PRO:HG3	1.86	0.58
7:I:88:ARG:NH1	7:I:1040:ASP:OD2	2.37	0.57
7:I:694:ARG:O	7:I:798:GLN:NE2	2.36	0.57
10:D:85:GLN:NE2	10:D:113:LEU:O	2.36	0.57
10:C:85:GLN:NE2	10:C:113:LEU:O	2.34	0.57
9:G:60:ARG:NH1	9:G:72:THR:O	2.37	0.57
7:I:67:GLU:OE1	7:I:105:TYR:OH	2.22	0.57
8:J:1150:PRO:HG3	8:J:1214:PRO:HB2	1.87	0.57
6:H:91:ARG:NH2	6:H:210:THR:O	2.38	0.57
8:J:492:SER:OG	8:J:495:ASN:OD1	2.21	0.57
8:J:1027:VAL:HG21	8:J:1122:ALA:HB3	1.87	0.57
10:D:149:ARG:HE	10:D:194:SER:HA	1.68	0.57
10:D:234:GLU:OE2	10:D:238:ARG:NH1	2.38	0.57
7:I:1246:ARG:NH2	7:I:1250:SER:O	2.37	0.56
7:I:811:ASN:O	7:I:1099:ASN:ND2	2.37	0.56
7:I:968:GLU:O	7:I:972:PHE:N	2.31	0.56
10:A:220:GLN:HA	10:A:227:VAL:HG21	1.88	0.56
10:B:220:GLN:HA	10:B:227:VAL:HG21	1.86	0.56
10:E:207:LEU:HD13	10:E:246:VAL:HG21	1.86	0.56
8:J:1038:THR:HG21	8:J:1079:LYS:HE2	1.87	0.56
8:J:245:LEU:HB3	8:J:250:ARG:HD3	1.88	0.56
10:A:138:PRO:HG2	10:B:213:PRO:HB2	1.88	0.56
7:I:60:GLN:HG2	7:I:67:GLU:HG3	1.86	0.56
10:F:80:TYR:N	10:F:111:PHE:O	2.38	0.56
10:F:244:GLU:OE2	10:F:296:ARG:NH2	2.38	0.56
6:H:59:VAL:HG21	6:H:85:LEU:HD13	1.86	0.56
6:H:124:VAL:HG13	6:H:125:LYS:HG3	1.88	0.56
7:I:88:ARG:NH2	7:I:1035:LYS:O	2.38	0.56
7:I:529:ARG:HD2	7:I:572:ILE:HG22	1.87	0.56
10:E:98:SER:HB2	10:E:118:GLU:HB3	1.88	0.56
7:I:241:LEU:HD21	7:I:246:LEU:HD11	1.88	0.56
7:I:317:LEU:HA	7:I:321:LEU:HD12	1.87	0.56
2:N:16:DG:H2"	2:N:17:DA:H5"	1.88	0.55
6:K:75:GLN:NE2	7:I:771:VAL:O	2.39	0.55
10:C:266:SER:HB2	10:C:269:ARG:HB2	1.87	0.55
1:L:65:PHE:CE2	8:J:291:ILE:HG13	2.42	0.55
6:H:206:GLU:OE1	8:J:531:LYS:NZ	2.36	0.55
8:J:121:PRO:O	8:J:123:ARG:NH1	2.40	0.55
8:J:394:ILE:HG22	8:J:398:LYS:HE3	1.89	0.55
8:J:648:GLU:N	8:J:648:GLU:OE1	2.39	0.55
9:G:148:ASP:OD1	9:G:164:ARG:HD3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:99:ILE:HD11	6:H:143:ARG:HB3	1.88	0.55
8:J:381:ILE:HD11	8:J:412:LEU:HD13	1.87	0.55
7:I:314:ASN:O	7:I:352:ARG:NH1	2.39	0.55
7:I:34:SER:HG	7:I:457:GLY:H	1.54	0.55
7:I:1304:MET:HE3	7:I:1308:ILE:HD11	1.88	0.55
8:J:513:MET:HG2	8:J:544:LEU:HD21	1.88	0.55
9:G:127:VAL:HG13	9:G:195:LEU:HD21	1.89	0.55
10:B:119:VAL:HG12	10:B:120:ASN:HD22	1.72	0.55
6:H:181:GLU:OE1	8:J:535:ARG:NH2	2.39	0.55
7:I:68:LEU:HD11	7:I:100:LEU:HB3	1.89	0.55
7:I:408:SER:O	7:I:431:LYS:NZ	2.38	0.55
8:J:848:VAL:HG11	8:J:880:VAL:HG12	1.89	0.55
10:A:128:ARG:HB2	10:B:28:ARG:HG2	1.89	0.55
10:E:207:LEU:HG	10:E:264:LEU:HD13	1.89	0.55
7:I:802:VAL:HG12	7:I:1096:ILE:HB	1.89	0.54
10:B:266:SER:HB2	10:B:269:ARG:HB2	1.89	0.54
10:E:349:ILE:HD11	10:E:392:GLU:HB3	1.89	0.54
2:N:6:DA:H2''	2:N:7:DC:H5'	1.87	0.54
2:N:16:DG:N3	2:N:16:DG:H2'	2.22	0.54
7:I:120:GLN:HE22	7:I:489:PRO:HG2	1.72	0.54
8:J:661:VAL:HA	8:J:664:ILE:HG22	1.88	0.54
6:H:180:VAL:O	8:J:535:ARG:NH1	2.40	0.54
10:B:80:TYR:N	10:B:111:PHE:O	2.39	0.54
1:L:107:GLU:HB3	8:J:288:PRO:HB3	1.90	0.54
10:A:80:TYR:N	10:A:111:PHE:O	2.40	0.54
6:K:231:PHE:HD1	6:K:231:PHE:H	1.56	0.54
7:I:255:ILE:HB	7:I:263:VAL:HB	1.88	0.54
8:J:91:GLU:OE1	8:J:92:VAL:N	2.41	0.54
1:L:87:PRO:HG3	7:I:477:GLU:HG3	1.90	0.54
7:I:18:ARG:HH12	7:I:621:SER:N	2.06	0.54
10:D:179:PRO:HB2	10:D:347:ARG:HH11	1.71	0.54
6:K:18:GLN:NE2	6:K:20:SER:O	2.40	0.54
7:I:1298:VAL:HG22	7:I:1301:ARG:HH22	1.73	0.54
8:J:514:THR:HG21	8:J:596:LEU:HD12	1.90	0.54
8:J:644:MET:O	8:J:764:ARG:NH1	2.41	0.54
1:L:66:PRO:HG2	8:J:278:ARG:NH2	2.22	0.54
10:E:176:ILE:HA	10:E:343:LEU:HB3	1.90	0.54
7:I:68:LEU:HD21	7:I:100:LEU:HD13	1.89	0.54
10:A:85:GLN:NE2	10:A:113:LEU:O	2.40	0.54
10:A:244:GLU:OE2	10:A:296:ARG:NH2	2.40	0.53
10:B:244:GLU:OE2	10:B:296:ARG:NH2	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:26:ARG:HG3	5:W:30:MET:HE3	1.89	0.53
8:J:836:ARG:HH22	8:J:873:GLU:HG2	1.73	0.53
9:G:145:VAL:HG12	9:G:145:VAL:O	2.08	0.53
8:J:1005:LYS:HG3	8:J:1011:VAL:HG12	1.91	0.53
10:B:234:GLU:OE2	10:B:238:ARG:NH1	2.39	0.53
8:J:1158:GLU:OE2	8:J:1222:ARG:NH2	2.42	0.53
8:J:1172:LYS:HB3	8:J:1189:MET:HB3	1.90	0.53
8:J:1322:ALA:HA	8:J:1325:PHE:CZ	2.44	0.53
6:H:86:LYS:NZ	8:J:526:VAL:O	2.42	0.53
7:I:1246:ARG:HH11	7:I:1266:GLY:HA2	1.74	0.53
8:J:1155:ILE:HG13	8:J:1210:ILE:HB	1.91	0.53
8:J:1317:GLU:N	8:J:1317:GLU:OE1	2.41	0.53
10:A:67:SER:OG	10:A:69:ASP:OD1	2.25	0.53
7:I:814:ASP:OD1	7:I:1106:ARG:NH1	2.41	0.53
6:H:83:LEU:HD23	8:J:528:THR:HA	1.90	0.53
7:I:1120:ALA:HB1	7:I:1198:LEU:HG	1.91	0.53
6:K:167:PRO:HD2	6:K:170:ARG:HE	1.74	0.52
10:C:66:ARG:NH1	10:C:78:ASP:OD2	2.41	0.52
10:B:15:ILE:HG23	10:B:26:LEU:HB2	1.91	0.52
5:W:31:GLN:HB2	5:W:46:THR:HG21	1.90	0.52
7:I:1269:ARG:HH11	7:I:1271:GLY:HA2	1.75	0.52
10:C:79:ILE:HD13	10:C:101:ILE:HG21	1.89	0.52
10:A:149:ARG:HH21	10:A:193:GLN:HB3	1.74	0.52
7:I:808:ASN:HD21	7:I:1216:ARG:HH22	1.57	0.52
8:J:268:LEU:HD23	8:J:306:LEU:HA	1.90	0.52
7:I:9:LYS:HG2	7:I:1171:ARG:HH11	1.74	0.52
9:G:43:ILE:O	9:G:60:ARG:NH2	2.43	0.52
8:J:118:LYS:NZ	8:J:311:ARG:O	2.39	0.52
6:H:19:VAL:HB	6:H:23:HIS:HB3	1.92	0.52
7:I:979:LEU:HD12	7:I:1011:LEU:HD21	1.92	0.52
10:D:290:ASP:OD1	10:D:291:ALA:N	2.43	0.52
3:T:2:DG:OP1	8:J:212:THR:OG1	2.28	0.52
8:J:1060:VAL:HG22	8:J:1106:ILE:HG23	1.92	0.52
10:E:379:LYS:HD3	10:E:413:PHE:HB3	1.91	0.51
7:I:34:SER:OG	7:I:457:GLY:N	2.38	0.51
10:E:299:ARG:NH2	10:F:233:ASP:HB3	2.24	0.51
10:C:264:LEU:HD22	10:C:300:PHE:HE1	1.75	0.51
10:B:66:ARG:NH1	10:B:78:ASP:OD2	2.43	0.51
5:W:48:VAL:HG21	8:J:418:GLU:HG2	1.92	0.51
7:I:1295:SER:OG	7:I:1296:ASP:N	2.39	0.51
10:E:65:LEU:HB2	10:E:79:ILE:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1105:SER:HB2	8:J:731:ARG:HG2	1.93	0.51
7:I:1288:GLN:HE21	8:J:1355:ARG:HA	1.75	0.51
8:J:811:GLU:OE2	8:J:890:THR:OG1	2.25	0.51
8:J:844:THR:HA	8:J:882:VAL:HA	1.93	0.51
6:H:27:THR:HG23	6:H:202:VAL:HG22	1.92	0.51
10:E:261:ILE:HG12	10:E:314:THR:HB	1.92	0.51
7:I:823:VAL:HG22	7:I:1060:ILE:HG21	1.92	0.51
10:D:80:TYR:N	10:D:111:PHE:O	2.40	0.51
8:J:644:MET:HG2	8:J:722:ILE:HD13	1.93	0.51
10:E:49:ILE:HD12	10:E:103:PRO:HD3	1.91	0.51
2:N:12:DC:OP1	7:I:201:ARG:NH2	2.43	0.51
7:I:1155:VAL:O	7:I:1158:LYS:NZ	2.43	0.51
7:I:6:THR:HG21	7:I:782:VAL:H	1.76	0.51
7:I:817:LEU:HD11	7:I:1080:ASN:HB2	1.93	0.51
10:B:79:ILE:HG12	10:B:101:ILE:HG21	1.93	0.51
5:W:28:ARG:O	5:W:32:VAL:HG23	2.11	0.50
9:G:51:ARG:HH12	9:G:52:LYS:HE2	1.76	0.50
10:C:188:LEU:HD21	10:C:263:LEU:HB3	1.92	0.50
10:E:188:LEU:HD21	10:E:263:LEU:HB3	1.94	0.50
10:F:73:LEU:HD13	10:F:238:ARG:HE	1.76	0.50
10:F:173:ARG:HE	10:F:339:GLY:HA2	1.76	0.50
7:I:22:LEU:HD22	7:I:603:ILE:HD13	1.92	0.50
8:J:988:PHE:CD1	8:J:988:PHE:N	2.78	0.50
10:C:96:THR:N	10:C:120:ASN:OD1	2.41	0.50
10:C:207:LEU:HD13	10:C:246:VAL:HG21	1.92	0.50
1:L:14:ALA:HB2	1:L:89:VAL:HA	1.92	0.50
1:L:64:PHE:HB3	8:J:281:ARG:NH1	2.20	0.50
6:K:29:GLU:CG	6:K:30:PRO:CA	2.89	0.50
7:I:693:LEU:HB2	7:I:829:THR:HG23	1.93	0.50
7:I:318:SER:OG	7:I:320:ASP:OD1	2.21	0.50
7:I:615:VAL:HG12	7:I:638:SER:HB3	1.93	0.50
7:I:689:ALA:HB2	7:I:1233:LEU:HD23	1.94	0.50
10:E:79:ILE:HD13	10:E:101:ILE:HG21	1.94	0.50
3:T:20:DC:H2'	3:T:21:DT:C6	2.46	0.50
8:J:1167:LYS:HD3	8:J:1170:LYS:HD2	1.94	0.50
7:I:18:ARG:HH12	7:I:621:SER:H	1.59	0.50
8:J:1028:ILE:HB	8:J:1118:GLY:HA2	1.93	0.50
8:J:1046:ILE:HG22	8:J:1061:VAL:HA	1.93	0.50
10:E:244:GLU:OE2	10:E:296:ARG:NH2	2.45	0.50
10:E:170:ARG:NH1	10:E:259:ASP:OD2	2.45	0.50
7:I:74:ARG:N	7:I:97:ARG:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:250:ARG:NE	8:J:266:ASN:OD1	2.40	0.49
8:J:601:ILE:HA	8:J:604:MET:HG2	1.94	0.49
10:D:140:HIS:O	10:D:142:ASN:ND2	2.45	0.49
8:J:1321:SER:HB2	8:J:1348:LYS:HD2	1.94	0.49
10:E:176:ILE:HB	10:E:318:THR:HG22	1.94	0.49
6:H:191:ARG:HB3	6:H:196:THR:HG23	1.93	0.49
7:I:116:ASP:OD1	7:I:116:ASP:N	2.44	0.49
7:I:1142:ARG:NH2	7:I:1166:ASP:OD1	2.46	0.49
8:J:264:ASP:HB3	8:J:324:LEU:HB3	1.92	0.49
10:F:254:VAL:HG21	10:F:313:LEU:HB2	1.94	0.49
6:K:28:LEU:HB2	6:K:201:LEU:HB3	1.94	0.49
7:I:725:GLN:HB3	7:I:733:VAL:HG12	1.92	0.49
7:I:915:ASP:OD2	7:I:919:ARG:NH2	2.45	0.49
8:J:102:MET:HG2	8:J:246:PRO:HD3	1.94	0.49
10:B:14:LEU:HB3	10:B:34:ILE:HG21	1.93	0.49
10:F:56:GLU:OE1	10:F:66:ARG:NE	2.45	0.49
6:K:104:LYS:HD3	6:K:110:VAL:HG22	1.93	0.49
8:J:338:PHE:HA	8:J:342:LEU:HB2	1.95	0.49
8:J:709:ARG:HB2	8:J:714:GLU:HB2	1.95	0.49
5:W:4:VAL:HG12	5:W:5:THR:HG23	1.95	0.49
10:A:147:MET:HE1	10:A:195:ILE:HG13	1.95	0.49
8:J:504:GLN:OE1	8:J:731:ARG:NH1	2.46	0.49
10:F:207:LEU:HD13	10:F:246:VAL:HG21	1.95	0.49
10:C:212:ARG:NE	10:B:338:THR:O	2.44	0.48
10:F:14:LEU:HB3	10:F:34:ILE:HG21	1.94	0.48
1:L:64:PHE:CD1	1:L:64:PHE:N	2.78	0.48
10:D:379:LYS:HD3	10:D:413:PHE:HB3	1.95	0.48
10:E:160:ARG:NH1	10:E:407:LYS:O	2.46	0.48
