



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 01:57 PM EST

PDB ID : 6PSS  
EMDB ID : EMD-20462  
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi1.5a) with TraR and mutant rpsT P2 promoter  
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2019-07-13  
Resolution : 3.50 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](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2



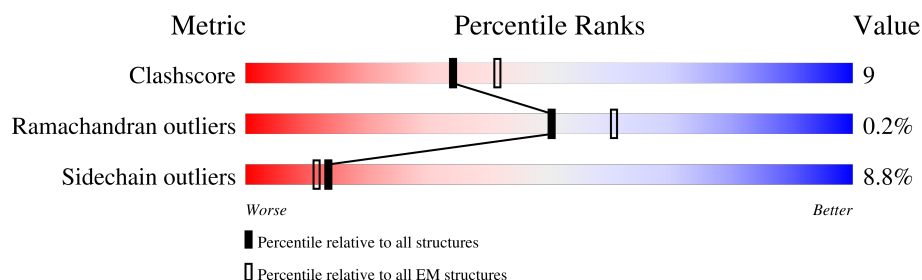
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	G	329	
1	H	329	
1	M	329	
2	I	1342	
3	J	1430	
4	K	91	
5	L	616	
6	N	72	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
7	O	85	<div><div></div><div></div><div></div><div></div></div>
8	P	85	<div><div></div><div></div><div></div><div></div></div>



## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32361 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	232	Total	C	N	O	S	0	0
			1769	1106	315	342	6		
1	H	218	Total	C	N	O	S	0	0
			1669	1044	293	326	6		
1	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1337	Total	C	N	O	S	0	0
			10502	6594	1830	2035	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1343	Total	C	N	O	S	0	0
			10449	6567	1864	1968	50		

There are 24 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	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	72	Total	C	N	O	S	0	0
			577	352	110	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	558	Total	C	N	O	S	0	0
			4489	2801	785	876	27		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	72	Total	C	N	O	S	0	0
			566	350	103	108	5		

- Molecule 7 is a DNA chain called DNA (85-MER).



Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	43	Total	C	N	O	P	0	0
			883	420	174	246	43		

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	43	Total	C	N	O	P	0	0
			881	422	148	268	43		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

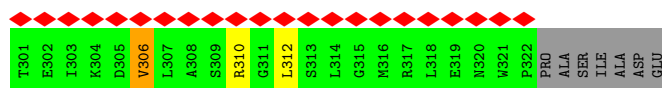
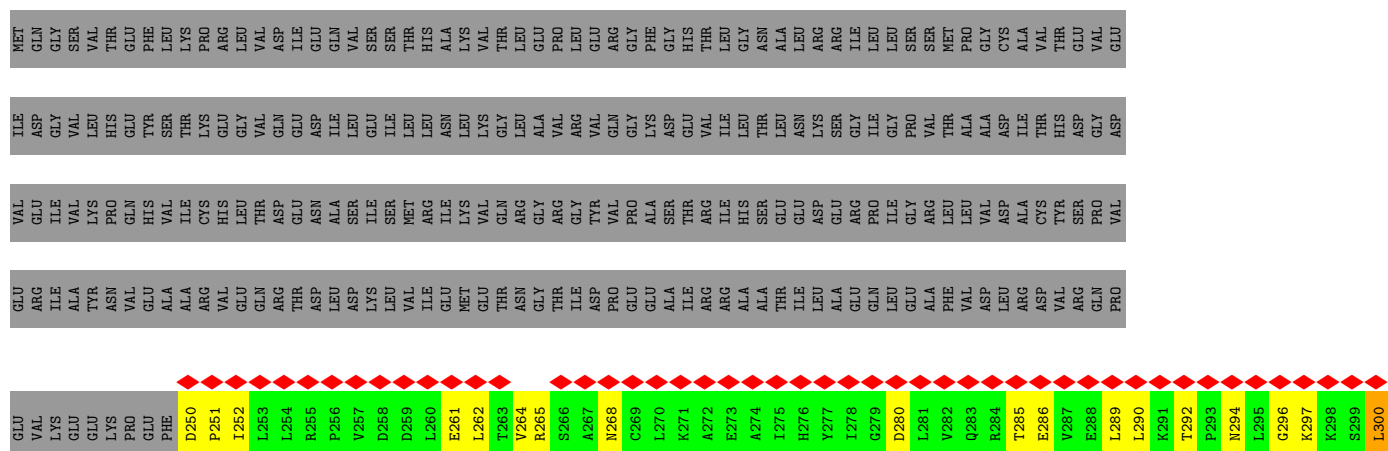
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total	Zn	0
			2	2	
10	N	1	Total	Zn	0
			1	1	

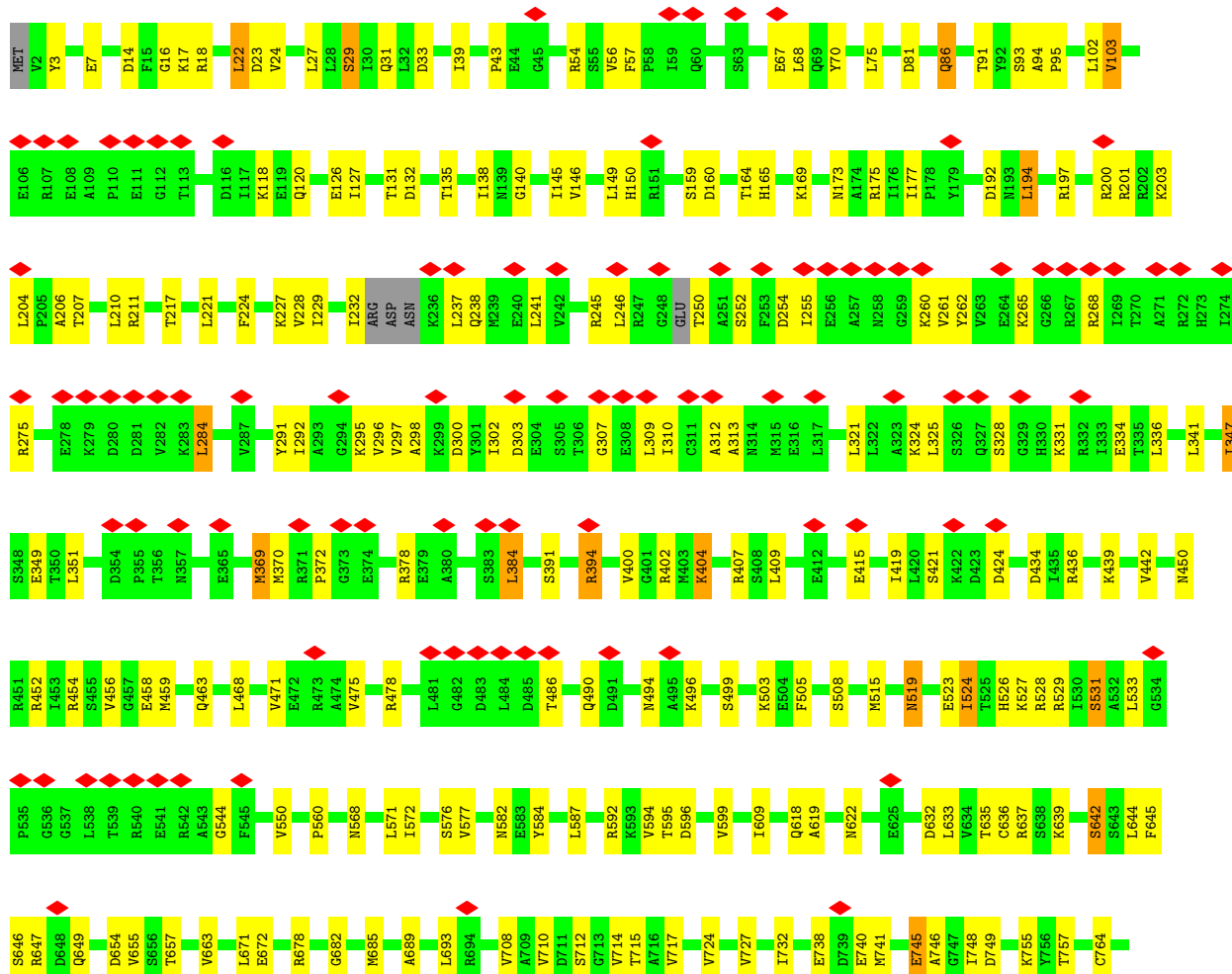




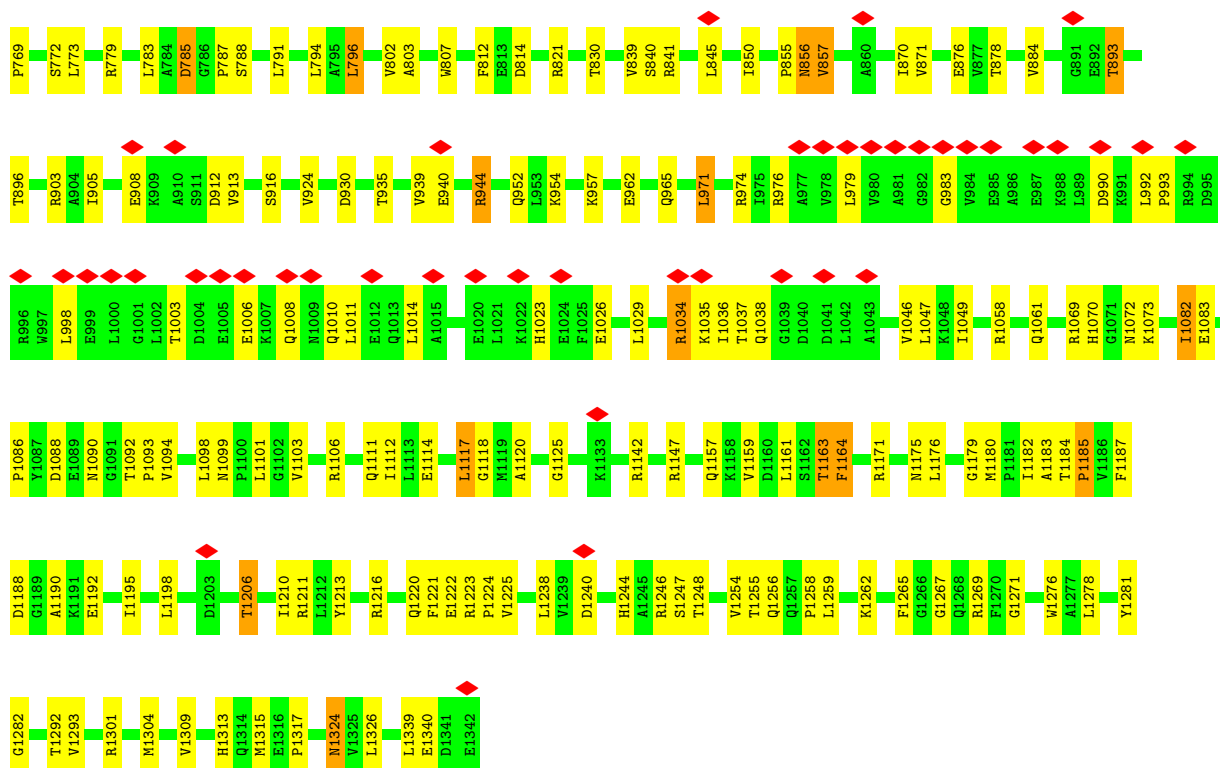




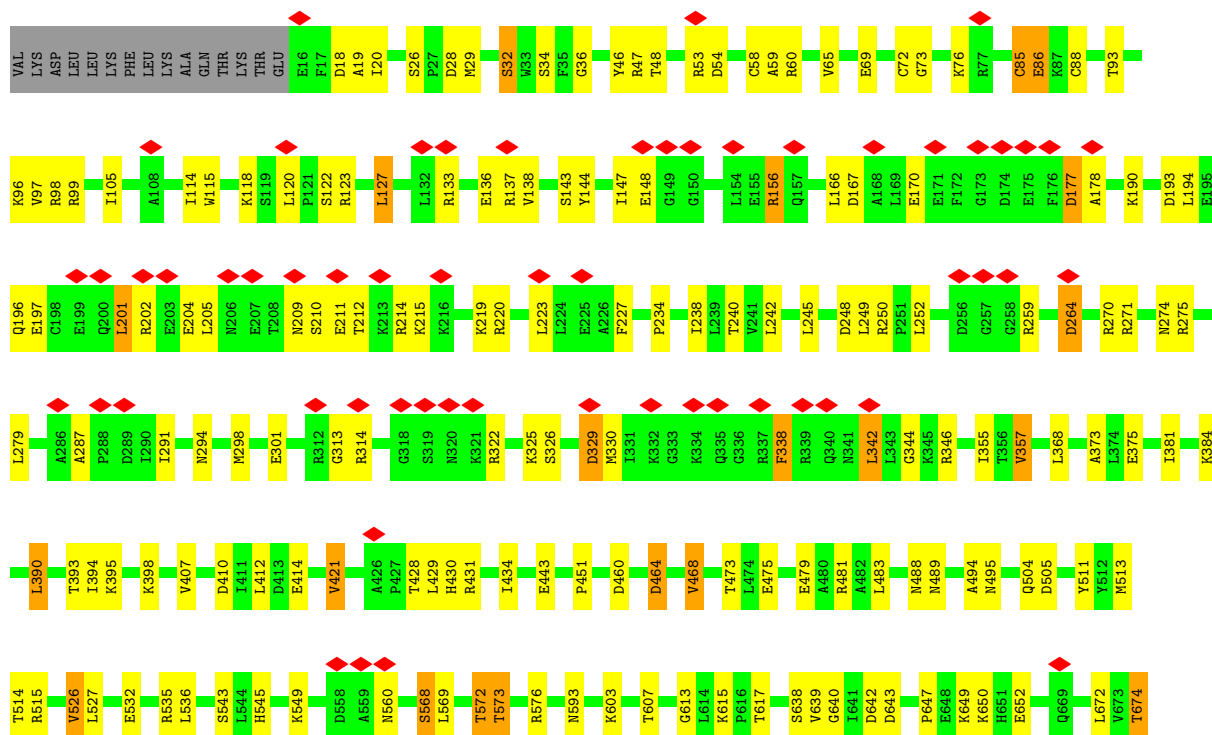
• Molecule 2: DNA-directed RNA polymerase subunit beta