10:B:290:ASP:HB3	10:B:293:ALA:HB2	1.95	0.48
8:J:118:LYS:HD3	8:J:311:ARG:HG2	1.96	0.48
8:J:131:PRO:HB2	8:J:133:ARG:CG	2.43	0.48
8:J:317:THR:OG1	8:J:318:GLY:N	2.47	0.48
10:D:188:LEU:HD21	10:D:263:LEU:HB3	1.96	0.48
10:A:138:PRO:HG3	10:A:305:ARG:HD3	1.95	0.48
2:N:9:DT:OP1	7:I:473:ARG:NH2	2.47	0.48
7:I:850:ILE:HG12	7:I:1048:LYS:HD3	1.96	0.48
7:I:1006:GLU:O	7:I:1010:GLN:N	2.46	0.48
9:G:95:ASP:OD1	9:G:96:GLN:N	2.47	0.48
6:K:62:ASP:OD1	6:K:63:GLY:N	2.47	0.48
8:J:393:THR:HG23	8:J:396:ALA:H	1.79	0.48
8:J:865:HIS:CE1	8:J:867:GLN:HB2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:147:MET:HE1	10:B:195:ILE:HG13	1.95	0.48
7:I:675:ASP:OD1	7:I:675:ASP:N	2.42	0.48
8:J:712:GLN:OE1	8:J:712:GLN:N	2.47	0.48
10:C:49:ILE:HD12	10:C:103:PRO:HG3	1.96	0.48
7:I:714:VAL:HB	7:I:787:PRO:HD2	1.94	0.47
7:I:1041:ASP:OD1	7:I:1041:ASP:N	2.46	0.47
10:E:147:MET:HE1	10:E:195:ILE:HG13	1.96	0.47
10:C:349:ILE:HG12	10:C:393:ILE:HG12	1.96	0.47
6:H:93:GLN:HG3	6:H:94:GLY:H	1.79	0.47
7:I:520:PRO:HG3	7:I:714:VAL:HG21	1.95	0.47
10:F:176:ILE:HB	10:F:318:THR:HG22	1.96	0.47
6:H:44:ARG:HA	6:H:183:ILE:HD13	1.96	0.47
7:I:817:LEU:HB3	7:I:1097:VAL:HB	1.96	0.47
10:A:56:GLU:OE1	10:A:66:ARG:NE	2.41	0.47
5:W:37:PRO:C	5:W:39:VAL:H	2.22	0.47
6:H:83:LEU:HB3	8:J:528:THR:HG23	1.96	0.47
10:A:212:ARG:NH1	10:A:215:GLU:OE2	2.46	0.47
7:I:225:PHE:HB2	7:I:336:LEU:HD22	1.96	0.47
8:J:318:GLY:N	8:J:322:ARG:O	2.44	0.47
8:J:1263:LYS:HG2	8:J:1281:GLU:HA	1.95	0.47
9:G:58:THR:H	9:G:100:VAL:HG22	1.79	0.47
10:D:264:LEU:HD22	10:D:300:PHE:HE1	1.79	0.47
10:F:15:ILE:HD13	10:F:27:ALA:HA	1.97	0.47
1:L:110:ALA:HB1	1:L:114:ARG:HH12	1.80	0.47
6:H:19:VAL:HG12	6:H:20:SER:H	1.79	0.47
7:I:207:THR:OG1	7:I:354:ASP:OD1	2.32	0.47
7:I:539:THR:HG23	7:I:541:GLU:H	1.79	0.47
7:I:720:ARG:NH2	7:I:749:ASP:OD1	2.47	0.47
9:G:30:ALA:HB1	9:G:110:ALA:HA	1.95	0.47
10:C:387:ILE:HG23	10:C:395:ALA:HB1	1.96	0.47
10:E:298:LYS:HB3	10:F:232:PHE:HD1	1.80	0.47
10:F:206:VAL:HG22	10:F:263:LEU:HD23	1.97	0.47
10:F:264:LEU:HD22	10:F:300:PHE:HE1	1.80	0.47
10:A:160:ARG:NE	10:A:409:ASN:OD1	2.44	0.47
10:B:67:SER:OG	10:B:69:ASP:OD1	2.30	0.47
7:I:726:TYR:HB3	7:I:733:VAL:HB	1.96	0.47
10:D:2:ASN:OD1	10:D:3:LEU:N	2.47	0.47
7:I:232:ILE:HG12	7:I:237:LEU:HG	1.97	0.47
8:J:515:ARG:NH2	8:J:718:SER:O	2.36	0.47
6:H:212:ASP:OD1	6:H:212:ASP:N	2.48	0.46
10:C:244:GLU:OE2	10:C:296:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:220:GLN:HG2	10:D:227:VAL:HB	1.98	0.46
7:I:777:VAL:HG11	7:I:783:LEU:HD21	1.97	0.46
7:I:1119:MET:HB2	7:I:1228:GLY:HA2	1.96	0.46
8:J:1261:LEU:O	8:J:1304:ARG:NH1	2.48	0.46
10:A:148:GLU:O	10:A:198:ASN:ND2	2.47	0.46
10:D:147:MET:HE1	10:D:195:ILE:HG13	1.97	0.46
10:E:298:LYS:HB3	10:F:232:PHE:CD1	2.50	0.46
3:T:2:DG:H2''	3:T:3:DG:C8	2.50	0.46
6:H:102:LEU:HD13	6:H:115:ILE:HG12	1.97	0.46
10:C:348:LYS:HG2	10:C:393:ILE:HD11	1.97	0.46
7:I:698:PRO:HA	7:I:799:ASN:HD21	1.81	0.46
7:I:452:ARG:NH2	7:I:458:GLU:OE2	2.42	0.46
8:J:795:TYR:HB3	8:J:799:ARG:HH12	1.79	0.46
8:J:957:SER:N	8:J:985:ILE:O	2.47	0.46
9:G:130:PHE:HZ	9:G:138:ILE:HG21	1.80	0.46
10:B:26:LEU:HD23	10:B:34:ILE:HG12	1.98	0.46
8:J:131:PRO:HB2	8:J:133:ARG:HG2	1.97	0.46
10:B:64:PHE:HB3	10:B:78:ASP:HB3	1.98	0.46
6:H:215:GLU:OE1	6:H:219:ARG:NE	2.47	0.46
7:I:1283:ALA:HB1	7:I:1286:THR:HB	1.98	0.46
8:J:704:GLU:H	8:J:718:SER:HB2	1.81	0.46
1:L:47:GLU:HG3	1:L:64:PHE:CE1	2.45	0.46
7:I:1255:THR:OG1	7:I:1296:ASP:OD1	2.33	0.46
8:J:516:ASP:OD1	8:J:516:ASP:N	2.48	0.46
8:J:1062:LEU:O	8:J:1067:ARG:NH2	2.48	0.46
6:K:29:GLU:HG2	6:K:30:PRO:CA	2.46	0.46
6:H:18:GLN:HA	6:H:24:ALA:HA	1.98	0.46
7:I:1154:ASP:OD1	7:I:1154:ASP:N	2.48	0.46
8:J:844:THR:HA	8:J:882:VAL:HG12	1.97	0.46
8:J:1136:GLY:HA2	8:J:1140:ARG:HB2	1.97	0.46
9:G:126:VAL:HG11	9:G:158:ALA:HB2	1.96	0.46
10:E:14:LEU:HB3	10:E:34:ILE:HG21	1.96	0.46
2:N:22:DG:H1'	2:N:23:DA:H5'	1.98	0.45
6:H:19:VAL:N	6:H:23:HIS:O	2.49	0.45
7:I:696:ASP:O	7:I:697:LYS:HG3	2.16	0.45
7:I:488:MET:HE3	7:I:489:PRO:HD2	1.98	0.45
8:J:1059:LEU:O	8:J:1107:VAL:N	2.49	0.45
1:L:65:PHE:CZ	8:J:291:ILE:HG13	2.52	0.45
6:K:102:LEU:HD13	6:K:115:ILE:HG12	1.98	0.45
7:I:1307:ASN:HB3	7:I:1312:ASN:O	2.17	0.45
8:J:586:GLY:HA3	8:J:612:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:733:SER:OG	8:J:736:GLN:OE1	2.26	0.45
10:C:145:LEU:HD21	10:C:170:ARG:HE	1.80	0.45
10:B:379:LYS:HD3	10:B:413:PHE:HB3	1.98	0.45
8:J:816:THR:OG1	8:J:818:GLU:OE1	2.33	0.45
10:C:96:THR:HB	10:C:120:ASN:HA	1.98	0.45
4:R:18:A:OP1	7:I:1073:LYS:NZ	2.37	0.45
7:I:211:ARG:NH2	7:I:357:ASN:O	2.50	0.45
7:I:1127:LYS:HE3	7:I:1131:MET:HE3	1.97	0.45
10:C:4:THR:O	10:C:8:ASN:ND2	2.50	0.45
7:I:839:VAL:HG12	7:I:1049:ILE:HD12	1.99	0.45
10:D:160:ARG:NE	10:D:409:ASN:OD1	2.44	0.45
10:D:178:ALA:HB3	10:D:184:LYS:HD3	1.99	0.45
10:E:85:GLN:NE2	10:E:113:LEU:O	2.46	0.45
6:H:100:LEU:HB2	6:H:144:ILE:HG23	1.99	0.45
7:I:9:LYS:O	7:I:1175:ASN:ND2	2.35	0.45
8:J:517:CYS:SG	8:J:518:VAL:N	2.89	0.45
8:J:1190:ILE:HG21	8:J:1196:LEU:HD21	1.99	0.45
1:L:65:PHE:N	1:L:65:PHE:HD1	2.14	0.45
5:W:16:ARG:NE	8:J:905:ARG:HH21	2.15	0.45
7:I:21:VAL:HG21	7:I:592:ARG:HD2	1.99	0.45
10:A:138:PRO:HB3	10:A:305:ARG:HB2	1.98	0.45
7:I:1313:HIS:HB2	8:J:474:LEU:HD12	1.99	0.45
8:J:319:SER:OG	8:J:322:ARG:NH2	2.50	0.45
8:J:495:ASN:ND2	8:J:1247:LYS:O	2.50	0.45
8:J:527:LEU:HD21	8:J:536:LEU:HD22	1.98	0.45
10:C:14:LEU:HB3	10:C:34:ILE:HG21	1.99	0.45
10:A:176:ILE:HB	10:A:318:THR:HG22	1.99	0.45
10:F:147:MET:HE1	10:F:195:ILE:HG13	1.99	0.45
6:K:207:THR:HG21	6:K:211:ILE:HG22	1.99	0.45
7:I:720:ARG:HH21	7:I:736:VAL:HG21	1.82	0.45
7:I:838:CYS:HB3	7:I:1050:VAL:HG13	1.99	0.45
10:C:102:ARG:HD3	10:C:114:LEU:HD13	1.99	0.45
10:B:349:ILE:HG12	10:B:393:ILE:HG12	1.99	0.45
6:K:154:PRO:HG2	6:K:157:THR:HG23	2.00	0.44
6:K:224:LEU:HD23	6:H:228:LEU:HD11	1.99	0.44
7:I:621:SER:HB2	7:I:653:MET:HE3	1.99	0.44
8:J:422:LEU:HB2	8:J:469:HIS:HB2	1.99	0.44
10:C:212:ARG:NH1	10:C:215:GLU:OE2	2.50	0.44
10:A:356:PRO:HB2	10:A:358:ILE:HG13	1.99	0.44
10:D:65:LEU:HB2	10:D:79:ILE:HB	1.99	0.44
7:I:539:THR:HG23	7:I:542:ARG:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:975:ILE:HD13	8:J:980:THR:HG21	1.99	0.44
10:C:17:LEU:HD12	10:C:38:ILE:HD13	1.99	0.44
10:C:65:LEU:HB2	10:C:79:ILE:HB	1.99	0.44
10:D:340:ASN:ND2	10:E:214:GLU:OE2	2.51	0.44
10:F:212:ARG:HA	10:F:232:PHE:HE2	1.81	0.44
2:N:17:DA:H1'	7:I:542:ARG:HG3	1.99	0.44
8:J:64:PRO:HG3	8:J:93:THR:H	1.82	0.44
10:C:90:ASN:ND2	10:D:28:ARG:HD2	2.33	0.44
10:B:160:ARG:NE	10:B:409:ASN:OD1	2.41	0.44
7:I:889:PRO:HA	7:I:913:VAL:HA	1.99	0.44
8:J:115:TRP:HE1	8:J:308:ASP:HB2	1.83	0.44
8:J:1101:LEU:HD13	8:J:1124:ILE:HD11	1.98	0.44
8:J:1344:LEU:HD22	8:J:1349:GLU:HB3	1.99	0.44
10:C:232:PHE:CD1	10:B:298:LYS:HG3	2.52	0.44
10:F:187:LEU:HD13	10:F:345:LEU:HD11	1.99	0.44
1:L:65:PHE:N	1:L:65:PHE:CD1	2.85	0.44
5:W:37:PRO:C	5:W:39:VAL:N	2.75	0.44
7:I:73:TYR:HA	7:I:98:VAL:HA	2.00	0.44
10:C:290:ASP:HB3	10:C:293:ALA:HB2	2.00	0.44
1:L:64:PHE:CB	8:J:281:ARG:HH12	2.22	0.44
1:L:65:PHE:CZ	8:J:288:PRO:HD2	2.48	0.44
3:T:15:DT:H2'	3:T:16:DA:C8	2.53	0.44
6:H:75:GLN:HB2	6:H:132:HIS:HB2	2.00	0.44
8:J:1000:GLY:HA3	8:J:1026:PRO:HG3	1.99	0.44
9:G:152:LEU:N	9:G:160:ALA:O	2.48	0.44
8:J:484:MET:HA	8:J:489:ASN:HD21	1.82	0.44
8:J:510:LEU:HA	8:J:513:MET:HE2	1.99	0.44
8:J:826:ILE:HG21	8:J:992:LYS:C	2.36	0.44
8:J:926:PRO:HG3	8:J:1248:ILE:HD11	2.00	0.44
8:J:959:LYS:NZ	8:J:960:LEU:O	2.50	0.44
10:E:299:ARG:HD2	10:F:233:ASP:OD2	2.17	0.44
6:K:45:ARG:HA	7:I:1083:GLU:HB2	2.00	0.44
6:H:115:ILE:HD11	6:H:130:ILE:HD11	1.98	0.44
7:I:250:THR:HA	7:I:268:ARG:HA	1.99	0.44
7:I:454:ARG:HG2	7:I:459:MET:HG3	2.00	0.44
10:D:208:LEU:HB3	10:D:211:GLU:HG3	2.00	0.44
10:E:356:PRO:HB2	10:E:358:ILE:HG13	2.00	0.44
10:F:79:ILE:HD13	10:F:101:ILE:HG21	2.00	0.44
7:I:1123:GLY:HA3	7:I:1204:LEU:HD11	2.00	0.44
8:J:1202:GLU:HB3	8:J:1204:VAL:HG13	2.00	0.44
8:J:1036:ARG:HH21	8:J:1081:VAL:HG11	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:186:VAL:HB	9:G:195:LEU:HD23	1.99	0.43
10:C:299:ARG:HG2	10:D:233:ASP:HB3	2.00	0.43
7:I:99:LYS:HG2	7:I:121:GLU:HB3	2.00	0.43
7:I:972:PHE:HA	7:I:975:ILE:HB	1.99	0.43
9:G:139:THR:OG1	9:G:178:ARG:NH2	2.46	0.43
2:N:21:DC:H2"	2:N:22:DG:N7	2.33	0.43
6:K:60:GLU:OE1	6:K:143:ARG:NH2	2.51	0.43
7:I:515:MET:HE3	7:I:517:GLN:HB2	2.00	0.43
7:I:741:MET:HE3	7:I:747:GLY:H	1.83	0.43
10:D:133:PHE:N	10:D:255:GLU:OE2	2.51	0.43
10:E:154:THR:HG23	10:E:155:GLU:OE1	2.19	0.43
1:L:28:GLU:HB3	7:I:481:LEU:HD22	2.00	0.43
7:I:251:ALA:HB2	7:I:269:ILE:HD11	2.01	0.43
10:A:264:LEU:HD22	10:A:300:PHE:HE1	1.82	0.43
4:R:14:A:H2'	4:R:15:G:C8	2.53	0.43
6:K:29:GLU:HG2	6:K:30:PRO:HA	1.98	0.43
7:I:519:ASN:OD1	7:I:522:SER:N	2.50	0.43
10:C:80:TYR:N	10:C:111:PHE:O	2.48	0.43
10:C:153:SER:OG	10:C:155:GLU:OE1	2.36	0.43
10:E:147:MET:HG3	10:E:162:LEU:HD22	2.01	0.43
10:E:173:ARG:NH1	10:F:214:GLU:OE2	2.51	0.43
10:F:179:PRO:HB2	10:F:347:ARG:HH11	1.83	0.43
8:J:1098:GLN:NE2	8:J:1200:GLU:OE1	2.52	0.43
9:G:183:LEU:HB3	9:G:197:VAL:HG22	1.99	0.43
10:A:264:LEU:HD22	10:A:300:PHE:CE1	2.53	0.43
7:I:1087:TYR:HE2	7:I:1215:GLY:HA2	1.84	0.43
8:J:505:ASP:N	8:J:505:ASP:OD1	2.51	0.43
10:C:172:GLN:NE2	10:C:340:ASN:OD1	2.52	0.43
10:E:54:VAL:HG21	10:E:249:LYS:HD2	2.00	0.43
6:K:86:LYS:HE2	6:K:176:CYS:SG	2.59	0.43
7:I:152:SER:HB3	7:I:452:ARG:HG3	1.99	0.43
7:I:623:LEU:HD13	7:I:627:GLY:HA2	2.00	0.43
8:J:204:GLU:N	8:J:204:GLU:OE1	2.52	0.43
9:G:103:ASP:OD1	9:G:104:ARG:N	2.52	0.43
10:A:179:PRO:HB3	10:A:347:ARG:HH11	1.84	0.43
7:I:935:THR:HA	7:I:1048:LYS:HA	2.01	0.43
10:C:55:LEU:HD13	10:C:81:VAL:HG21	2.01	0.43
7:I:454:ARG:HH22	7:I:536:GLY:HA3	1.82	0.43
8:J:615:LYS:HB2	8:J:616:PRO:HD3	2.01	0.43
8:J:990:ARG:HE	8:J:990:ARG:HB3	1.66	0.43
9:G:148:ASP:HA	9:G:164:ARG:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:173:ARG:NH2	10:D:338:THR:O	2.41	0.43
10:E:80:TYR:HB2	10:E:110:TYR:HB2	2.01	0.43
8:J:416:ILE:HG23	8:J:439:PRO:HB2	2.01	0.42
9:G:43:ILE:HG12	9:G:44:ASP:H	1.84	0.42
10:C:176:ILE:HB	10:C:318:THR:HG22	2.01	0.42
10:D:406:THR:OG1	10:D:407:LYS:N	2.52	0.42
2:N:5:DT:H1'	2:N:6:DA:C8	2.54	0.42
6:K:23:HIS:NE2	6:K:204:GLU:OE2	2.50	0.42
7:I:80:PHE:HB3	7:I:84:GLU:HB3	2.00	0.42
7:I:86:GLN:HA	7:I:140:GLY:HA2	2.02	0.42
7:I:673:HIS:HB3	7:I:1109:ILE:HB	2.00	0.42
8:J:60:ARG:HG2	8:J:90:VAL:HG12	2.00	0.42
8:J:1150:PRO:HG2	8:J:1153:PRO:HA	2.00	0.42
7:I:1085:MET:SD	7:I:1086:PRO:HD2	2.59	0.42
10:C:214:GLU:CD	10:C:214:GLU:H	2.27	0.42
10:C:254:VAL:HG21	10:C:313:LEU:HB2	2.01	0.42
10:A:379:LYS:HD3	10:A:413:PHE:HB3	2.01	0.42
1:L:103:ILE:HG23	1:L:104:SER:H	1.83	0.42
7:I:99:LYS:HA	7:I:121:GLU:HA	2.02	0.42
7:I:1296:ASP:HB3	7:I:1321:GLU:H	1.84	0.42
8:J:192:MET:HE3	8:J:197:GLU:HG2	2.00	0.42
8:J:342:LEU:HD13	8:J:1352:ILE:HG23	2.00	0.42
10:F:71:SER:HB2	10:F:238:ARG:HH22	1.85	0.42
10:F:133:PHE:N	10:F:255:GLU:OE2	2.51	0.42
10:F:166:SER:HB2	10:F:341:MET:HE2	2.02	0.42
7:I:9:LYS:HG2	7:I:1171:ARG:NH1	2.34	0.42
7:I:192:ASP:OD2	7:I:436:ARG:NH2	2.50	0.42
8:J:282:LEU:HD21	8:J:291:ILE:HG22	2.02	0.42
8:J:1145:PHE:HB3	8:J:1309:ILE:HD11	2.00	0.42
1:L:17:GLY:O	2:N:6:DA:H3'	2.20	0.42
8:J:131:PRO:O	8:J:135:ILE:HG13	2.20	0.42
8:J:1322:ALA:HA	8:J:1325:PHE:CE1	2.54	0.42
10:B:387:ILE:HG23	10:B:395:ALA:HB1	2.01	0.42
6:H:46:ILE:HD11	6:H:224:LEU:HD13	2.02	0.42
7:I:972:PHE:HD1	7:I:975:ILE:HD12	1.84	0.42
10:C:349:ILE:HD11	10:C:392:GLU:HB3	2.02	0.42
10:F:213:PRO:HD3	10:F:232:PHE:CE2	2.55	0.42
7:I:12:ARG:NH2	7:I:698:PRO:O	2.45	0.42
8:J:215:LYS:O	8:J:218:THR:OG1	2.34	0.42
8:J:1146:GLU:HB3	8:J:1148:ARG:HG3	2.02	0.42
9:G:123:ARG:NH2	9:G:159:GLU:O	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:220:GLN:HG2	10:C:227:VAL:HB	2.01	0.42
10:B:289:VAL:HG22	10:B:327:MET:HG3	2.02	0.42
10:E:174:GLY:HA2	10:E:341:MET:HB3	2.02	0.42
5:W:28:ARG:NH1	7:I:1314:GLN:HB2	2.35	0.41
8:J:111:THR:O	8:J:239:LEU:N	2.53	0.41
10:C:406:THR:OG1	10:C:407:LYS:N	2.53	0.41
10:E:264:LEU:HD11	10:E:266:SER:HB3	2.02	0.41
5:W:16:ARG:H	5:W:19:LEU:HD23	1.85	0.41
8:J:591:ILE:O	8:J:594:GLN:NE2	2.53	0.41
8:J:1163:VAL:HG12	8:J:1202:GLU:H	1.85	0.41
8:J:1178:THR:HG23	8:J:1184:ASP:HB3	2.02	0.41
10:A:247:ILE:HB	10:A:300:PHE:CE2	2.55	0.41
10:E:170:ARG:O	10:E:306:ASN:ND2	2.50	0.41
10:F:96:THR:N	10:F:120:ASN:OD1	2.51	0.41
8:J:259:ARG:HD3	8:J:259:ARG:H	1.85	0.41
8:J:841:GLY:HA3	8:J:901:ARG:HG2	2.01	0.41
10:D:73:LEU:HD13	10:D:238:ARG:NH1	2.35	0.41
6:K:17:GLU:HB3	6:K:25:LYS:HB3	2.02	0.41
8:J:668:PHE:CG	8:J:678:ARG:HD3	2.55	0.41
9:G:183:LEU:HD23	9:G:183:LEU:H	1.84	0.41
10:A:406:THR:OG1	10:A:407:LYS:N	2.52	0.41
5:W:26:ARG:HH12	5:W:35:LYS:NZ	2.18	0.41
7:I:840:SER:OG	7:I:1048:LYS:N	2.37	0.41
7:I:1010:GLN:HA	7:I:1013:GLN:HB3	2.02	0.41
8:J:123:ARG:HA	8:J:123:ARG:HD3	1.91	0.41
8:J:709:ARG:C	8:J:711:GLY:H	2.27	0.41
8:J:850:LYS:HG3	8:J:852:GLY:H	1.85	0.41
8:J:930:LEU:HD11	8:J:1241:TYR:CE1	2.56	0.41
10:D:67:SER:OG	10:D:69:ASP:OD1	2.34	0.41
10:F:147:MET:HE3	10:F:194:SER:HB2	2.02	0.41
2:N:2:DG:N2	3:T:29:DC:O2	2.53	0.41
8:J:317:THR:HA	8:J:323:PRO:HA	2.03	0.41
8:J:1265:THR:O	8:J:1303:SER:N	2.53	0.41
10:D:212:ARG:HA	10:D:232:PHE:HE2	1.86	0.41
10:E:406:THR:OG1	10:E:407:LYS:N	2.52	0.41
1:L:6:LYS:NZ	1:L:7:LYS:O	2.45	0.41
6:H:100:LEU:HD21	6:H:121:VAL:HG11	2.03	0.41
7:I:81:ASP:OD1	7:I:84:GLU:N	2.49	0.41
7:I:138:ILE:HG23	7:I:139:ASN:H	1.85	0.41
7:I:618:GLN:OE1	8:J:768:ASN:ND2	2.53	0.41
7:I:1219:GLU:OE1	8:J:634:ARG:NH1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:133:PHE:N	10:A:255:GLU:OE2	2.54	0.41
10:D:195:ILE:HD13	10:D:261:ILE:HG21	2.02	0.41
7:I:1124:ILE:HD12	7:I:1201:LEU:HD23	2.02	0.41
8:J:504:GLN:HG2	8:J:731:ARG:HB2	2.02	0.41
8:J:1275:LEU:HB2	8:J:1278:GLU:HB2	2.03	0.41
10:A:79:ILE:HG12	10:A:101:ILE:HG21	2.03	0.41
10:F:253:LEU:HB3	10:F:258:LYS:HB2	2.03	0.41
3:T:26:DG:H8	3:T:26:DG:H5'	1.85	0.41
6:H:182:ARG:HD2	8:J:581:MET:HE1	2.03	0.41
7:I:1223:ARG:NH2	8:J:719:PHE:O	2.54	0.41
8:J:152:THR:HG23	8:J:154:LEU:H	1.86	0.41
8:J:361:LEU:HD13	8:J:366:CYS:HA	2.02	0.41
8:J:363:LEU:HD23	8:J:618:VAL:HG13	2.02	0.41
3:T:18:DC:H2'	3:T:19:DT:C6	2.55	0.41
6:H:52:PRO:HA	6:H:150:ARG:HG2	2.03	0.41
6:H:197:ASP:OD1	6:H:197:ASP:N	2.52	0.41
7:I:554:HIS:HB3	7:I:558:VAL:HB	2.01	0.41
7:I:606:LEU:HD23	7:I:610:GLU:HB3	2.03	0.41
7:I:695:ALA:HB1	7:I:795:ALA:HB3	2.03	0.41
7:I:755:LYS:HA	7:I:755:LYS:HD3	1.79	0.41
8:J:959:LYS:HB3	8:J:983:LYS:HB2	2.03	0.41
10:D:207:LEU:HD13	10:D:246:VAL:HG21	2.02	0.41
10:E:266:SER:OG	10:E:269:ARG:HB2	2.21	0.41
1:L:45:PRO:CB	1:L:64:PHE:CE2	2.94	0.40
5:W:45:LYS:NZ	8:J:415:VAL:HA	2.36	0.40
6:K:106:GLY:HA2	6:K:136:GLU:HA	2.03	0.40
7:I:1176:LEU:HD22	7:I:1180:MET:HA	2.03	0.40
10:C:147:MET:HE1	10:C:195:ILE:HG13	2.03	0.40
3:T:17:DC:H2'	3:T:18:DC:C6	2.57	0.40
6:H:28:LEU:HB2	6:H:201:LEU:HB3	2.02	0.40
6:H:37:HIS:CD2	7:I:1216:ARG:HD2	2.56	0.40
10:B:96:THR:HB	10:B:120:ASN:HA	2.03	0.40
10:D:266:SER:HB2	10:D:269:ARG:HB2	2.04	0.40
3:T:16:DA:H2'	3:T:17:DC:C6	2.56	0.40
7:I:120:GLN:NE2	7:I:489:PRO:HG2	2.34	0.40
7:I:243:PRO:HA	7:I:246:LEU:HD12	2.03	0.40
7:I:1244:HIS:NE2	7:I:1266:GLY:O	2.44	0.40
8:J:17:PHE:HZ	8:J:1353:VAL:HG21	1.87	0.40
8:J:985:ILE:CG2	8:J:989:GLY:HA2	2.45	0.40
10:B:296:ARG:HB2	10:B:297:PRO:HD3	2.02	0.40
10:F:148:GLU:O	10:F:198:ASN:ND2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:27:LEU:HD13	7:I:663:VAL:HG11	2.04	0.40
7:I:593:LYS:HB3	7:I:602:GLU:CD	2.46	0.40
7:I:1007:LYS:HE2	7:I:1007:LYS:HB3	1.96	0.40
7:I:1214:ASP:OD1	7:I:1215:GLY:N	2.55	0.40
8:J:137:ARG:O	8:J:142:GLU:N	2.53	0.40
8:J:189:LEU:HD23	8:J:235:GLU:HA	2.02	0.40
9:G:141:VAL:HB	9:G:153:ASP:HB3	2.03	0.40
10:A:247:ILE:HB	10:A:300:PHE:HE2	1.87	0.40
5:W:28:ARG:HH12	7:I:1314:GLN:HB2	1.86	0.40
7:I:1082:ILE:HD12	7:I:1082:ILE:H	1.86	0.40
8:J:129:ASP:OD2	8:J:220:ARG:NH1	2.54	0.40
8:J:332:LYS:HE2	8:J:332:LYS:HB3	1.92	0.40
10:C:276:THR:HG23	10:B:291:ALA:HB1	2.02	0.40
10:D:39:LEU:HD22	10:D:49:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	W	53/91 (58%)	51 (96%)	2 (4%)	0	100	100
6	H	214/329 (65%)	206 (96%)	8 (4%)	0	100	100
6	K	273/329 (83%)	266 (97%)	7 (3%)	0	100	100
7	I	1298/1342 (97%)	1247 (96%)	51 (4%)	0	100	100
8	J	654/1416 (46%)	630 (96%)	24 (4%)	0	100	100
10	A	349/419 (83%)	346 (99%)	3 (1%)	0	100	100
10	B	399/419 (95%)	395 (99%)	4 (1%)	0	100	100
10	C	125/419 (30%)	125 (100%)	0	0	100	100
10	D	411/419 (98%)	411 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	E	411/419 (98%)	408 (99%)	3 (1%)	0	100	100
10	F	339/419 (81%)	339 (100%)	0	0	100	100
All	All	4526/6021 (75%)	4424 (98%)	102 (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	L	83/158 (52%)	78 (94%)	5 (6%)	17	39
5	W	46/75 (61%)	46 (100%)	0	100	100
6	H	186/286 (65%)	182 (98%)	4 (2%)	45	64
6	K	192/286 (67%)	185 (96%)	7 (4%)	31	52
7	I	1125/1157 (97%)	1110 (99%)	15 (1%)	61	74
8	J	1115/1177 (95%)	1084 (97%)	31 (3%)	38	59
9	G	145/409 (36%)	135 (93%)	10 (7%)	14	36
10	A	305/359 (85%)	303 (99%)	2 (1%)	76	81
10	B	350/359 (98%)	348 (99%)	2 (1%)	78	83
10	C	354/359 (99%)	353 (100%)	1 (0%)	86	86
10	D	355/359 (99%)	352 (99%)	3 (1%)	73	80
10	E	355/359 (99%)	352 (99%)	3 (1%)	73	80
10	F	293/359 (82%)	291 (99%)	2 (1%)	76	81
All	All	4904/5702 (86%)	4819 (98%)	85 (2%)	52	69