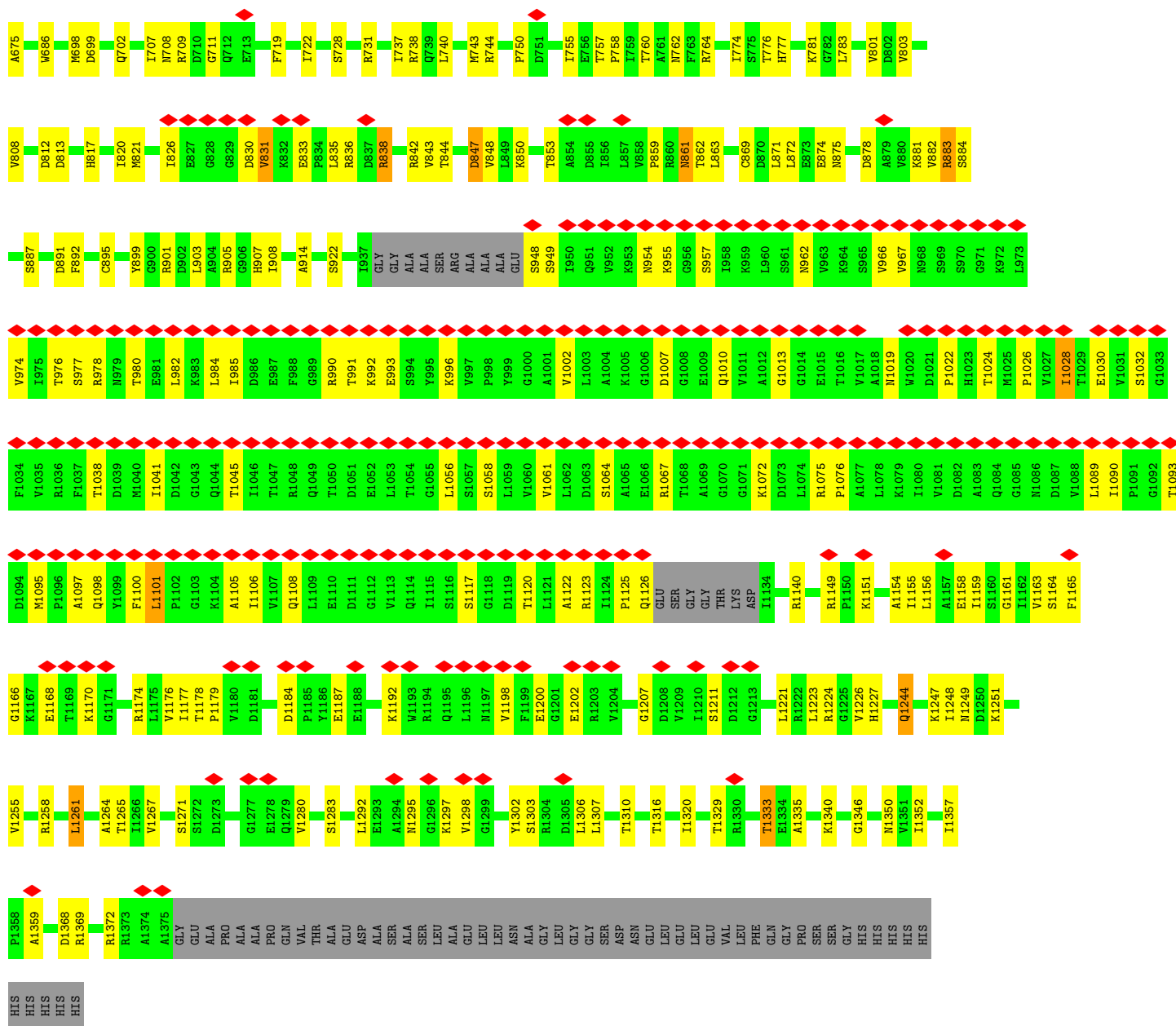




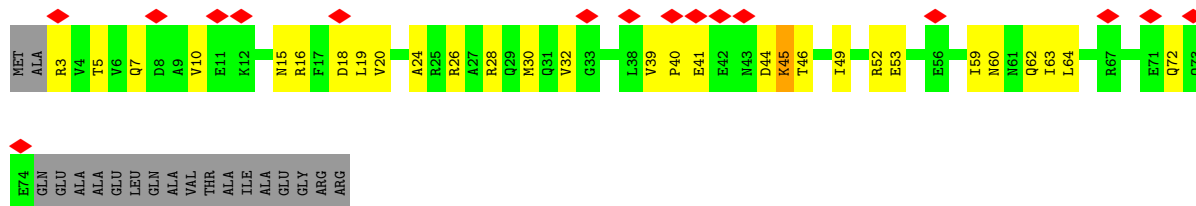
• Molecule 3: DNA-directed RNA polymerase subunit beta'





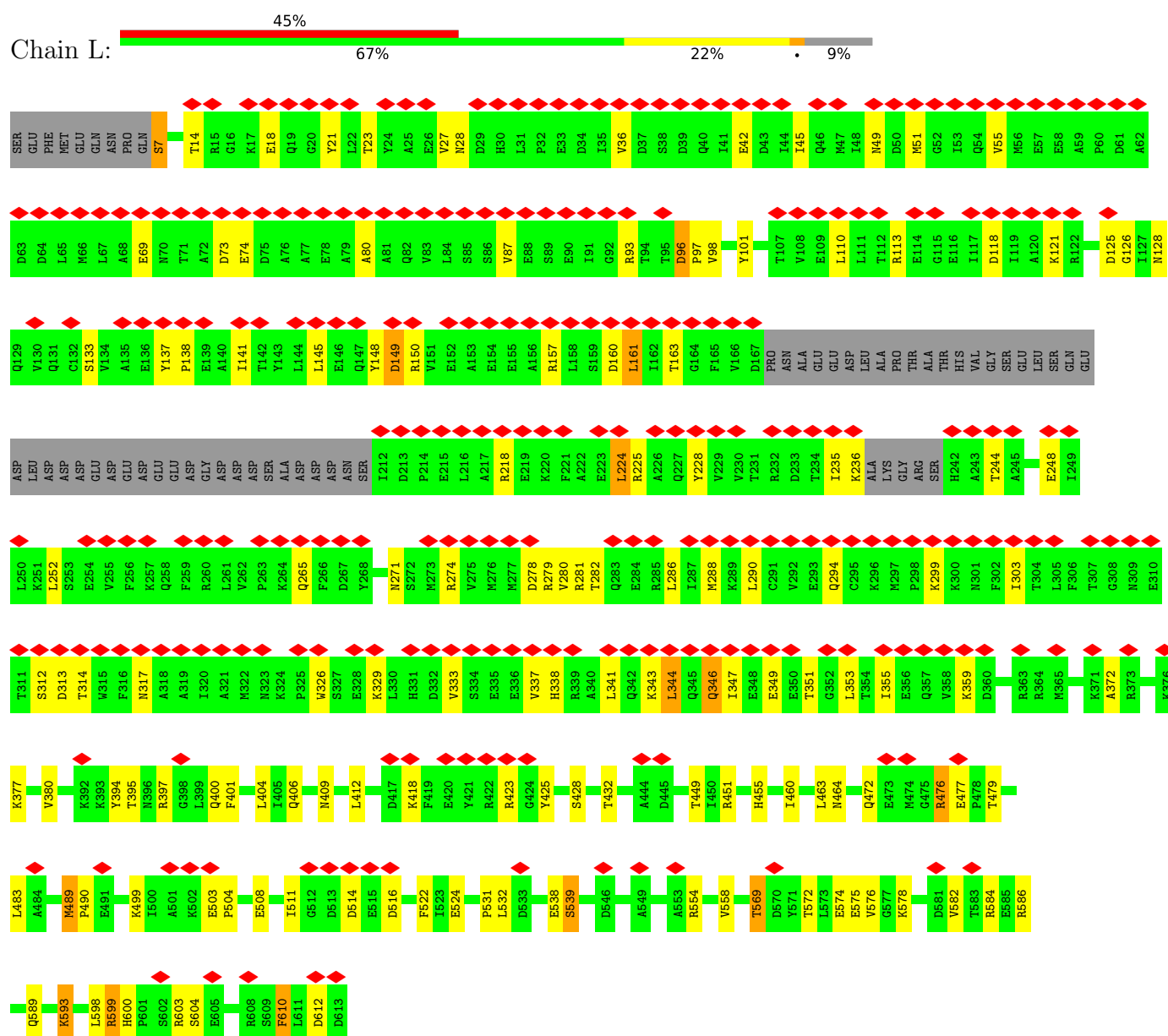


- Molecule 4: DNA-directed RNA polymerase subunit omega

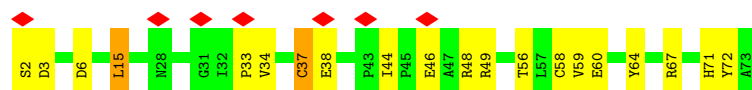


- Molecule 5: RNA polymerase sigma factor RpoD

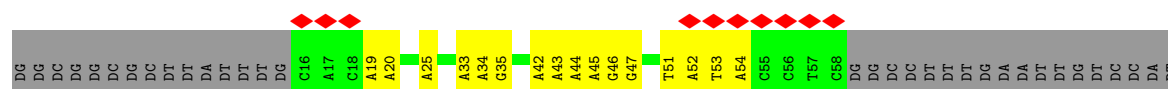
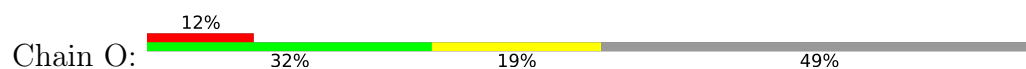




- Molecule 6: Protein TraR



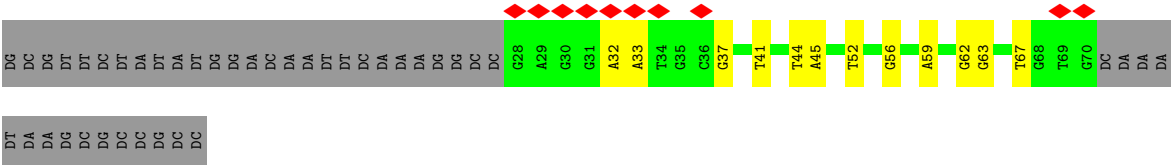
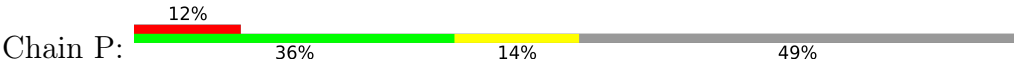
- Molecule 7: DNA (85-MER)





DA  
DT  
DA  
DG  
DA  
DA  
DC  
DG  
DC

● Molecule 8: DNA (85-MER)



DT  
DA  
DA  
DG  
DC  
DG  
DC  
DC  
DC  
DC



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56721	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 K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3, 1.3, 1.3	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	G	0.43	0/1791	0.60	0/2431
1	H	0.39	0/1688	0.59	0/2289
1	M	0.35	0/579	0.66	0/784
2	I	0.45	0/10667	0.60	3/14393 (0.0%)
3	J	0.43	0/10608	0.60	1/14323 (0.0%)
4	K	0.36	0/579	0.58	0/779
5	L	0.31	0/4546	0.58	4/6123 (0.1%)
6	N	0.42	0/575	0.63	0/777
7	O	0.71	0/994	1.00	1/1530 (0.1%)
8	P	0.69	0/984	1.08	2/1518 (0.1%)
All	All	0.44	0/33011	0.64	11/44947 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	I	0	4
5	L	0	1
6	N	0	1
All	All	0	7

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	550	VAL	C-N-CA	6.74	138.56	121.70
2	I	998	LEU	CA-CB-CG	6.17	129.50	115.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	569	THR	C-N-CA	6.05	136.83	121.70
7	O	47	DG	O5'-P-OP1	-6.01	100.29	105.70
5	L	344	LEU	CA-CB-CG	5.76	128.55	115.30
2	I	544	GLY	C-N-CA	5.47	135.39	121.70
3	J	707	ILE	C-N-CA	5.26	134.85	121.70
5	L	149	ASP	CB-CG-OD2	5.19	122.97	118.30
5	L	51	MET	C-N-CA	5.13	133.07	122.30
8	P	37	DG	P-O3'-C3'	5.08	125.79	119.70
8	P	59	DA	P-O3'-C3'	5.04	125.74	119.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	78	ILE	Peptide
2	I	1185	PRO	Peptide
2	I	261	VAL	Peptide
2	I	857	VAL	Peptide
2	I	893	THR	Peptide
5	L	503	GLU	Peptide
6	N	33	PRO	Peptide

## 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	G	1769	0	1789	34	0
1	H	1669	0	1698	39	0
1	M	572	0	602	11	0
2	I	10502	0	10510	204	0
3	J	10449	0	10673	213	0
4	K	577	0	588	19	0
5	L	4489	0	4506	90	0
6	N	566	0	553	11	0
7	O	883	0	481	11	0
8	P	881	0	491	8	0
9	J	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	2	0	0	0	0
10	N	1	0	0	0	0
All	All	32361	0	31891	570	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 9.