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	44	VAL
1	L	64	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	86	VAL
1	L	97	SER
1	L	103	ILE
6	K	13	LEU
6	K	26	VAL
6	K	74	VAL
6	K	166	ARG
6	K	177	TYR
6	K	196	THR
6	K	231	PHE
6	H	6	THR
6	H	13	LEU
6	H	47	LEU
6	H	144	ILE
7	I	111	GLU
7	I	116	ASP
7	I	138	ILE
7	I	382	GLU
7	I	483	ASP
7	I	486	THR
7	I	490	GLN
7	I	493	ILE
7	I	514	PHE
7	I	697	LYS
7	I	862	LEU
7	I	888	THR
7	I	1050	VAL
7	I	1106	ARG
7	I	1159	VAL
8	J	76	LYS
8	J	84	ILE
8	J	92	VAL
8	J	93	THR
8	J	95	THR
8	J	133	ARG
8	J	134	ASP
8	J	197	GLU
8	J	253	VAL
8	J	430	HIS
8	J	442	ILE
8	J	528	THR
8	J	552	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	J	564	VAL
8	J	593	ASN
8	J	639	VAL
8	J	663	GLU
8	J	684	ASP
8	J	706	VAL
8	J	757	THR
8	J	774	ILE
8	J	831	VAL
8	J	839	VAL
8	J	847	ASP
8	J	907	HIS
8	J	987	GLU
8	J	990	ARG
8	J	1027	VAL
8	J	1261	LEU
8	J	1301	THR
8	J	1326	GLN
9	G	47	VAL
9	G	49	ILE
9	G	59	PHE
9	G	89	LEU
9	G	93	VAL
9	G	129	GLN
9	G	147	ARG
9	G	148	ASP
9	G	182	VAL
9	G	186	VAL
10	C	214	GLU
10	A	155	GLU
10	A	188	LEU
10	B	3	LEU
10	B	188	LEU
10	D	139	LEU
10	D	188	LEU
10	D	228	VAL
10	E	131	ILE
10	E	154	THR
10	E	155	GLU
10	F	188	LEU
10	F	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
5	W	31	GLN
6	K	147	GLN
6	K	186	ASN
6	H	75	GLN
6	H	132	HIS
6	H	194	GLN
7	I	150	HIS
7	I	214	ASN
7	I	490	GLN
7	I	649	GLN
7	I	658	GLN
7	I	659	GLN
7	I	799	ASN
7	I	808	ASN
7	I	856	ASN
7	I	932	GLN
7	I	952	GLN
7	I	965	GLN
7	I	1008	GLN
7	I	1017	GLN
7	I	1023	HIS
7	I	1061	GLN
7	I	1209	GLN
7	I	1256	GLN
7	I	1288	GLN
8	J	45	ASN
8	J	196	GLN
8	J	341	ASN
8	J	365	GLN
8	J	465	GLN
8	J	488	ASN
8	J	489	ASN
8	J	593	ASN
8	J	897	HIS
8	J	910	ASN
8	J	954	ASN
8	J	1098	GLN
8	J	1108	GLN
8	J	1326	GLN
9	G	194	GLN
10	C	8	ASN
10	C	42	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	C	90	ASN
10	C	172	GLN
10	C	241	GLN
10	C	361	ASN
10	C	388	HIS
10	A	172	GLN
10	A	190	ASN
10	A	295	HIS
10	B	172	GLN
10	B	193	GLN
10	B	241	GLN
10	D	172	GLN
10	D	256	HIS
10	E	90	ASN
10	E	239	HIS
10	E	361	ASN
10	F	172	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	9/18 (50%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	10	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

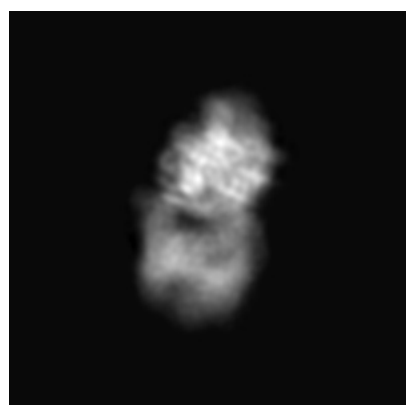
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22115. These allow visual inspection of the internal detail of the map and identification of artifacts.

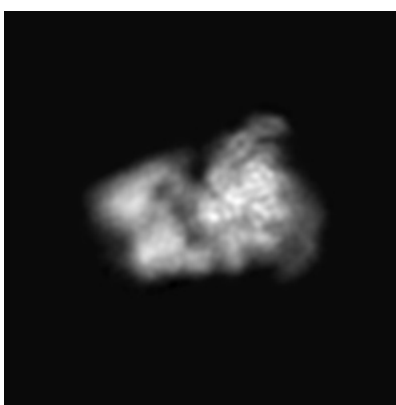
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

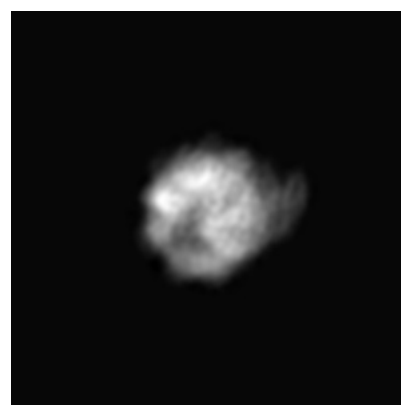
6.1.1 Primary map



X



Y



Z

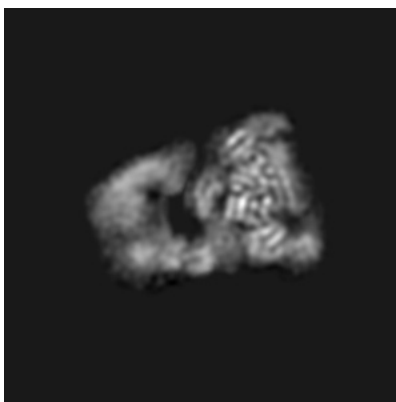
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