All (570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:149:ASP:OD1	5:L:225:ARG:NH2	1.66	1.26
5:L:149:ASP:CG	5:L:225:ARG:HH22	1.58	1.07
5:L:149:ASP:CG	5:L:225:ARG:NH2	2.15	0.95
5:L:45:ILE:O	5:L:49:ASN:HB2	1.75	0.87
2:I:29:SER:O	2:I:33:ASP:HB3	1.88	0.72
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.72	0.71
1:G:234:LEU:HD22	1:H:14:VAL:HG21	1.73	0.71
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.72	0.71
2:I:232:ILE:HG12	2:I:237:LEU:H	1.56	0.69
2:I:238:GLN:HE21	2:I:284:LEU:HB3	1.58	0.67
5:L:455:HIS:HE1	7:O:44:DA:H2'	1.59	0.67
2:I:22:LEU:HB2	2:I:655:VAL:HG11	1.76	0.66
3:J:136:GLU:HG3	5:L:93:ARG:HH22	1.58	0.66
1:M:264:VAL:O	1:M:268:ASN:HB2	1.95	0.66
1:G:45:ARG:HE	2:I:1083:GLU:HG3	1.60	0.65
5:L:351:THR:HG23	5:L:353:LEU:H	1.62	0.65
3:J:120:LEU:HD21	5:L:80:ALA:HB2	1.80	0.64
2:I:255:ILE:HG21	2:I:262:TYR:HB2	1.80	0.64
2:I:250:THR:HA	2:I:268:ARG:HA	1.79	0.64
1:G:62:ASP:OD1	1:G:143:ARG:NH2	2.31	0.64
2:I:31:GLN:HG3	2:I:527:LYS:HB3	1.80	0.64
5:L:394:TYR:HA	5:L:397:ARG:HH21	1.62	0.64
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.31	0.63
3:J:1165:PHE:HB3	3:J:1200:GLU:HG2	1.80	0.63
2:I:478:ARG:O	2:I:478:ARG:NH1	2.32	0.63
3:J:144:TYR:HB3	3:J:178:ALA:HB1	1.81	0.62
3:J:833:GLU:OE1	3:J:838:ARG:NH1	2.32	0.62
3:J:1176:VAL:HG22	3:J:1187:GLU:HB3	1.81	0.62
3:J:338:PHE:HA	3:J:342:LEU:HD22	1.80	0.62
3:J:955:LYS:HE2	3:J:1013:GLY:H	1.65	0.62
3:J:1105:ALA:HB1	3:J:1122:ALA:HB1	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.82	0.61
2:I:618:GLN:HE22	2:I:637:ARG:HG2	1.65	0.61
2:I:1256:GLN:O	2:I:1301:ARG:NH2	2.34	0.61
5:L:45:ILE:HD12	5:L:55:VAL:HG11	1.83	0.61
1:H:191:ARG:HG3	1:H:196:THR:HG22	1.83	0.60
3:J:53:ARG:NH1	3:J:88:CYS:O	2.34	0.60
5:L:14:THR:O	5:L:18:GLU:HB3	2.01	0.60
2:I:1271:GLY:HA2	3:J:344:GLY:HA2	1.83	0.60
3:J:209:ASN:HA	3:J:214:ARG:HD2	1.82	0.60
2:I:197:ARG:HH22	2:I:200:ARG:HH21	1.48	0.60
1:H:29:GLU:HA	1:H:200:LYS:HG3	1.83	0.60
3:J:647:PRO:HG2	3:J:650:LYS:HB2	1.84	0.60
3:J:1335:ALA:HA	3:J:1340:LYS:HE3	1.83	0.60
3:J:127:LEU:O	3:J:220:ARG:NH2	2.35	0.59
1:H:233:ASP:OD1	1:H:233:ASP:N	2.34	0.59
3:J:708:ASN:HB3	3:J:711:GLY:H	1.67	0.59
3:J:821:MET:HA	3:J:881:LYS:HA	1.84	0.59
2:I:745:GLU:O	2:I:974:ARG:NH1	2.35	0.59
2:I:839:VAL:HG13	2:I:1049:ILE:HG12	1.85	0.59
2:I:1073:LYS:NZ	6:N:3:ASP:OD1	2.36	0.59
5:L:97:PRO:O	5:L:101:TYR:HB2	2.01	0.59
1:H:180:VAL:HA	1:H:207:THR:HA	1.84	0.59
3:J:1093:THR:HG22	3:J:1095:MET:H	1.67	0.58
1:M:306:VAL:O	1:M:310:ARG:NH1	2.36	0.58
3:J:750:PRO:HD3	3:J:777:HIS:HB3	1.84	0.58
3:J:948:SER:OG	3:J:949:SER:N	2.37	0.58
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.35	0.58
2:I:321:LEU:HA	2:I:324:LYS:HD2	1.84	0.58
3:J:1166:GLY:HA3	3:J:1174:ARG:HB2	1.84	0.58
3:J:1002:VAL:O	3:J:1019:ASN:ND2	2.37	0.58
2:I:341:LEU:HD21	6:N:67:ARG:HD3	1.86	0.58
3:J:572:THR:OG1	3:J:573:THR:N	2.36	0.58
5:L:344:LEU:HG	5:L:355:ILE:HG13	1.84	0.57
2:I:632:ASP:OD1	2:I:647:ARG:NH2	2.37	0.57
3:J:215:LYS:O	3:J:219:LYS:HB2	2.04	0.57
3:J:568:SER:OG	3:J:569:LEU:N	2.35	0.57
2:I:1069:ARG:NH2	2:I:1114:GLU:OE2	2.37	0.57
3:J:460:ASP:OD2	6:N:2:SER:N	2.37	0.57
2:I:131:THR:OG1	2:I:132:ASP:N	2.38	0.57
3:J:1061:VAL:HG21	3:J:1101:LEU:HD13	1.86	0.57
3:J:1024:THR:HG23	3:J:1123:ARG:HG2	1.86	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.37	0.57
1:G:180:VAL:HG12	1:G:207:THR:HG22	1.87	0.57
5:L:584:ARG:NH2	8:P:56:DG:N7	2.51	0.57
2:I:67:GLU:HB3	2:I:103:VAL:HG23	1.86	0.56
2:I:43:PRO:O	2:I:54:ARG:NH2	2.39	0.56
2:I:528:ARG:NH2	2:I:576:SER:O	2.36	0.56
2:I:983:GLY:HA3	2:I:1003:THR:H	1.70	0.56
3:J:638:SER:OG	3:J:639:VAL:N	2.38	0.56
1:G:18:GLN:NE2	1:G:20:SER:O	2.39	0.56
1:G:45:ARG:NH2	1:H:34:GLY:O	2.39	0.56
2:I:519:ASN:ND2	2:I:689:ALA:O	2.38	0.56
2:I:436:ARG:O	2:I:436:ARG:NH1	2.37	0.56
3:J:275:ARG:NH2	5:L:400:GLN:OE1	2.39	0.56
3:J:294:ASN:OD1	5:L:406:GLN:NE2	2.38	0.56
3:J:357:VAL:HG12	3:J:451:PRO:HG3	1.88	0.56
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.87	0.56
2:I:1120:ALA:HB1	2:I:1198:LEU:HG	1.87	0.56
3:J:481:ARG:NH1	4:K:3:ARG:O	2.40	0.55
2:I:1142:ARG:NH1	2:I:1164:PHE:O	2.37	0.55
3:J:264:ASP:N	3:J:264:ASP:OD1	2.39	0.55
3:J:325:LYS:HD3	3:J:330:MET:HG2	1.89	0.55
3:J:1022:PRO:HG2	3:J:1126:GLN:HE21	1.72	0.55
5:L:554:ARG:NH2	7:O:25:DA:OP2	2.39	0.55
6:N:38:GLU:HG3	6:N:56:THR:HB	1.87	0.55
2:I:3:TYR:HB3	2:I:7:GLU:HB3	1.89	0.55
2:I:1259:LEU:HD11	5:L:524:GLU:HB3	1.89	0.55
6:N:44:ILE:O	6:N:49:ARG:NH2	2.37	0.55
3:J:699:ASP:HA	3:J:702:GLN:HE21	1.72	0.54
3:J:887:SER:HB3	3:J:1227:HIS:HE1	1.72	0.54
3:J:847:ASP:OD1	3:J:847:ASP:N	2.39	0.54
1:M:251:PRO:HD2	1:M:252:ILE:HD12	1.89	0.54
2:I:594:VAL:HG22	2:I:599:VAL:HG12	1.90	0.54
5:L:278:ASP:O	5:L:282:THR:N	2.40	0.54
3:J:1056:LEU:HD21	3:J:1108:GLN:HB2	1.88	0.54
1:G:77:ASP:OD1	1:G:77:ASP:N	2.40	0.54
3:J:390:LEU:HD22	3:J:407:VAL:HG21	1.87	0.54
3:J:820:ILE:HG12	3:J:884:SER:HB2	1.90	0.54
3:J:1158:GLU:HA	3:J:1223:LEU:HD21	1.90	0.54
5:L:145:LEU:O	5:L:225:ARG:NH2	2.41	0.54
5:L:141:ILE:HG12	5:L:224:LEU:HD21	1.90	0.54
2:I:421:SER:H	2:I:424:ASP:HB2	1.71	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:177:ASP:OD1	3:J:177:ASP:N	2.40	0.54
3:J:878:ASP:HB3	3:J:990:ARG:HG2	1.89	0.54
2:I:194:LEU:HB3	2:I:206:ALA:HB3	1.90	0.54
1:G:20:SER:OG	1:G:21:SER:N	2.40	0.53
3:J:1120:THR:O	3:J:1123:ARG:NH1	2.41	0.53
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.89	0.53
5:L:326:TRP:HA	5:L:329:LYS:HB2	1.89	0.53
1:H:9:LEU:HB2	1:H:32:GLU:HG2	1.91	0.53
3:J:674:THR:OG1	3:J:675:ALA:N	2.41	0.53
3:J:843:VAL:O	3:J:883:ARG:N	2.38	0.53
1:H:8:PHE:HD2	1:H:32:GLU:HG3	1.74	0.53
2:I:391:SER:OG	2:I:394:ARG:NH1	2.42	0.53
3:J:54:ASP:OD1	3:J:60:ARG:NH1	2.42	0.53
4:K:40:PRO:O	4:K:52:ARG:NH2	2.37	0.53
7:O:53:DT:H2"	7:O:54:DA:C8	2.43	0.53
2:I:1103:VAL:HG21	2:I:1112:ILE:HD11	1.90	0.53
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.90	0.53
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.34	0.53
3:J:835:LEU:HD22	3:J:990:ARG:HH21	1.72	0.53
5:L:278:ASP:HA	5:L:281:ARG:HB2	1.91	0.53
2:I:1313:HIS:O	4:K:28:ARG:NH2	2.42	0.53
1:H:78:ILE:HG12	1:H:81:ILE:HD12	1.91	0.53
2:I:159:SER:OG	2:I:160:ASP:N	2.42	0.53
2:I:229:ILE:HG12	2:I:334:GLU:HG3	1.91	0.53
2:I:1006:GLU:O	2:I:1010:GLN:N	2.41	0.53
3:J:966:VAL:HG11	3:J:1030:GLU:HA	1.90	0.53
3:J:270:ARG:O	3:J:274:ASN:ND2	2.42	0.52
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.90	0.52
3:J:649:LYS:NZ	3:J:652:GLU:OE2	2.42	0.52
3:J:871:LEU:O	3:J:875:ASN:ND2	2.42	0.52
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.92	0.52
3:J:1022:PRO:HB2	3:J:1126:GLN:HG2	1.91	0.52
1:G:100:LEU:HD21	1:G:121:VAL:HG11	1.90	0.52
1:H:76:GLU:OE2	1:H:132:HIS:ND1	2.42	0.52
2:I:1171:ARG:O	2:I:1175:ASN:ND2	2.43	0.52
5:L:126:GLY:HA3	5:L:372:ALA:HB2	1.91	0.52
5:L:463:LEU:HD11	5:L:483:LEU:HD13	1.91	0.52
6:N:46:GLU:HG2	6:N:49:ARG:HH22	1.74	0.52
1:M:297:LYS:HA	1:M:300:LEU:HB2	1.91	0.52
2:I:642:SER:O	2:I:642:SER:OG	2.26	0.52
1:G:166:ARG:NH1	2:I:876:GLU:OE1	2.40	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:93:SER:OG	2:I:126:GLU:OE1	2.28	0.52
2:I:939:VAL:HG21	2:I:1047:LEU:HB3	1.92	0.52
2:I:576:SER:OG	2:I:577:VAL:N	2.43	0.51
2:I:903:ARG:NH1	2:I:908:GLU:O	2.43	0.51
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.92	0.51
3:J:1075:ARG:HB3	3:J:1100:PHE:HB2	1.93	0.51
1:H:104:LYS:HD2	1:H:110:VAL:HB	1.93	0.51
2:I:619:ALA:HB2	2:I:654:ASP:HB2	1.91	0.51
3:J:393:THR:HG22	3:J:395:LYS:H	1.75	0.51
3:J:1310:THR:HG21	5:L:69:GLU:HB3	1.90	0.51
3:J:431:ARG:NH2	3:J:489:ASN:OD1	2.44	0.51
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.75	0.51
3:J:984:LEU:HB3	3:J:993:GLU:H	1.76	0.51
1:G:33:ARG:NH2	1:G:199:ASP:OD2	2.44	0.51
1:H:22:THR:OG1	1:H:207:THR:O	2.29	0.51
5:L:42:GLU:HA	5:L:45:ILE:HB	1.93	0.51
1:H:41:ASN:OD1	1:H:44:ARG:NH2	2.39	0.51
1:H:118:ASP:OD2	1:H:118:ASP:N	2.43	0.51
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.92	0.51
5:L:149:ASP:OD2	5:L:225:ARG:NH2	2.37	0.51
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.93	0.51
2:I:905:ILE:O	5:L:599:ARG:NH1	2.44	0.51
5:L:455:HIS:NE2	7:O:44:DA:OP2	2.42	0.50
1:G:212:ASP:N	1:G:212:ASP:OD1	2.44	0.50
2:I:1088:ASP:HB3	2:I:1210:ILE:HD12	1.93	0.50
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.92	0.50
3:J:640:GLY:N	3:J:643:ASP:OD2	2.43	0.50
3:J:762:ASN:OD1	3:J:762:ASN:N	2.42	0.50
2:I:372:PRO:HD2	5:L:36:VAL:HG13	1.94	0.50
3:J:133:ARG:HB3	3:J:137:ARG:HH21	1.77	0.50
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.91	0.50
5:L:539:SER:HB3	5:L:610:PHE:HZ	1.76	0.50
1:M:265:ARG:HH21	1:M:294:ASN:HB2	1.75	0.50
1:H:114:ASP:OD1	1:H:114:ASP:N	2.45	0.50
2:I:1184:THR:HG23	2:I:1190:ALA:H	1.75	0.50
5:L:401:PHE:HA	5:L:404:LEU:HD12	1.94	0.50
5:L:489:MET:SD	5:L:489:MET:N	2.84	0.50
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.94	0.50
2:I:636:CYS:HB2	2:I:645:PHE:HD2	1.76	0.50
3:J:1261:LEU:HD23	3:J:1306:LEU:HD13	1.93	0.50