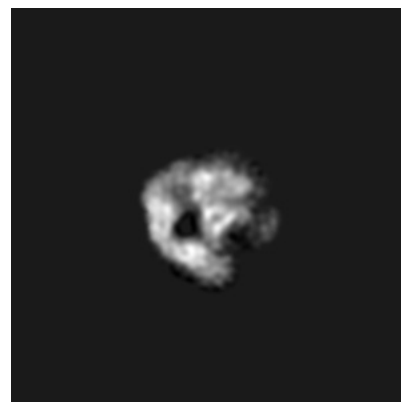
6.2.1 Primary map



X Index: 175



Y Index: 175

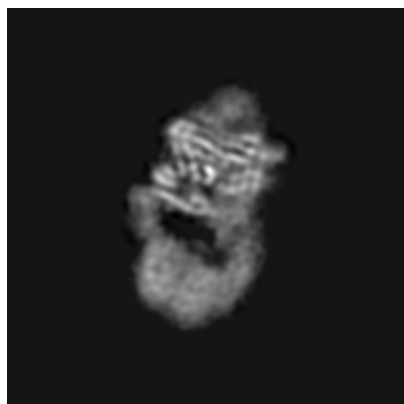


Z Index: 175

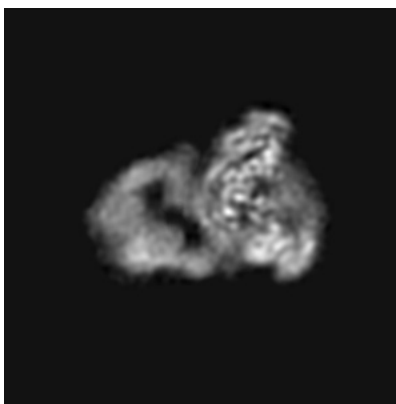
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

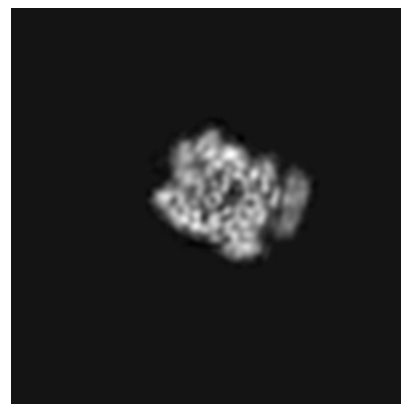
6.3.1 Primary map



X Index: 180



Y Index: 185

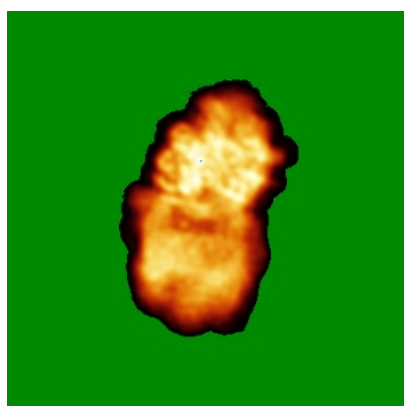


Z Index: 223

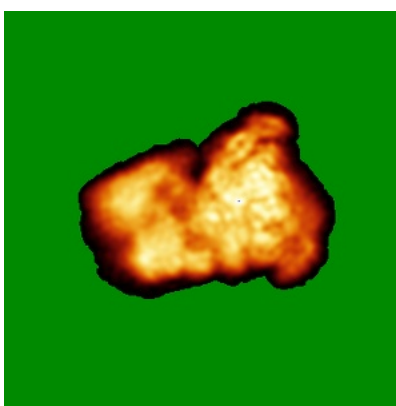
The images above show the largest variance slices of the map in three orthogonal directions.

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

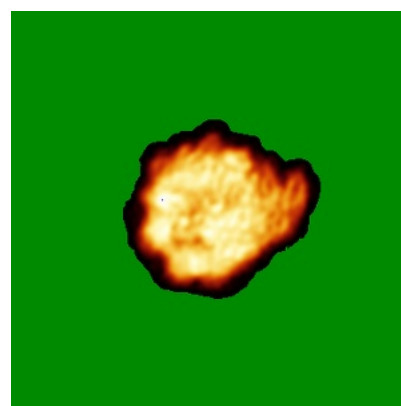
6.4.1 Primary map



X



Y

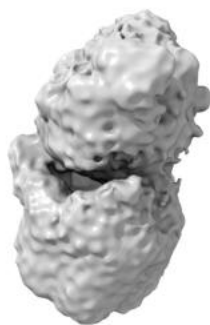


Z

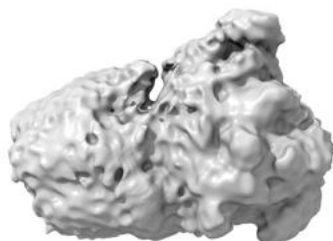
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

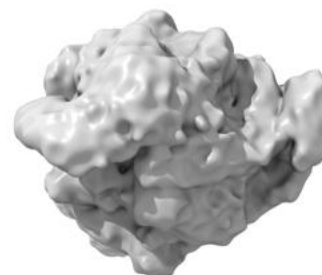
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

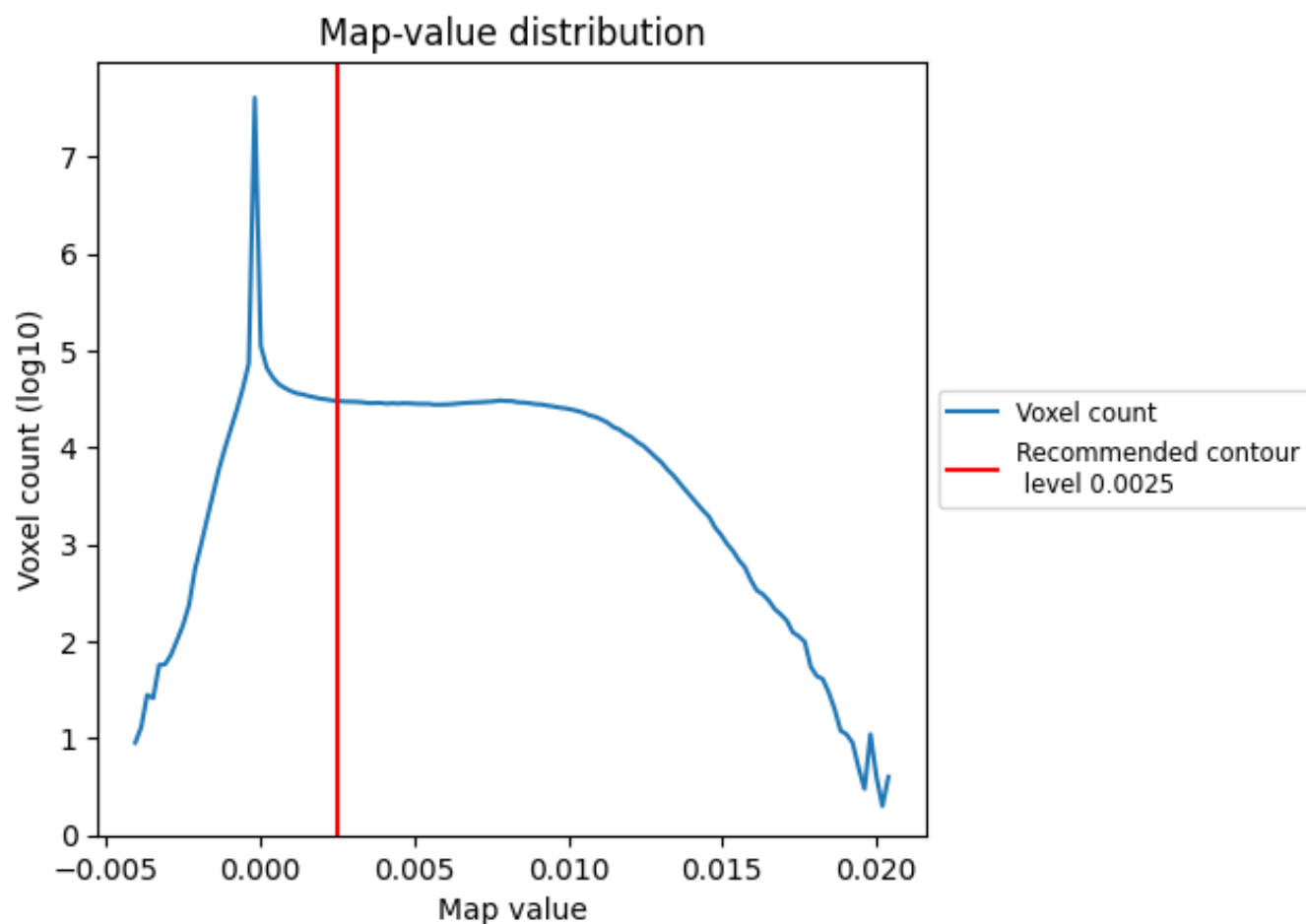
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