6:N:37:CYS:SG	6:N:38:GLU:N	2.85	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.94	0.50
2:I:714:VAL:HB	2:I:787:PRO:HD2	1.93	0.50
2:I:1244:HIS:HB2	2:I:1262:LYS:HG3	1.92	0.50
1:G:102:LEU:HB2	1:G:144:ILE:HD11	1.93	0.50
5:L:572:THR:OG1	8:P:56:DG:OP2	2.30	0.50
1:H:215:GLU:OE2	1:H:219:ARG:NH2	2.45	0.50
3:J:58:CYS:SG	3:J:59:ALA:N	2.85	0.50
3:J:504:GLN:HE22	3:J:731:ARG:HH21	1.60	0.50
2:I:18:ARG:NH2	2:I:622:ASN:OD1	2.45	0.49
7:O:35:DG:N2	8:P:52:DT:O2	2.45	0.49
5:L:428:SER:O	5:L:432:THR:OG1	2.29	0.49
1:H:181:GLU:O	3:J:535:ARG:NH1	2.45	0.49
2:I:1213:TYR:HA	2:I:1220:GLN:HA	1.94	0.49
3:J:808:VAL:HG12	3:J:914:ALA:HA	1.93	0.49
2:I:1246:ARG:NH1	2:I:1265:PHE:O	2.44	0.49
3:J:275:ARG:NH1	3:J:298:MET:O	2.42	0.49
5:L:279:ARG:HH21	5:L:343:LYS:HB3	1.78	0.49
5:L:281:ARG:HH21	5:L:359:LYS:HG2	1.77	0.49
1:G:98:VAL:HG21	1:G:121:VAL:HG21	1.95	0.49
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.45	0.49
3:J:1041:ILE:O	3:J:1045:THR:OG1	2.28	0.49
3:J:1064:SER:OG	3:J:1168:GLU:OE1	2.31	0.49
3:J:1329:THR:O	3:J:1333:THR:OG1	2.28	0.49
5:L:148:TYR:HE1	5:L:218:ARG:HE	1.59	0.49
5:L:589:GLN:O	5:L:593:LYS:N	2.43	0.49
2:I:954:LYS:HG2	2:I:957:LYS:HE3	1.95	0.49
3:J:202:ARG:HA	3:J:205:LEU:HB2	1.94	0.49
1:G:180:VAL:HA	1:G:207:THR:HA	1.94	0.49
3:J:576:ARG:HD3	3:J:593:ASN:HA	1.94	0.49
5:L:337:VAL:O	5:L:341:LEU:N	2.46	0.49
5:L:558:VAL:HG23	5:L:576:VAL:HG11	1.95	0.49
2:I:232:ILE:O	2:I:331:LYS:NZ	2.45	0.48
2:I:633:LEU:HB3	2:I:644:LEU:HD12	1.94	0.48
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.95	0.48
2:I:1281:TYR:OH	3:J:434:ILE:O	2.30	0.48
7:O:46:DG:N2	8:P:41:DT:O2	2.46	0.48
2:I:682:GLY:HA2	2:I:685:MET:HE2	1.95	0.48
5:L:312:SER:OG	5:L:313:ASP:N	2.46	0.48
1:G:44:ARG:HG3	1:G:183:ILE:HB	1.94	0.48
1:H:113:ALA:HB2	1:H:126:PRO:HB2	1.96	0.48
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.45	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1117:LEU:HG	2:I:1195:ILE:HG12	1.94	0.48
3:J:572:THR:OG1	3:J:573:THR:O	2.32	0.48
1:M:310:ARG:HG3	1:M:312:LEU:HD12	1.95	0.48
2:I:577:VAL:HG22	2:I:663:VAL:HG12	1.94	0.48
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.46	0.48
3:J:686:TRP:CD2	3:J:758:PRO:HG3	2.49	0.48
3:J:1178:THR:HA	3:J:1184:ASP:HB3	1.95	0.48
3:J:1265:THR:OG1	3:J:1303:SER:OG	2.30	0.48
2:I:91:THR:HG23	2:I:138:ILE:HD13	1.95	0.48
5:L:149:ASP:OD1	5:L:225:ARG:CZ	2.55	0.48
2:I:86:GLN:NE2	2:I:140:GLY:O	2.41	0.48
2:I:207:THR:HG22	2:I:210:LEU:HD12	1.96	0.48
3:J:613:GLY:O	3:J:617:THR:OG1	2.29	0.48
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.96	0.48
3:J:210:SER:OG	3:J:211:GLU:N	2.46	0.48
3:J:842:ARG:HD3	3:J:882:VAL:HG21	1.94	0.48
3:J:1292:LEU:HD23	3:J:1297:LYS:HE3	1.96	0.48
3:J:475:GLU:HG3	4:K:24:ALA:HB1	1.96	0.48
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.95	0.48
3:J:738:ARG:NH2	3:J:744:ARG:O	2.47	0.48
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.42	0.48
2:I:1267:GLY:O	3:J:346:ARG:NH1	2.47	0.48
3:J:72:CYS:SG	3:J:73:GLY:N	2.87	0.47
3:J:830:ASP:OD1	3:J:830:ASP:N	2.47	0.47
5:L:290:LEU:HA	5:L:294:GLN:HB2	1.96	0.47
1:H:196:THR:OG1	3:J:443:GLU:OE2	2.31	0.47
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.96	0.47
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.96	0.47
2:I:1023:HIS:HA	2:I:1026:GLU:HB2	1.95	0.47
3:J:69:GLU:HG3	3:J:76:LYS:HG2	1.96	0.47
1:H:47:LEU:HA	1:H:51:MET:HG3	1.95	0.47
2:I:870:ILE:HG23	2:I:884:VAL:HG22	1.96	0.47
3:J:475:GLU:OE2	4:K:28:ARG:NH1	2.34	0.47
5:L:574:GLU:O	5:L:578:LYS:N	2.48	0.47
2:I:29:SER:O	2:I:33:ASP:CB	2.61	0.47
1:G:10:LYS:NZ	1:H:229:GLU:OE1	2.47	0.47
2:I:56:VAL:HG11	2:I:468:LEU:HB3	1.96	0.47
2:I:252:SER:O	2:I:265:LYS:NZ	2.42	0.47
5:L:7:SER:O	5:L:7:SER:OG	2.32	0.47
2:I:27:LEU:HD22	2:I:663:VAL:HG11	1.96	0.47
2:I:871:VAL:O	2:I:944:ARG:NH2	2.47	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:169:LYS:NZ	2:I:192:ASP:OD1	2.47	0.47
2:I:1326:LEU:HD22	3:J:342:LEU:HD21	1.95	0.47
3:J:672:LEU:O	6:N:48:ARG:NH1	2.44	0.47
3:J:1207:GLY:H	3:J:1223:LEU:HD23	1.80	0.47
5:L:118:ASP:HA	5:L:121:LYS:HG2	1.95	0.47
5:L:600:HIS:ND1	1:M:261:GLU:OE1	2.44	0.47
2:I:164:THR:O	5:L:21:TYR:OH	2.33	0.47
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.48	0.47
3:J:398:LYS:HG3	5:L:532:LEU:HD21	1.96	0.47
1:G:8:PHE:HD1	1:G:32:GLU:HG3	1.80	0.47
2:I:68:LEU:HD22	2:I:475:VAL:HG11	1.97	0.47
3:J:342:LEU:HB3	3:J:1352:ILE:HG12	1.97	0.47
2:I:1324:ASN:N	2:I:1324:ASN:OD1	2.48	0.46
3:J:245:LEU:O	3:J:250:ARG:NH2	2.44	0.46
3:J:287:ALA:HB1	3:J:291:ILE:HD11	1.97	0.46
2:I:224:PHE:HB2	2:I:347:ILE:HG21	1.96	0.46
2:I:1247:SER:HB2	3:J:375:GLU:O	2.15	0.46
3:J:148:GLU:H	3:J:156:ARG:HG3	1.79	0.46
4:K:46:THR:HA	4:K:49:ILE:HD12	1.95	0.46
5:L:409:ASN:HA	5:L:412:LEU:HB3	1.97	0.46
5:L:460:ILE:O	5:L:464:ASN:N	2.43	0.46
5:L:575:GLU:HA	5:L:578:LYS:HD3	1.96	0.46
3:J:414:GLU:O	4:K:45:LYS:NZ	2.48	0.46
3:J:1108:GLN:OE1	3:J:1123:ARG:NH1	2.48	0.46
1:G:10:LYS:O	1:G:12:ARG:NH1	2.44	0.46
1:G:154:PRO:HG2	1:G:157:THR:HG23	1.97	0.46
2:I:16:GLY:HA3	2:I:1185:PRO:HG2	1.96	0.46
1:H:153:VAL:O	1:H:158:ARG:NH2	2.48	0.46
2:I:402:ARG:NH2	2:I:419:ILE:O	2.48	0.46
2:I:531:SER:HB2	2:I:572:ILE:HG12	1.98	0.46
3:J:1271:SER:O	3:J:1271:SER:OG	2.34	0.46
5:L:377:LYS:HA	5:L:380:VAL:HB	1.96	0.46
2:I:126:GLU:O	2:I:503:LYS:NZ	2.49	0.46
3:J:105:ILE:HB	3:J:242:LEU:HB3	1.96	0.46
3:J:1098:GLN:H	3:J:1098:GLN:HG2	1.50	0.46
3:J:1244:GLN:HE21	3:J:1244:GLN:HB2	1.48	0.46
3:J:1264:ALA:HB1	3:J:1302:TYR:HB2	1.98	0.46
5:L:125:ASP:HA	5:L:128:ASN:HB2	1.96	0.46
1:G:42:ALA:O	1:G:46:ILE:HG12	2.16	0.46
2:I:145:ILE:HG22	2:I:456:VAL:HG22	1.97	0.46
2:I:746:ALA:HA	2:I:971:LEU:HG	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:150:ARG:HE	5:L:150:ARG:HB3	1.61	0.46
1:G:134:THR:O	1:G:134:THR:OG1	2.34	0.45
2:I:992:LEU:HD12	2:I:993:PRO:HD2	1.97	0.45
2:I:496:LYS:HA	2:I:496:LYS:HD2	1.80	0.45
2:I:957:LYS:HB2	2:I:1029:LEU:HD11	1.98	0.45
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.98	0.45
5:L:343:LYS:HA	5:L:346:GLN:HB3	1.98	0.45
3:J:118:LYS:HD3	3:J:118:LYS:HA	1.76	0.45
3:J:615:LYS:NZ	4:K:7:GLN:OE1	2.39	0.45
3:J:962:ASN:O	3:J:980:THR:OG1	2.25	0.45
5:L:161:LEU:HG	5:L:265:GLN:HG3	1.98	0.45
5:L:511:ILE:HG13	5:L:522:PHE:HE2	1.81	0.45
7:O:51:DT:H1'	7:O:52:DA:C8	2.51	0.45
2:I:454:ARG:HD2	2:I:459:MET:HG2	1.98	0.45
3:J:488:ASN:HB3	4:K:16:ARG:HH21	1.82	0.45
3:J:869:CYS:HA	3:J:872:LEU:HG	1.99	0.45
3:J:1368:ASP:OD2	3:J:1372:ARG:NH1	2.49	0.45
8:P:44:DT:H2''	8:P:45:DA:C8	2.51	0.45
2:I:524:ILE:HG13	2:I:712:SER:HB2	1.97	0.45
2:I:639:LYS:H	2:I:639:LYS:HG3	1.49	0.45
5:L:343:LYS:HA	5:L:343:LYS:HD3	1.77	0.45
5:L:582:VAL:HG11	5:L:586:ARG:HB3	1.98	0.45
7:O:19:DA:H2''	7:O:20:DA:C8	2.51	0.45
1:G:76:GLU:OE1	1:G:132:HIS:N	2.44	0.44
1:H:76:GLU:H	1:H:76:GLU:HG2	1.53	0.44
2:I:341:LEU:HD22	6:N:64:TYR:HD1	1.83	0.44
2:I:962:GLU:HA	2:I:965:GLN:HG2	1.99	0.44
3:J:817:HIS:O	3:J:881:LYS:NZ	2.46	0.44
1:M:296:GLY:HA3	8:P:67:DT:H3'	1.98	0.44
1:H:35:PHE:HA	1:H:38:THR:HG22	1.99	0.44
2:I:1088:ASP:OD1	2:I:1088:ASP:N	2.41	0.44
3:J:1357:ILE:HD12	3:J:1359:ALA:HB3	1.99	0.44
5:L:244:THR:O	5:L:248:GLU:N	2.50	0.44
2:I:291:TYR:O	2:I:295:LYS:NZ	2.38	0.44
2:I:749:ASP:OD1	2:I:749:ASP:N	2.51	0.44
2:I:1248:THR:HG21	5:L:531:PRO:HG2	1.99	0.44
3:J:954:ASN:HD22	3:J:992:LYS:HE3	1.82	0.44
3:J:1075:ARG:NH2	3:J:1168:GLU:OE2	2.39	0.44
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.50	0.44
1:H:44:ARG:O	1:H:48:LEU:HB2	2.16	0.44
5:L:73:ASP:HA	5:L:74:GLU:HA	1.69	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:141:ILE:HG21	5:L:252:LEU:HD21	2.00	0.44
5:L:603:ARG:HA	5:L:603:ARG:HD3	1.82	0.44
2:I:400:VAL:HG23	2:I:584:TYR:HB3	2.00	0.44
2:I:515:MET:HA	2:I:526:HIS:HD2	1.82	0.44
2:I:1114:GLU:O	2:I:1118:GLY:N	2.47	0.44
2:I:1278:LEU:HD23	2:I:1278:LEU:HA	1.79	0.44
4:K:44:ASP:OD2	4:K:52:ARG:NH1	2.51	0.44
2:I:1309:VAL:HG11	3:J:394:ILE:HD12	1.99	0.44
3:J:355:ILE:HD11	3:J:464:ASP:HB2	1.98	0.44
3:J:891:ASP:OD1	3:J:1283:SER:OG	2.36	0.44
3:J:903:LEU:HD11	3:J:1251:LYS:HD2	1.98	0.44
8:P:32:DA:H2"	8:P:33:DA:C8	2.52	0.44
2:I:201:ARG:HA	5:L:28:ASN:HD22	1.82	0.44
2:I:241:LEU:HD11	2:I:246:LEU:HD22	1.99	0.44
2:I:657:THR:HB	2:I:1187:PHE:HB2	1.99	0.44
2:I:1034:ARG:HD2	2:I:1034:ARG:HA	1.77	0.44
3:J:368:LEU:HD23	3:J:373:ALA:HB2	2.00	0.44
3:J:1106:ILE:O	3:J:1123:ARG:NH2	2.50	0.44
1:H:97:GLU:HB3	1:H:147:GLN:HG3	1.99	0.44
3:J:122:SER:O	3:J:122:SER:OG	2.35	0.44
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	2.00	0.44
2:I:785:ASP:OD1	2:I:785:ASP:N	2.50	0.44
3:J:1295:ASN:HB3	3:J:1297:LYS:HG2	1.99	0.44
5:L:598:LEU:O	5:L:604:SER:OG	2.35	0.44
2:I:102:LEU:HB3	2:I:118:LYS:HB2	2.00	0.43
3:J:1072:LYS:HB3	3:J:1072:LYS:HE2	1.72	0.43
3:J:1090:ILE:HD11	3:J:1097:ALA:HA	2.00	0.43
2:I:1117:LEU:HD22	2:I:1182:ILE:HG13	1.99	0.43
2:I:1176:LEU:HD22	2:I:1180:MET:HA	2.00	0.43
3:J:99:ARG:NH1	3:J:248:ASP:OD2	2.46	0.43
2:I:370:MET:HG2	2:I:384:LEU:HD11	2.00	0.43
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.00	0.43
2:I:773:LEU:HD23	2:I:773:LEU:HA	1.88	0.43
2:I:794:LEU:HG	2:I:796:LEU:HD13	2.01	0.43
3:J:167:ASP:HA	3:J:170:GLU:HG3	2.01	0.43
3:J:861:ASN:N	3:J:861:ASN:OD1	2.52	0.43
5:L:282:THR:O	5:L:286:LEU:N	2.48	0.43
1:M:297:LYS:HA	1:M:297:LYS:HD3	1.84	0.43
8:P:62:DG:H2"	8:P:63:DG:C8	2.53	0.43
2:I:75:LEU:HD12	2:I:94:ALA:HB3	2.00	0.43
2:I:755:LYS:O	2:I:757:THR:N	2.51	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:29:MET:HA	3:J:32:SER:HB3	2.00	0.43
3:J:313:GLY:HA2	3:J:314:ARG:HA	1.61	0.43
5:L:451:ARG:NH2	7:O:45:DA:OP1	2.50	0.43
2:I:175:ARG:HD2	2:I:177:ILE:HD11	2.00	0.43
2:I:404:LYS:NZ	2:I:450:ASN:OD1	2.46	0.43
2:I:1315:MET:HG2	3:J:473:THR:HG21	1.99	0.43
3:J:1155:ILE:HG12	3:J:1211:SER:HB2	2.01	0.43
1:M:250:ASP:HA	1:M:251:PRO:HD3	1.81	0.43
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.99	0.43
1:H:61:ILE:HG22	1:H:142:MET:HB3	2.00	0.43
2:I:303:ASP:HB3	2:I:310:ILE:HD11	1.99	0.43
3:J:34:SER:OG	3:J:36:GLY:O	2.37	0.43
3:J:698:MET:O	3:J:702:GLN:NE2	2.51	0.43
3:J:957:SER:HB2	3:J:1010:GLN:HG2	2.01	0.43
3:J:743:MET:HE3	3:J:760:THR:HA	2.00	0.43
3:J:967:VAL:O	3:J:1117:SER:OG	2.37	0.43
3:J:985:ILE:HD13	3:J:991:THR:HA	2.01	0.43
1:H:65:LEU:HD22	1:H:65:LEU:HA	1.85	0.43
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.54	0.43
5:L:423:ARG:NH1	5:L:425:TYR:OH	2.52	0.43
1:H:46:ILE:HD11	1:H:224:LEU:HD13	2.00	0.43
2:I:490:GLN:HG3	5:L:472:GLN:HE21	1.84	0.43
3:J:511:TYR:CG	3:J:728:SER:HB3	2.53	0.43
3:J:755:ILE:HD12	3:J:774:ILE:HG23	2.01	0.43
3:J:826:ILE:HG12	3:J:831:VAL:HB	2.01	0.43
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	2.01	0.43
2:I:434:ASP:HB3	2:I:439:LYS:HB2	2.01	0.42
2:I:678:ARG:NH2	6:N:6:ASP:OD1	2.52	0.42
2:I:708:VAL:HG12	2:I:794:LEU:HD13	2.01	0.42
3:J:194:LEU:HD11	3:J:234:PRO:HG3	2.01	0.42
3:J:513:MET:HG3	3:J:514:THR:HG23	2.01	0.42
3:J:1089:LEU:HD12	3:J:1089:LEU:HA	1.91	0.42
3:J:1106:ILE:HD11	3:J:1125:PRO:HG3	1.99	0.42
5:L:27:VAL:HG11	5:L:45:ILE:HD11	2.01	0.42
1:G:228:LEU:HD11	1:H:224:LEU:HD23	2.01	0.42
2:I:197:ARG:HD3	2:I:203:LYS:HG2	2.00	0.42
2:I:830:THR:O	2:I:1058:ARG:N	2.52	0.42
2:I:952:GLN:HB3	2:I:1036:ILE:HD13	2.00	0.42
5:L:338:HIS:HA	5:L:341:LEU:HB2	1.99	0.42
1:G:69:SER:OG	1:G:70:THR:N	2.52	0.42
2:I:347:ILE:HD13	2:I:347:ILE:HA	1.86	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:515:MET:HB3	2:I:515:MET:HE2	1.94	0.42
2:I:1254:VAL:HG23	2:I:1255:THR:H	1.84	0.42
4:K:59:ILE:HG23	4:K:64:LEU:HG	2.02	0.42
2:I:710:VAL:HG13	2:I:717:VAL:HG21	2.01	0.42
2:I:740:GLU:H	2:I:740:GLU:HG2	1.76	0.42
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	2.02	0.42
2:I:1008:GLN:HA	2:I:1011:LEU:HB2	2.02	0.42
2:I:1098:LEU:HD23	2:I:1098:LEU:HA	1.90	0.42
3:J:1032:SER:OG	3:J:1117:SER:N	2.53	0.42
5:L:409:ASN:OD1	5:L:409:ASN:N	2.52	0.42
2:I:221:LEU:HD13	2:I:336:LEU:HD11	2.01	0.42
2:I:755:LYS:HA	2:I:755:LYS:HD2	1.72	0.42
5:L:157:ARG:O	5:L:161:LEU:N	2.50	0.42
5:L:476:ARG:NH2	5:L:477:GLU:H	2.18	0.42
1:H:86:LYS:NZ	3:J:526:VAL:O	2.45	0.42
2:I:533:LEU:HD21	2:I:571:LEU:HD13	2.02	0.42
2:I:637:ARG:HB3	2:I:642:SER:HB2	2.00	0.42
2:I:1163:THR:O	2:I:1163:THR:OG1	2.34	0.42
4:K:10:VAL:HG12	4:K:19:LEU:HD22	2.01	0.42
5:L:137:TYR:HA	5:L:138:PRO:HD3	1.89	0.42
2:I:120:GLN:NE2	2:I:490:GLN:OE1	2.52	0.42
4:K:39:VAL:HG12	4:K:53:GLU:HG3	2.01	0.42
1:G:113:ALA:HB2	1:G:126:PRO:HB2	2.01	0.42
5:L:96:ASP:OD1	5:L:96:ASP:N	2.51	0.42
2:I:1082:ILE:HD11	2:I:1093:PRO:HG3	2.01	0.42
2:I:1225:VAL:HA	3:J:638:SER:HB2	2.02	0.42
3:J:1140:ARG:HD2	3:J:1140:ARG:HA	1.77	0.42
1:H:120:ASP:OD2	1:H:120:ASP:N	2.52	0.41
2:I:138:ILE:HD13	2:I:138:ILE:HA	1.88	0.41
2:I:402:ARG:HA	2:I:402:ARG:HD3	1.84	0.41
3:J:421:VAL:HB	3:J:468:VAL:HG23	2.02	0.41
3:J:1156:LEU:HD11	3:J:1224:ARG:HH21	1.85	0.41
4:K:60:ASN:HB2	4:K:63:ILE:HD12	2.02	0.41
5:L:299:LYS:O	5:L:303:ILE:N	2.47	0.41
2:I:407:ARG:HD3	2:I:407:ARG:HA	1.92	0.41
3:J:245:LEU:HG	3:J:249:LEU:HB2	2.02	0.41
3:J:1072:LYS:HD2	3:J:1168:GLU:HB2	2.02	0.41
3:J:1163:VAL:HA	3:J:1177:ILE:HA	2.02	0.41
5:L:235:ILE:HD13	5:L:235:ILE:HA	1.91	0.41
1:G:158:ARG:HH22	1:G:175:ALA:H	1.68	0.41
2:I:1339:LEU:HD12	3:J:20:ILE:HG12	2.01	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:105:ILE:HD12	3:J:242:LEU:HD23	2.03	0.41
3:J:1076:PRO:HG2	3:J:1101:LEU:HD12	2.02	0.41
2:I:1340:GLU:HB2	3:J:19:ALA:HB3	2.00	0.41
3:J:18:ASP:OD2	3:J:1369:ARG:NH2	2.52	0.41
3:J:190:LYS:HE3	3:J:190:LYS:HB2	1.86	0.41
3:J:223:LEU:HD13	3:J:223:LEU:HA	1.89	0.41
3:J:1184:ASP:OD1	3:J:1184:ASP:N	2.53	0.41
3:J:1192:LYS:HE3	3:J:1192:LYS:HB3	1.80	0.41
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.47	0.41
2:I:57:PHE:CD2	2:I:70:TYR:HB2	2.56	0.41
2:I:300:ASP:HA	2:I:312:ALA:HA	2.02	0.41
2:I:568:ASN:HB2	2:I:571:LEU:HB2	2.02	0.41
3:J:86:GLU:H	3:J:86:GLU:HG3	1.64	0.41
5:L:97:PRO:O	5:L:101:TYR:CB	2.68	0.41
1:H:51:MET:HA	1:H:52:PRO:HD3	1.95	0.41
2:I:204:LEU:HD21	2:I:369:MET:HB2	2.03	0.41
2:I:325:LEU:HA	2:I:328:SER:HB2	2.01	0.41
2:I:515:MET:HA	2:I:526:HIS:CD2	2.56	0.41
2:I:649:GLN:H	2:I:649:GLN:HG2	1.59	0.41
2:I:1211:ARG:HD2	2:I:1224:PRO:HB3	2.03	0.41
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.42	0.41
3:J:996:LYS:HB3	3:J:996:LYS:HE3	1.86	0.41
3:J:1198:VAL:HG22	3:J:1202:GLU:HB3	2.01	0.41
5:L:489:MET:HA	5:L:490:PRO:HD3	1.80	0.41
1:H:39:LEU:HD23	1:H:39:LEU:HA	1.91	0.41
2:I:693:LEU:HD23	2:I:693:LEU:HA	1.86	0.41
2:I:710:VAL:HA	2:I:715:THR:HG21	2.03	0.41
2:I:1061:GLN:NE2	2:I:1240:ASP:OD1	2.53	0.41
2:I:1106:ARG:H	2:I:1106:ARG:HG3	1.70	0.41
3:J:114:ILE:HD12	3:J:114:ILE:HA	1.81	0.41
3:J:978:ARG:NH2	3:J:1202:GLU:OE1	2.51	0.41
3:J:1154:ALA:HA	3:J:1211:SER:HB3	2.02	0.41
5:L:228:TYR:HD1	5:L:252:LEU:HD11	1.86	0.41
1:M:286:GLU:H	1:M:286:GLU:HG2	1.70	0.41
1:G:83:LEU:HD11	2:I:693:LEU:HD13	2.01	0.41
1:H:47:LEU:HB3	1:H:180:VAL:HG11	2.02	0.41
1:H:152:TYR:CZ	3:J:536:LEU:HD21	2.56	0.41
2:I:149:LEU:HD12	2:I:149:LEU:HA	1.82	0.41
2:I:1223:ARG:NH1	3:J:719:PHE:O	2.53	0.41
3:J:193:ASP:HB3	3:J:196:GLN:HB3	2.03	0.41
3:J:238:ILE:HD13	3:J:238:ILE:HA	1.94	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:494:ALA:HA	3:J:922:SER:HB3	2.02	0.41
1:G:67:GLU:HG3	1:G:171:LEU:HD12	2.03	0.41
2:I:302:ILE:HD12	2:I:307:GLY:HA2	2.03	0.41
2:I:372:PRO:HG2	5:L:36:VAL:HG22	2.01	0.41
2:I:979:LEU:HD21	2:I:1011:LEU:HD21	2.02	0.41
2:I:1008:GLN:O	2:I:1008:GLN:NE2	2.54	0.41
2:I:1010:GLN:O	2:I:1014:LEU:N	2.39	0.41
2:I:1035:LYS:HA	2:I:1038:GLN:HG2	2.02	0.41
2:I:1282:GLY:H	3:J:483:LEU:HD13	1.85	0.41
3:J:326:SER:OG	3:J:329:ASP:OD1	2.37	0.41
3:J:488:ASN:OD1	3:J:488:ASN:N	2.52	0.41
3:J:603:LYS:O	3:J:607:THR:OG1	2.30	0.41
3:J:1007:ASP:OD1	3:J:1007:ASP:N	2.53	0.41
3:J:1174:ARG:HB3	3:J:1187:GLU:HB2	2.02	0.41
3:J:1221:LEU:HD11	3:J:1226:VAL:HG23	2.03	0.41
5:L:110:LEU:HD23	5:L:110:LEU:HA	1.97	0.41
5:L:499:LYS:HE3	5:L:499:LYS:HB2	1.94	0.41
7:O:42:DA:H1'	7:O:43:DA:C8	2.56	0.41
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.51	0.41
3:J:123:ARG:O	3:J:127:LEU:HB2	2.21	0.40
3:J:1164:SER:O	3:J:1176:VAL:N	2.54	0.40
1:H:152:TYR:OH	3:J:532:GLU:OE2	2.36	0.40
2:I:211:ARG:NH2	2:I:217:THR:OG1	2.35	0.40
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.86	0.40
2:I:1086:PRO:HB3	2:I:1221:PHE:HE2	1.87	0.40
3:J:197:GLU:O	3:J:201:LEU:HB2	2.22	0.40
3:J:836:ARG:HG3	3:J:869:CYS:SG	2.61	0.40
3:J:863:LEU:HD13	3:J:908:ILE:HG13	2.02	0.40
3:J:899:TYR:CZ	3:J:1251:LYS:HD3	2.56	0.40
4:K:49:ILE:H	4:K:49:ILE:HG13	1.74	0.40
1:H:67:GLU:HA	1:H:68:TYR:HA	1.82	0.40
2:I:207:THR:HG21	2:I:351:LEU:HG	2.03	0.40
2:I:298:ALA:HB3	2:I:334:GLU:HB3	2.04	0.40
3:J:781:LYS:HG2	6:N:15:LEU:HD11	2.02	0.40
3:J:878:ASP:OD1	3:J:878:ASP:N	2.50	0.40
3:J:1149:ARG:HD3	3:J:1149:ARG:HA	1.83	0.40
3:J:1170:LYS:HE3	3:J:1170:LYS:HB2	1.92	0.40
1:G:207:THR:HG21	1:G:211:ILE:HG22	2.03	0.40
2:I:297:VAL:HG13	2:I:313:ALA:HA	2.04	0.40
2:I:1206:THR:O	2:I:1206:THR:OG1	2.37	0.40
2:I:1293:VAL:HG11	2:I:1304:MET:HG2	2.03	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:85:CYS:SG	3:J:86:GLU:N	2.95	0.40
3:J:138:VAL:HG22	3:J:143:SER:HB2	2.03	0.40
3:J:722:ILE:HG23	3:J:737:ILE:HD12	2.03	0.40
4:K:41:GLU:HA	4:K:52:ARG:HH12	1.86	0.40
5:L:271:ASN:HA	5:L:274:ARG:HB2	2.04	0.40
7:O:33:DA:H2''	7:O:34:DA:C8	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	230/329 (70%)	213 (93%)	17 (7%)	0	100	100
1	H	214/329 (65%)	193 (90%)	21 (10%)	0	100	100
1	M	71/329 (22%)	59 (83%)	12 (17%)	0	100	100
2	I	1331/1342 (99%)	1221 (92%)	105 (8%)	5 (0%)	34	72
3	J	1337/1430 (94%)	1240 (93%)	96 (7%)	1 (0%)	51	84
4	K	70/91 (77%)	69 (99%)	1 (1%)	0	100	100
5	L	552/616 (90%)	514 (93%)	37 (7%)	1 (0%)	47	81
6	N	70/72 (97%)	61 (87%)	8 (11%)	1 (1%)	11	46
All	All	3875/4538 (85%)	3570 (92%)	297 (8%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	34	VAL
2	I	856	ASN
5	L	504	PRO
2	I	254	ASP