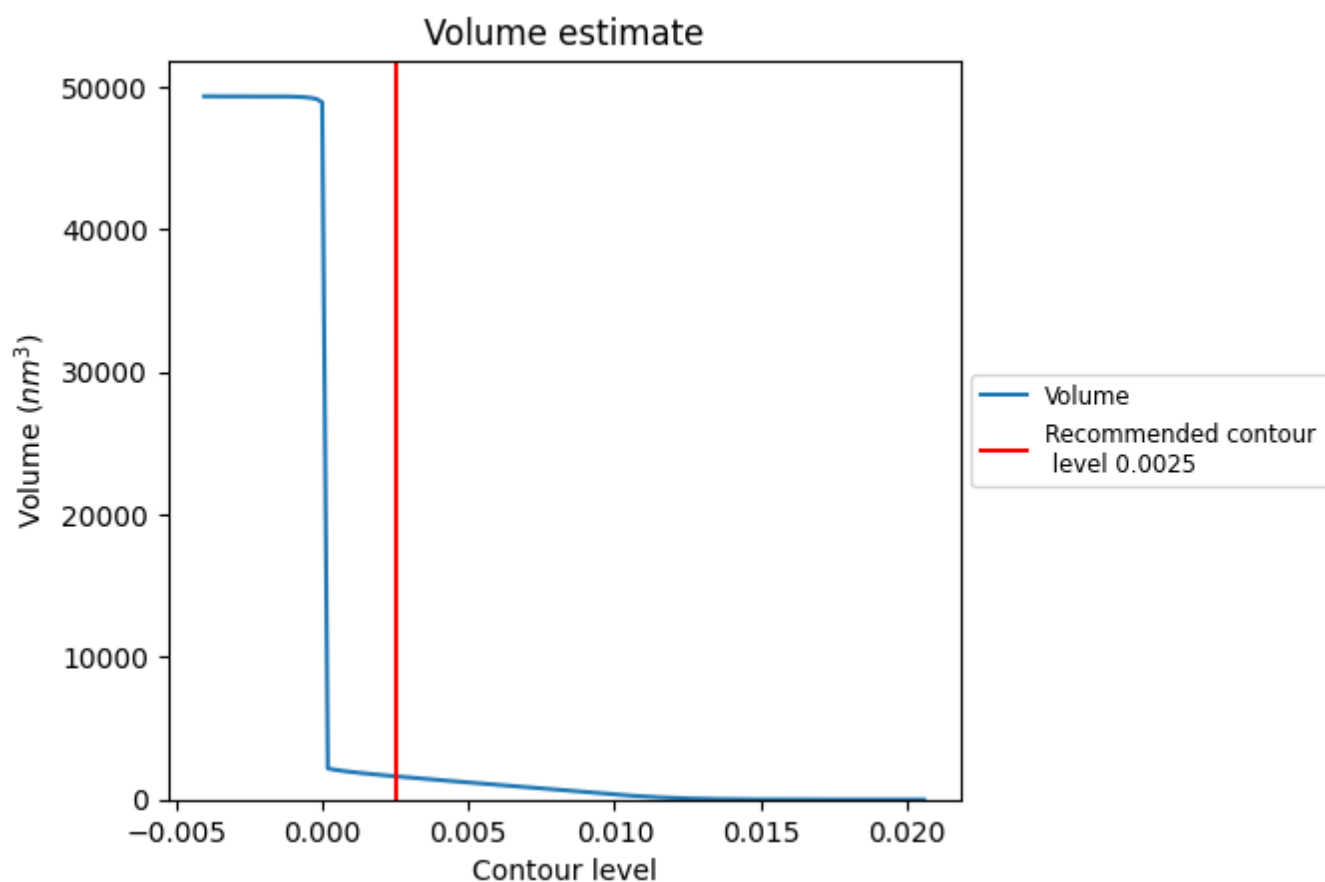
This section contains the results of statistical analysis of the map.

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.

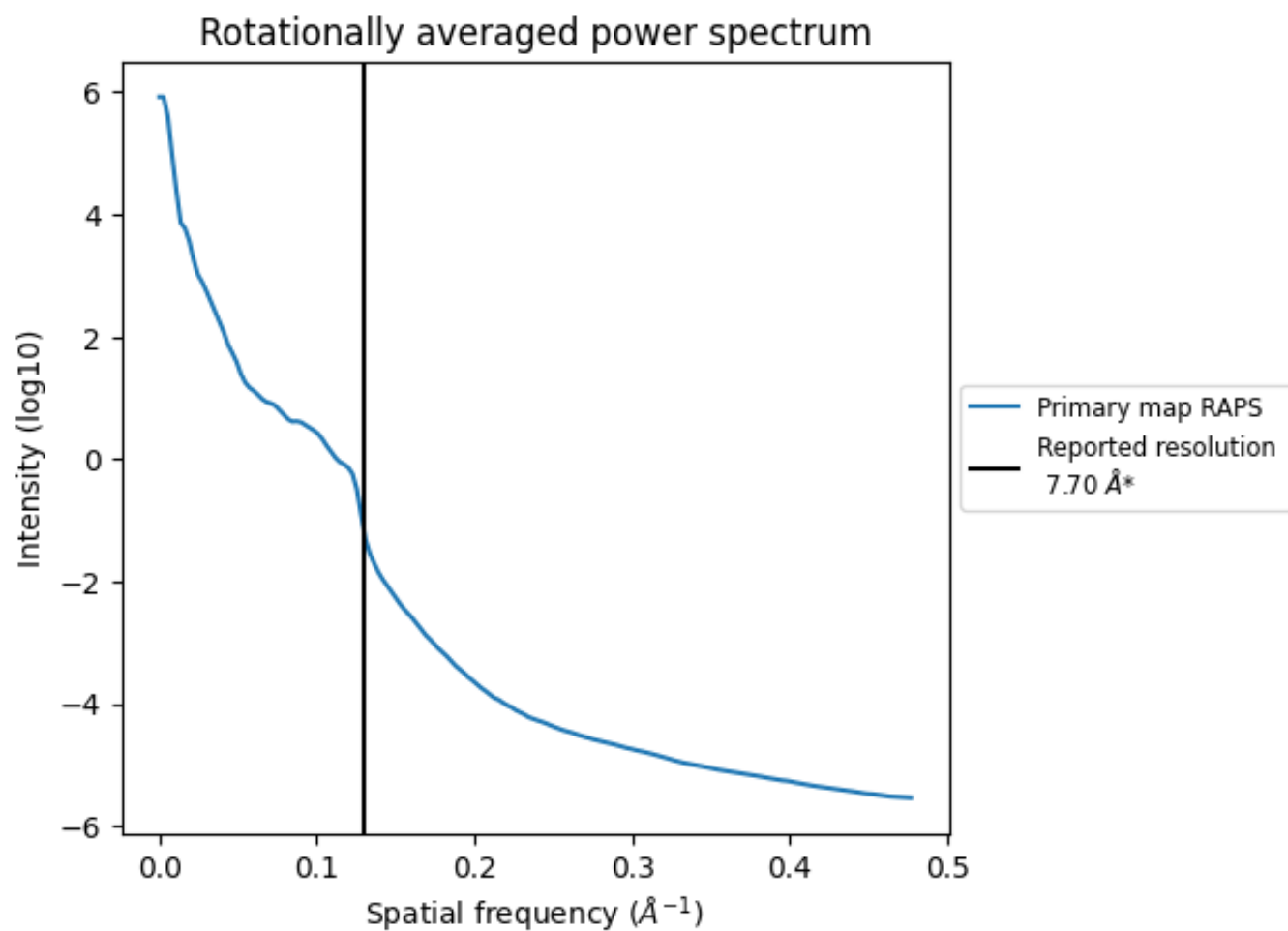
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1632 nm³; this corresponds to an approximate mass of 1474 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 ⓘ