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
3	J	859	PRO
2	I	855	PRO
2	I	940	GLU
2	I	1317	PRO

### 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	G	192/286 (67%)	175 (91%)	17 (9%)	9	37
1	H	184/286 (64%)	166 (90%)	18 (10%)	8	33
1	M	65/286 (23%)	57 (88%)	8 (12%)	4	23
2	I	1142/1157 (99%)	1039 (91%)	103 (9%)	9	37
3	J	1126/1189 (95%)	1026 (91%)	100 (9%)	9	37
4	K	63/75 (84%)	57 (90%)	6 (10%)	8	34
5	L	490/543 (90%)	456 (93%)	34 (7%)	15	47
6	N	60/61 (98%)	53 (88%)	7 (12%)	5	26
All	All	3322/3883 (86%)	3029 (91%)	293 (9%)	13	38

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	12	ARG
1	G	70	THR
1	G	77	ASP
1	G	96	ASP
1	G	98	VAL
1	G	102	LEU
1	G	124	VAL
1	G	132	HIS
1	G	134	THR
1	G	160	HIS
1	G	177	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	G	196	THR
1	G	199	ASP
1	G	211	ILE
1	G	212	ASP
1	G	224	LEU
1	G	231	PHE
1	H	9	LEU
1	H	12	ARG
1	H	14	VAL
1	H	20	SER
1	H	23	HIS
1	H	43	LEU
1	H	65	LEU
1	H	68	TYR
1	H	70	THR
1	H	76	GLU
1	H	114	ASP
1	H	118	ASP
1	H	127	GLN
1	H	157	THR
1	H	196	THR
1	H	210	THR
1	H	218	ARG
1	H	233	ASP
2	I	17	LYS
2	I	22	LEU
2	I	23	ASP
2	I	24	VAL
2	I	29	SER
2	I	39	ILE
2	I	81	ASP
2	I	86	GLN
2	I	103	VAL
2	I	146	VAL
2	I	150	HIS
2	I	165	HIS
2	I	173	ASN
2	I	194	LEU
2	I	227	LYS
2	I	228	VAL
2	I	245	ARG
2	I	260	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	I	275	ARG
2	I	284	LEU
2	I	292	ILE
2	I	296	VAL
2	I	347	ILE
2	I	349	GLU
2	I	369	MET
2	I	378	ARG
2	I	384	LEU
2	I	394	ARG
2	I	404	LYS
2	I	409	LEU
2	I	415	GLU
2	I	442	VAL
2	I	471	VAL
2	I	486	THR
2	I	494	ASN
2	I	499	SER
2	I	508	SER
2	I	519	ASN
2	I	523	GLU
2	I	524	ILE
2	I	529	ARG
2	I	531	SER
2	I	582	ASN
2	I	592	ARG
2	I	595	THR
2	I	596	ASP
2	I	609	ILE
2	I	635	THR
2	I	642	SER
2	I	646	SER
2	I	671	LEU
2	I	672	GLU
2	I	738	GLU
2	I	741	MET
2	I	745	GLU
2	I	748	ILE
2	I	764	CYS
2	I	772	SER
2	I	779	ARG
2	I	783	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	I	785	ASP
2	I	788	SER
2	I	791	LEU
2	I	796	LEU
2	I	802	VAL
2	I	807	TRP
2	I	814	ASP
2	I	821	ARG
2	I	845	LEU
2	I	856	ASN
2	I	857	VAL
2	I	878	THR
2	I	893	THR
2	I	896	THR
2	I	912	ASP
2	I	913	VAL
2	I	916	SER
2	I	924	VAL
2	I	930	ASP
2	I	935	THR
2	I	944	ARG
2	I	971	LEU
2	I	976	ARG
2	I	990	ASP
2	I	1034	ARG
2	I	1037	THR
2	I	1082	ILE
2	I	1092	THR
2	I	1111	GLN
2	I	1117	LEU
2	I	1147	ARG
2	I	1157	GLN
2	I	1159	VAL
2	I	1161	LEU
2	I	1163	THR
2	I	1164	PHE
2	I	1206	THR
2	I	1216	ARG
2	I	1222	GLU
2	I	1238	LEU
2	I	1269	ARG
2	I	1292	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	I	1324	ASN
3	J	26	SER
3	J	28	ASP
3	J	32	SER
3	J	46	TYR
3	J	47	ARG
3	J	48	THR
3	J	65	VAL
3	J	85	CYS
3	J	86	GLU
3	J	93	THR
3	J	96	LYS
3	J	97	VAL
3	J	98	ARG
3	J	115	TRP
3	J	127	LEU
3	J	147	ILE
3	J	156	ARG
3	J	166	LEU
3	J	177	ASP
3	J	201	LEU
3	J	204	GLU
3	J	212	THR
3	J	227	PHE
3	J	240	THR
3	J	252	LEU
3	J	259	ARG
3	J	264	ASP
3	J	271	ARG
3	J	279	LEU
3	J	301	GLU
3	J	322	ARG
3	J	329	ASP
3	J	338	PHE
3	J	342	LEU
3	J	357	VAL
3	J	384	LYS
3	J	390	LEU
3	J	410	ASP
3	J	421	VAL
3	J	428	THR
3	J	429	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	J	430	HIS
3	J	464	ASP
3	J	468	VAL
3	J	505	ASP
3	J	515	ARG
3	J	526	VAL
3	J	527	LEU
3	J	543	SER
3	J	545	HIS
3	J	560	ASN
3	J	568	SER
3	J	572	THR
3	J	573	THR
3	J	674	THR
3	J	709	ARG
3	J	740	LEU
3	J	757	THR
3	J	783	LEU
3	J	803	VAL
3	J	812	ASP
3	J	831	VAL
3	J	838	ARG
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	850	LYS
3	J	853	THR
3	J	861	ASN
3	J	862	THR
3	J	874	GLU
3	J	883	ARG
3	J	892	PHE
3	J	895	CYS
3	J	905	ARG
3	J	907	HIS
3	J	974	VAL
3	J	976	THR
3	J	977	SER
3	J	982	LEU
3	J	1028	ILE
3	J	1038	THR
3	J	1058	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	J	1067	ARG
3	J	1101	LEU
3	J	1151	LYS
3	J	1159	ILE
3	J	1244	GLN
3	J	1248	ILE
3	J	1249	ASN
3	J	1255	VAL
3	J	1258	ARG
3	J	1261	LEU
3	J	1267	VAL
3	J	1280	VAL
3	J	1298	VAL
3	J	1307	LEU
3	J	1316	THR
3	J	1320	ILE
3	J	1333	THR
4	K	5	THR
4	K	30	MET
4	K	32	VAL
4	K	45	LYS
4	K	62	GLN
4	K	72	GLN
5	L	7	SER
5	L	23	THR
5	L	87	VAL
5	L	96	ASP
5	L	98	VAL
5	L	113	ARG
5	L	133	SER
5	L	160	ASP
5	L	161	LEU
5	L	163	THR
5	L	224	LEU
5	L	236	LYS
5	L	288	MET
5	L	314	THR
5	L	317	ASN
5	L	333	VAL
5	L	346	GLN
5	L	349	GLU
5	L	395	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	L	418	LYS
5	L	449	THR
5	L	476	ARG
5	L	479	THR
5	L	489	MET
5	L	508	GLU
5	L	514	ASP
5	L	516	ASP
5	L	538	GLU
5	L	539	SER
5	L	569	THR
5	L	593	LYS
5	L	599	ARG
5	L	610	PHE
5	L	612	ASP
1	M	262	LEU
1	M	280	ASP
1	M	285	THR
1	M	289	LEU
1	M	290	LEU
1	M	292	THR
1	M	300	LEU
1	M	306	VAL
6	N	15	LEU
6	N	37	CYS
6	N	58	CYS
6	N	59	VAL
6	N	60	GLU
6	N	71	HIS
6	N	72	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	18	GLN
2	I	387	ASN
2	I	437	ASN
2	I	447	HIS
2	I	513	GLN
2	I	582	ASN
2	I	618	GLN
2	I	658	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	I	799	ASN
2	I	1061	GLN
2	I	1080	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1175	ASN
2	I	1264	GLN
3	J	206	ASN
3	J	294	ASN
3	J	477	GLN
3	J	545	HIS
3	J	680	ASN
3	J	702	GLN
3	J	910	ASN
3	J	962	ASN
3	J	1010	GLN
3	J	1023	HIS
3	J	1126	GLN
3	J	1227	HIS
4	K	72	GLN
5	L	8	GLN
5	L	28	ASN
5	L	406	GLN
6	N	68	GLN
6	N	71	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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.



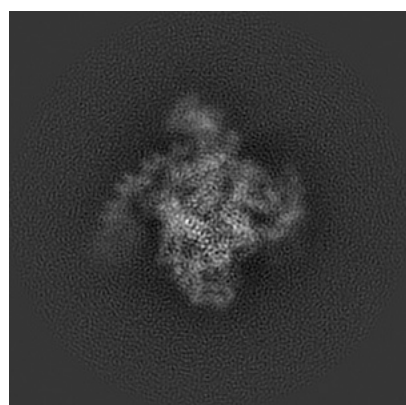
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20462. These allow visual inspection of the internal detail of the map and identification of artifacts.

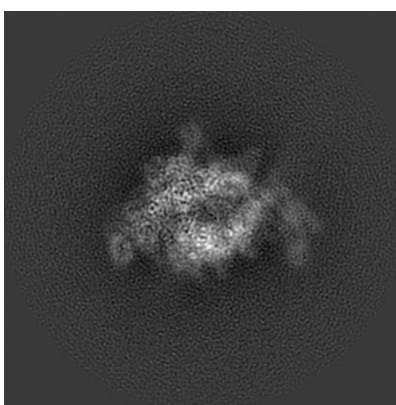
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

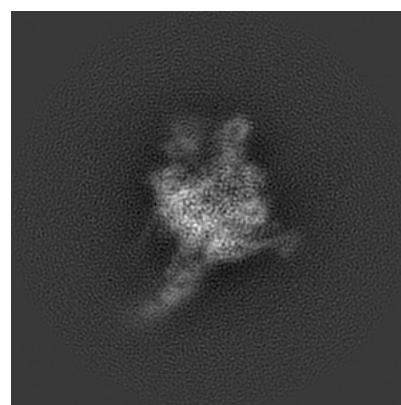
#### 6.1.1 Primary map



X



Y

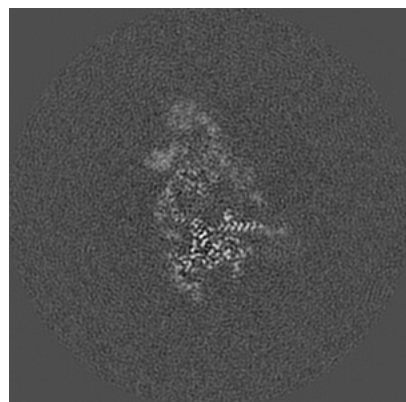


Z

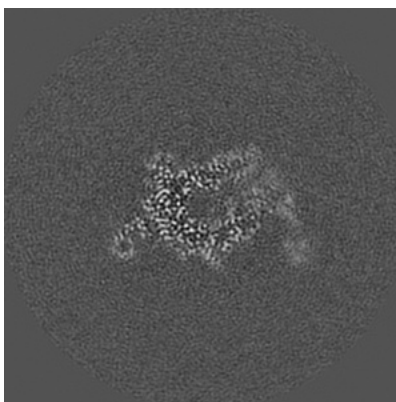
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

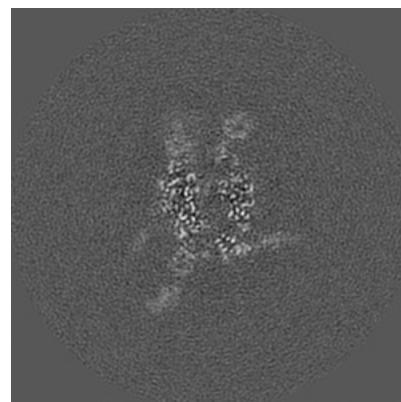
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



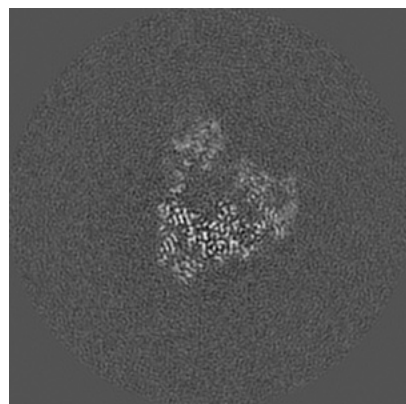
Z Index: 128



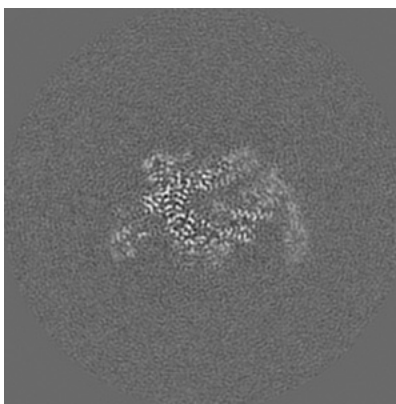
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

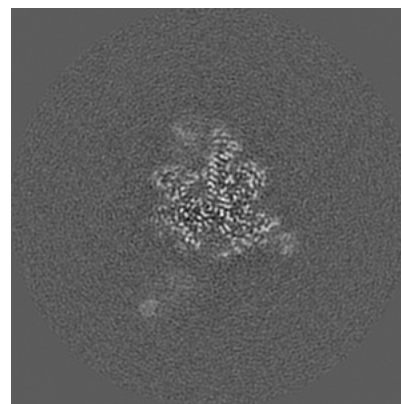
### 6.3.1 Primary map



X Index: 137



Y Index: 124

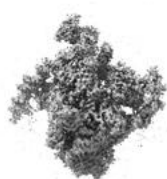


Z Index: 115

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

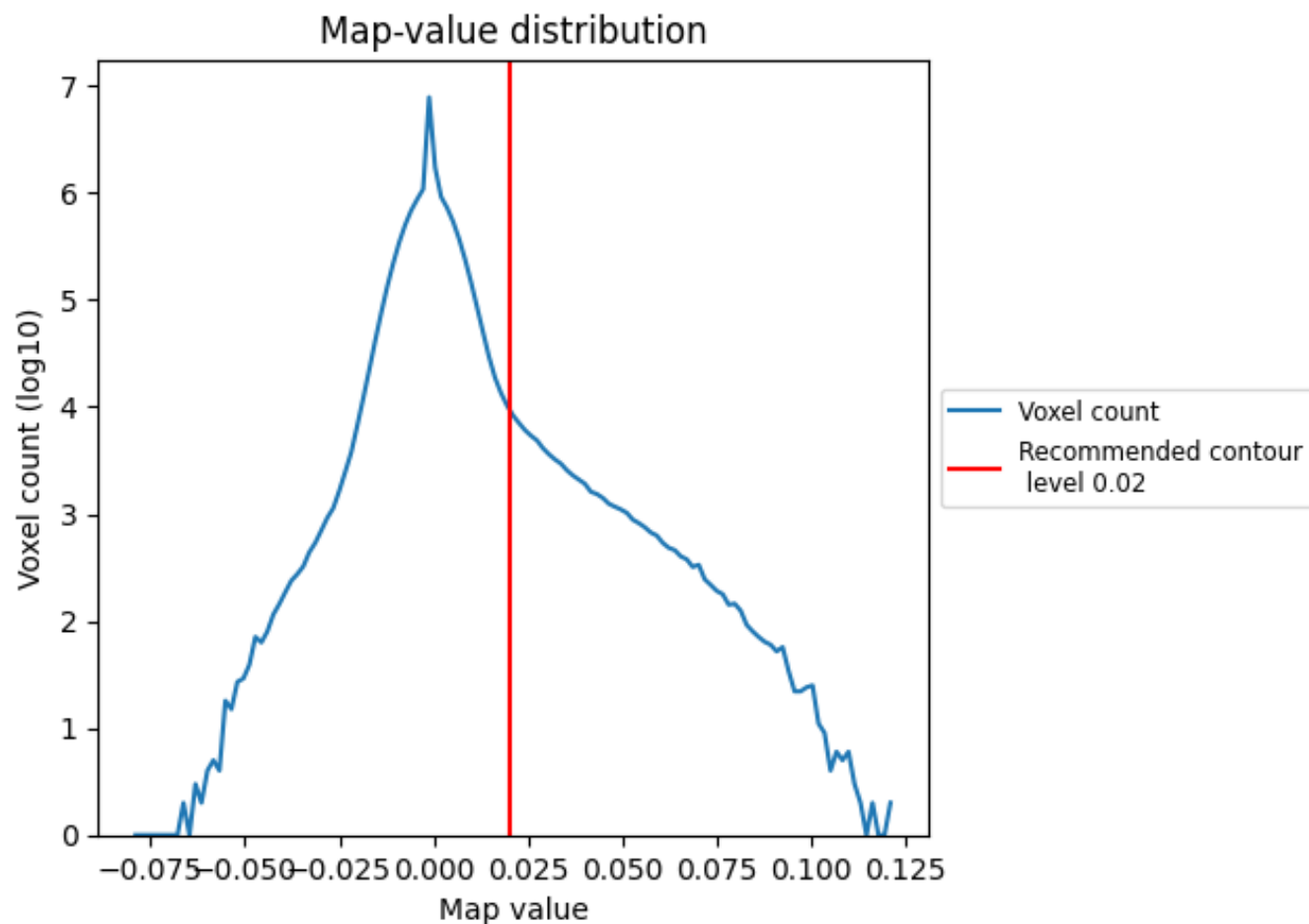
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

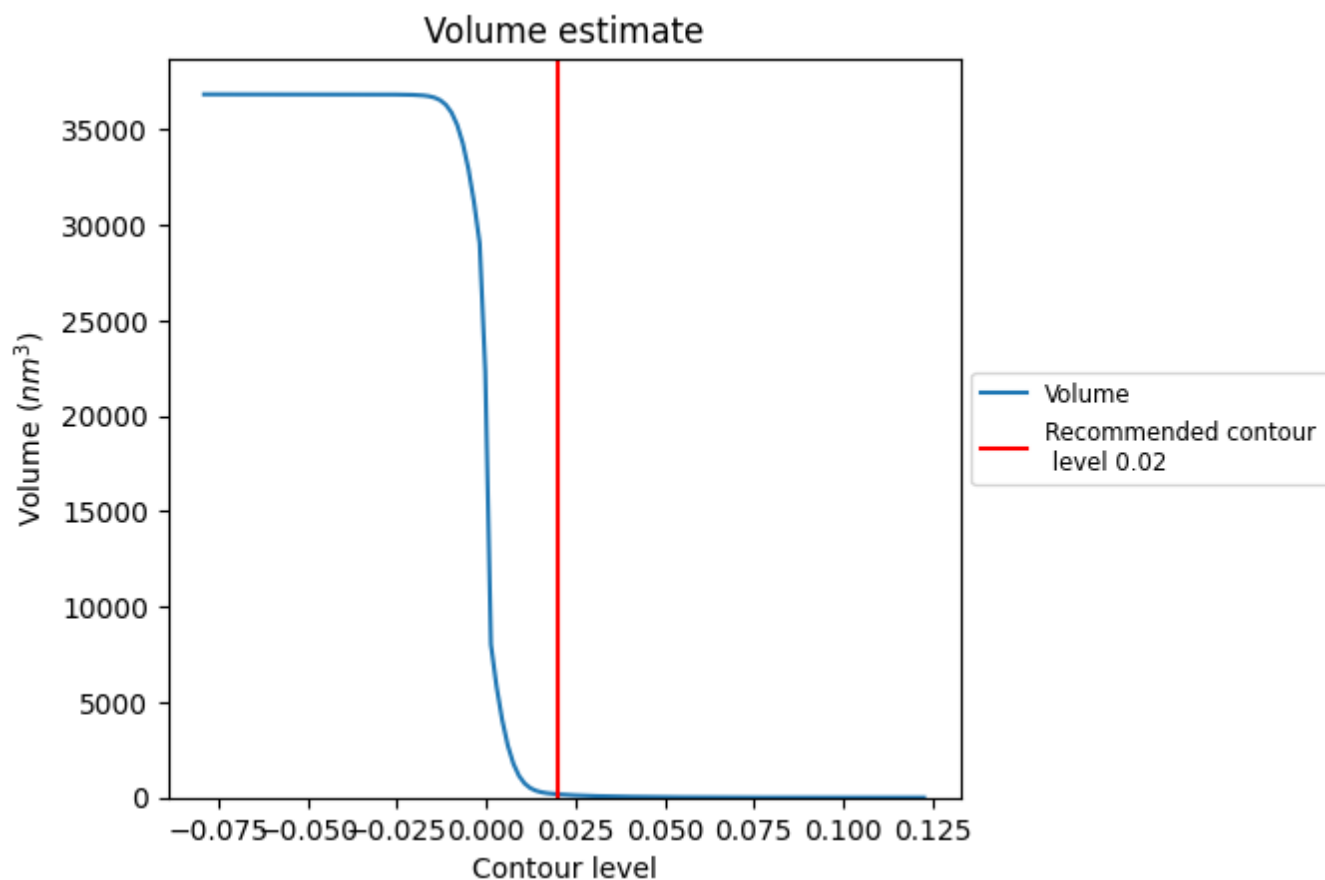
### 7.1 Map-value distribution [i](#)



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](#)

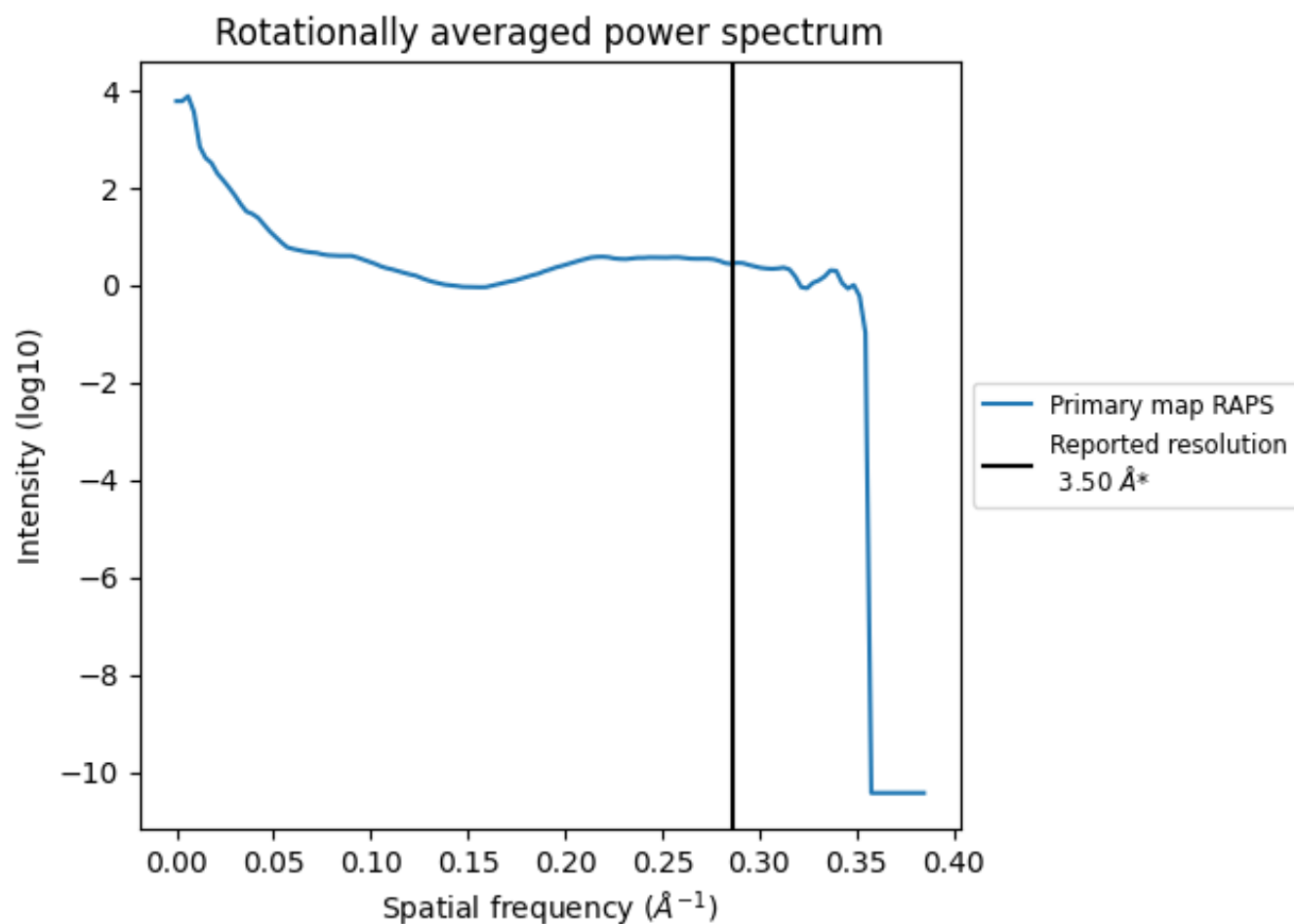


The volume at the recommended contour level is 173 nm<sup>3</sup>; this corresponds to an approximate mass of 156 kDa.