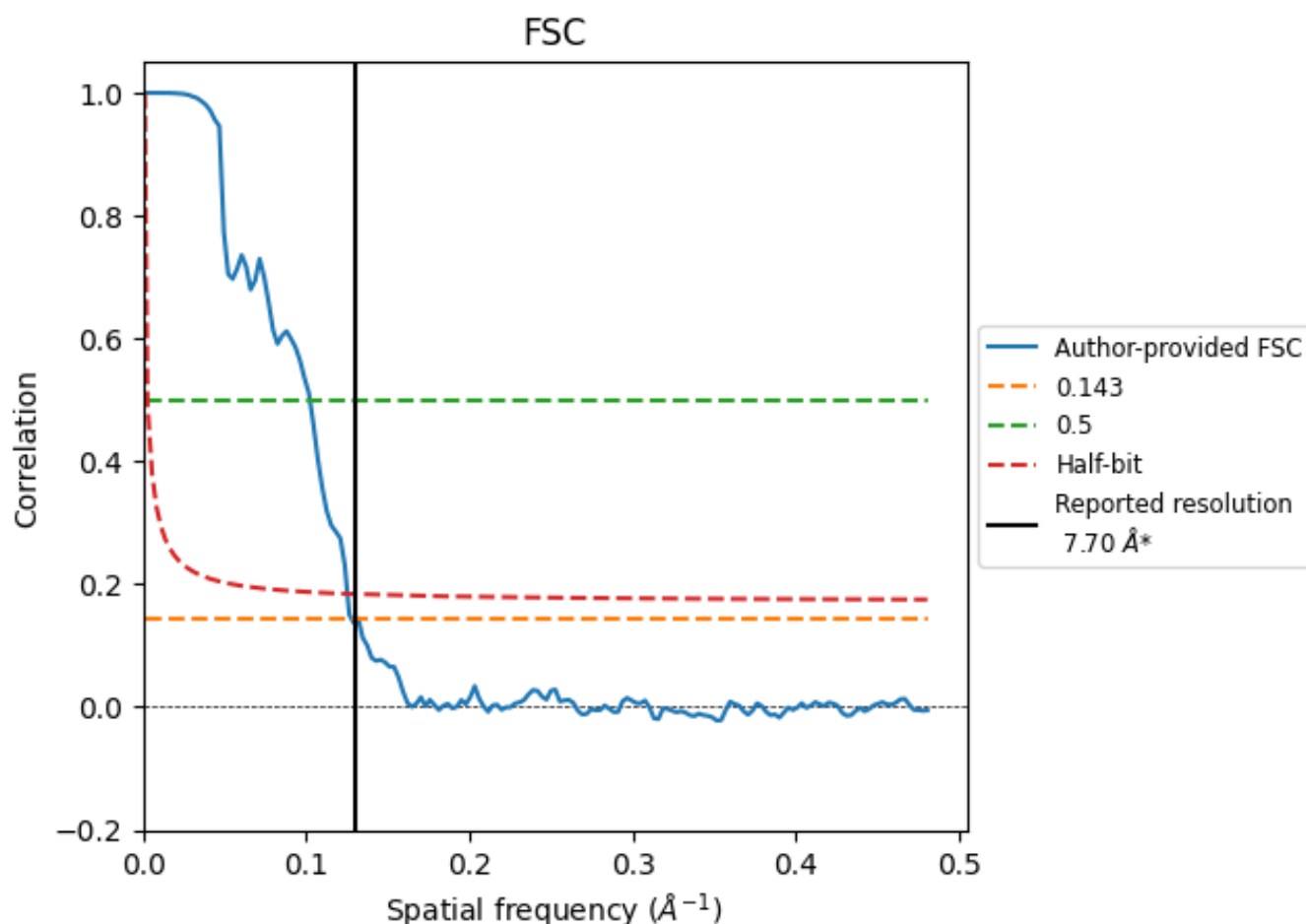


*Reported resolution corresponds to spatial frequency of 0.130 Å⁻¹

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 0.130 Å⁻¹

8.2 Resolution estimates [i](#)

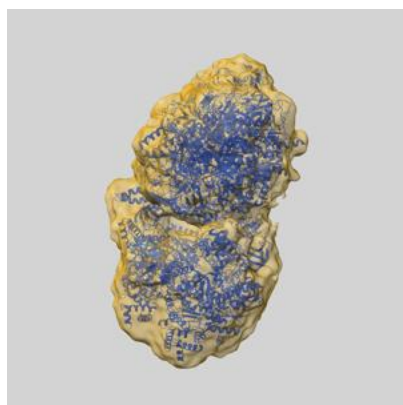
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.70	-	-
Author-provided FSC curve	7.82	9.78	7.99
Unmasked-calculated*	-	-	-

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

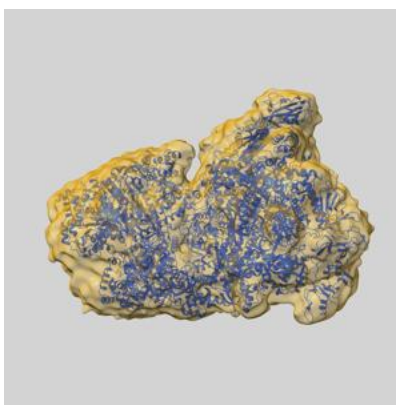
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22115 and PDB model 6XAV. Per-residue inclusion information can be found in section 3 on page 7.

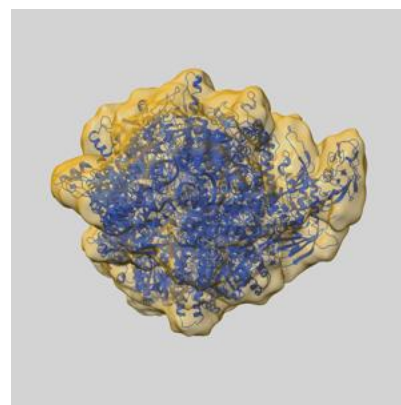
9.1 Map-model overlay [i](#)



X



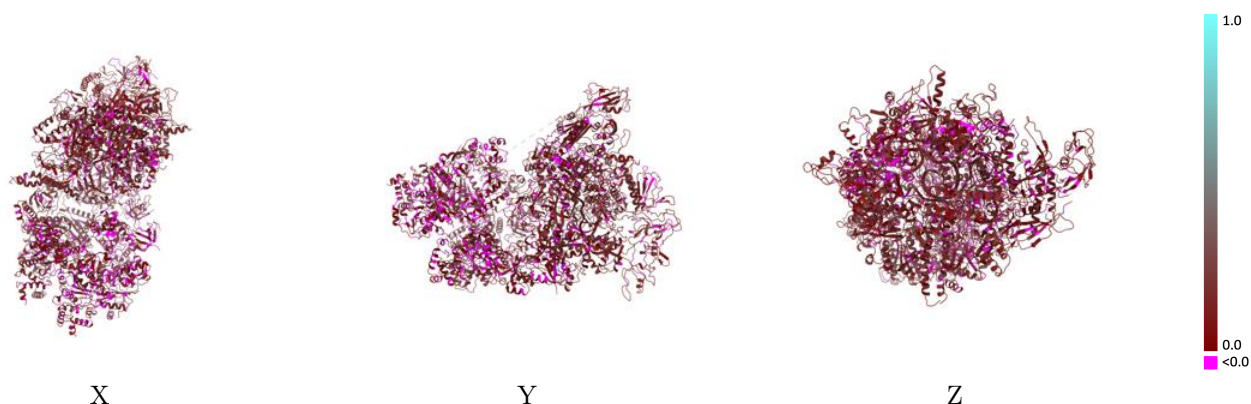
Y



Z

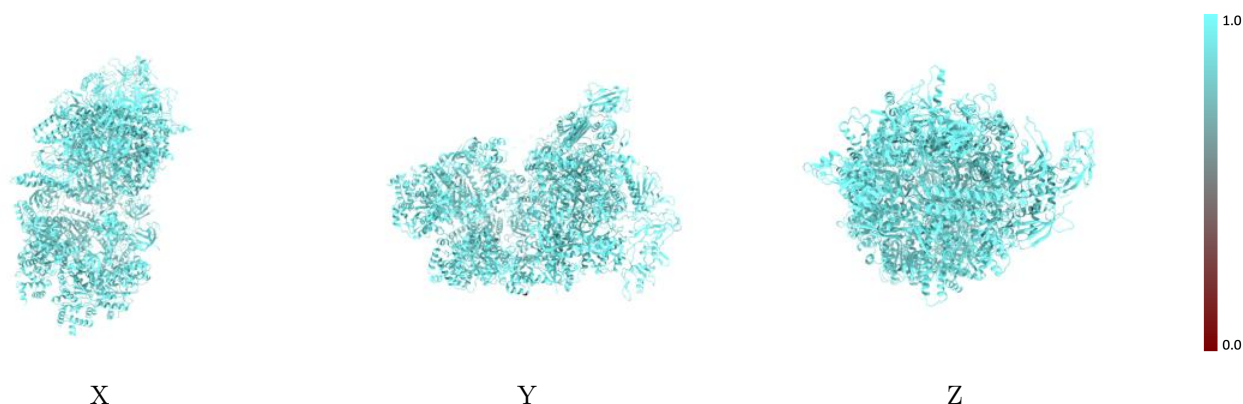
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



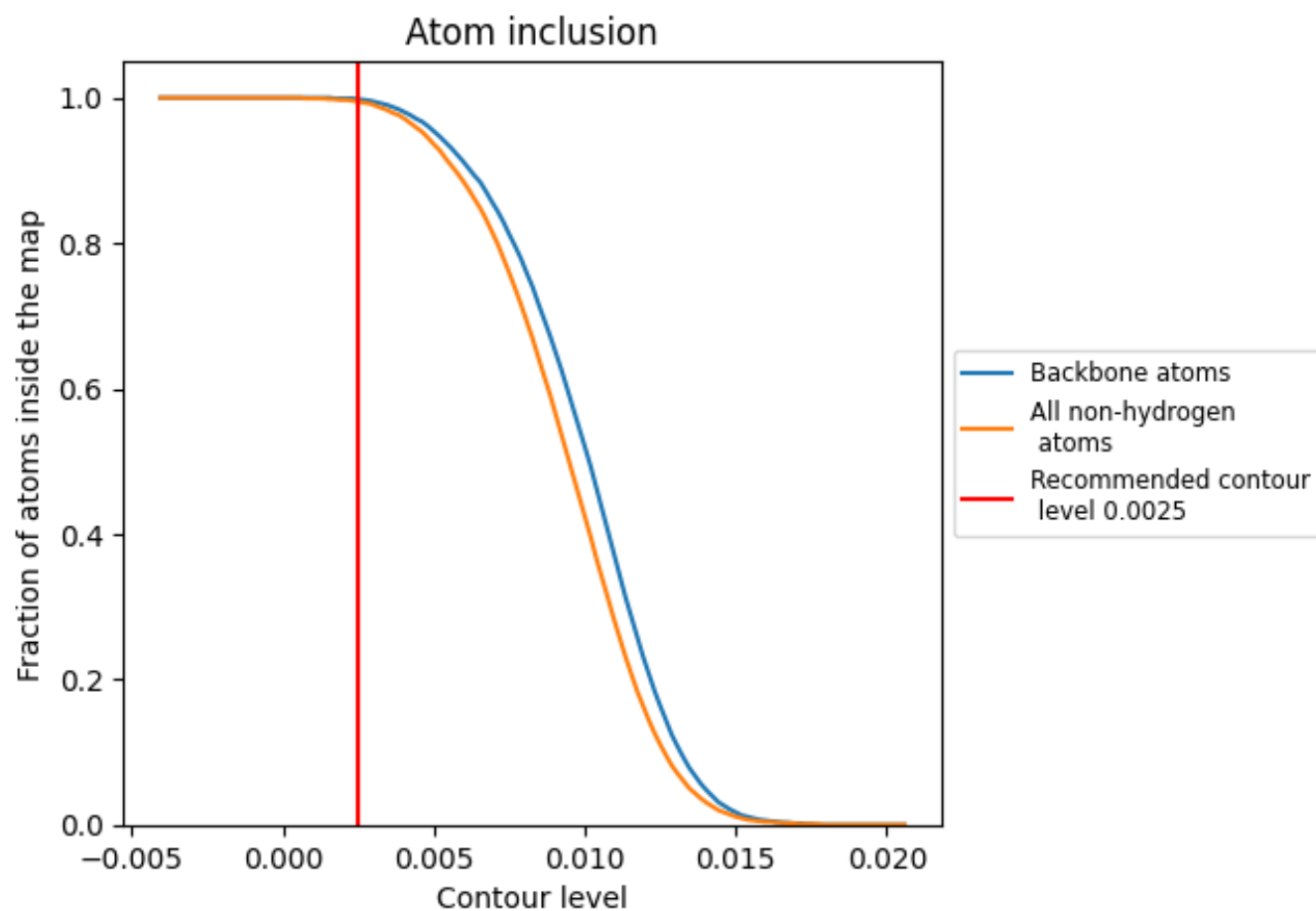
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.1030
A	 0.9920	 0.0650
B	 0.9940	 0.1070
C	 0.9940	 0.1120
D	 0.9950	 0.0820
E	 0.9940	 0.0770
F	 0.9940	 0.0500
G	 0.9780	 0.0650
H	 0.9950	 0.1150
I	 0.9970	 0.1280
J	 0.9970	 0.1170
K	 0.9980	 0.1170
L	 0.9930	 0.0370
N	 0.9840	 0.0860
R	 1.0000	 0.1990
T	 1.0000	 0.1510
W	 0.9710	 0.0270