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 ⓘ



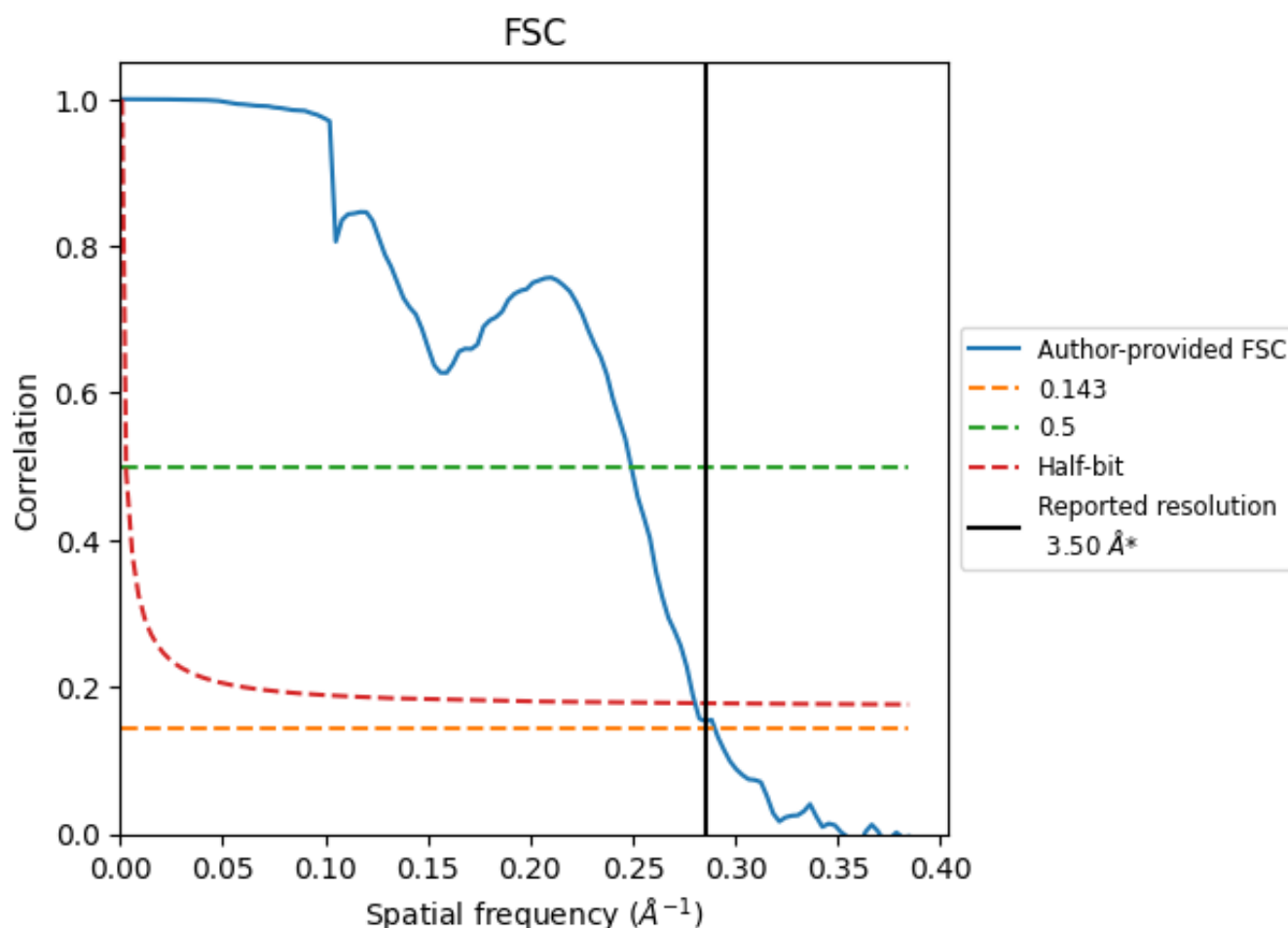
\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>



## 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 0.286 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	4.01	3.57
Unmasked-calculated*	-	-	-

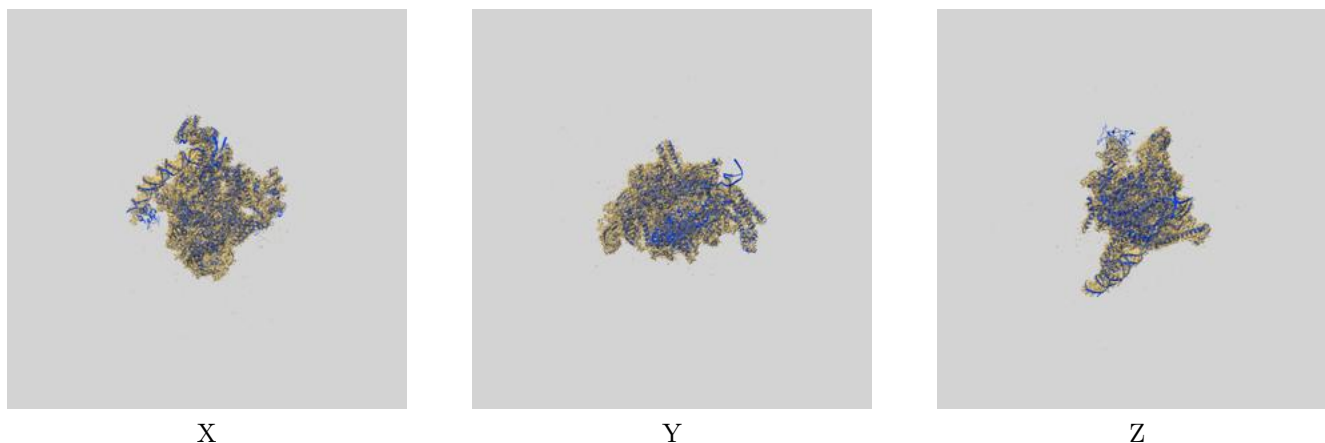
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20462 and PDB model 6PSS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

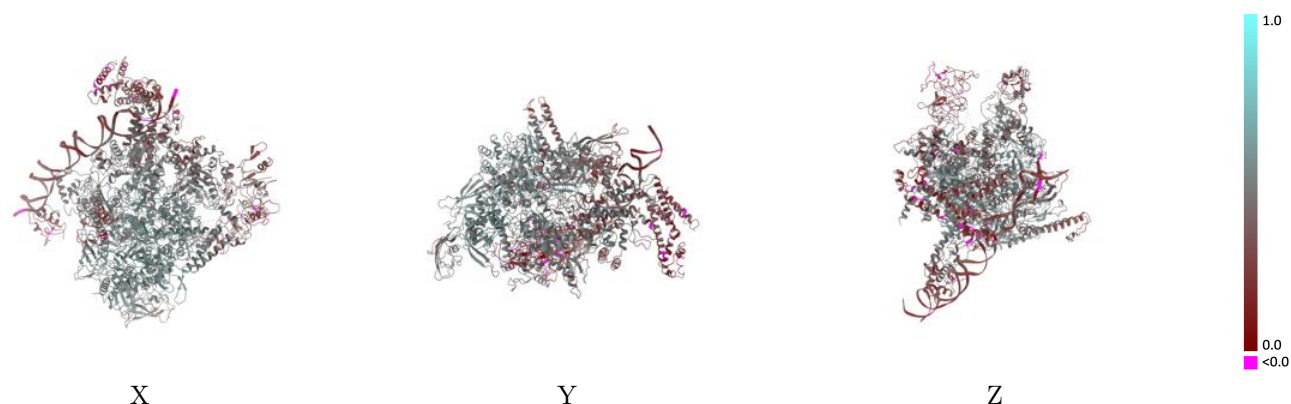
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

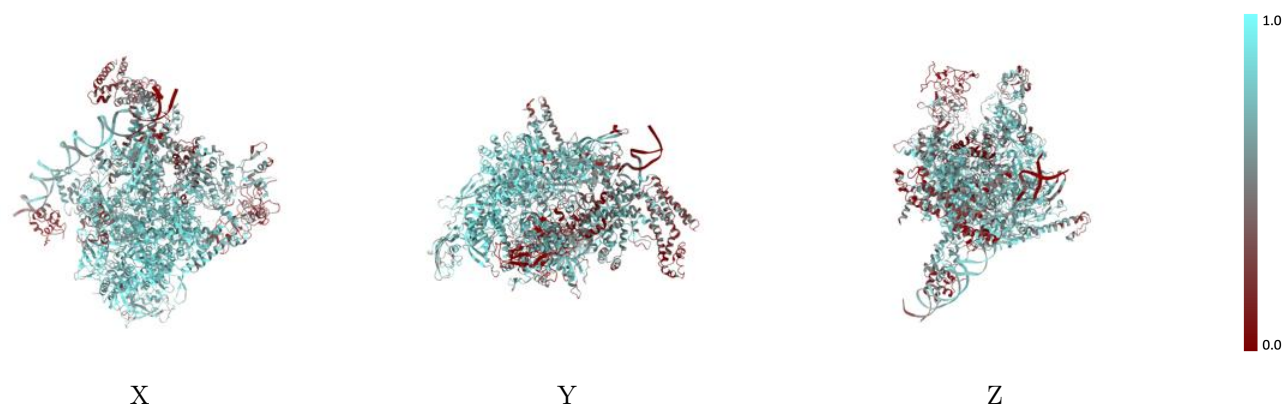


## 9.2 Q-score mapped to coordinate model [i](#)



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.

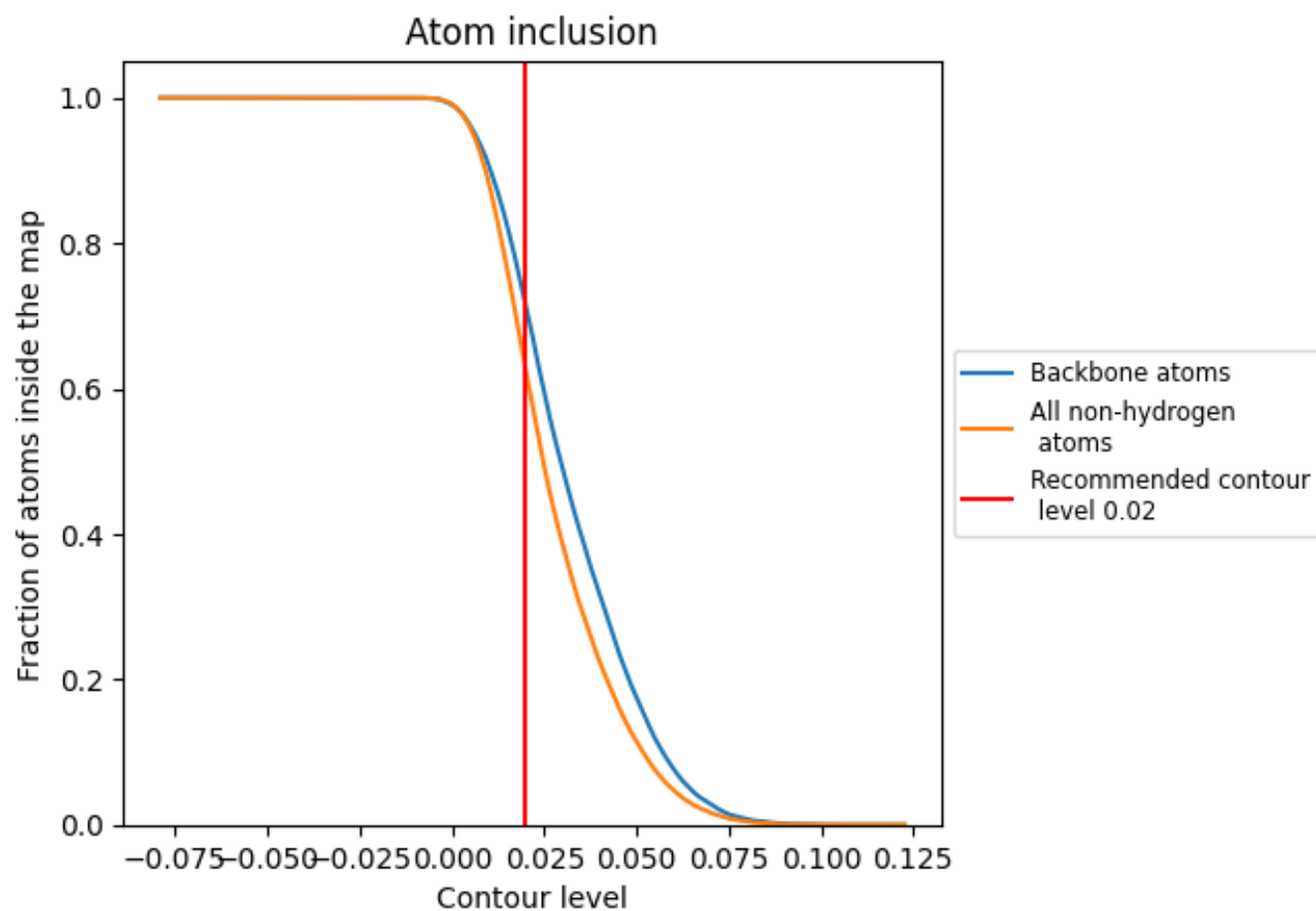
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6261	<div></div> 0.4460
G	<div></div> 0.7663	<div></div> 0.5190
H	<div></div> 0.7062	<div></div> 0.4790
I	<div></div> 0.7182	<div></div> 0.4930
J	<div></div> 0.6364	<div></div> 0.4620
K	<div></div> 0.5936	<div></div> 0.4850
L	<div></div> 0.4024	<div></div> 0.3450
M	<div></div> 0.0607	<div></div> 0.2650
N	<div></div> 0.7042	<div></div> 0.4730
O	<div></div> 0.5719	<div></div> 0.2720
P	<div></div> 0.5051	<div></div> 0.2640

1.0  
0.0  
<0.0