



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:18 AM UTC

PDB ID : 6WVJ / pdb_00006wvj
EMDB ID : EMD-21920
Title : Cryo-EM structure of Bacillus subtilis RNA Polymerase elongation complex
Authors : Newing, T.; Tolun, G.; Oakley, A.J.
Deposited on : 2020-05-06
Resolution : 3.36 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

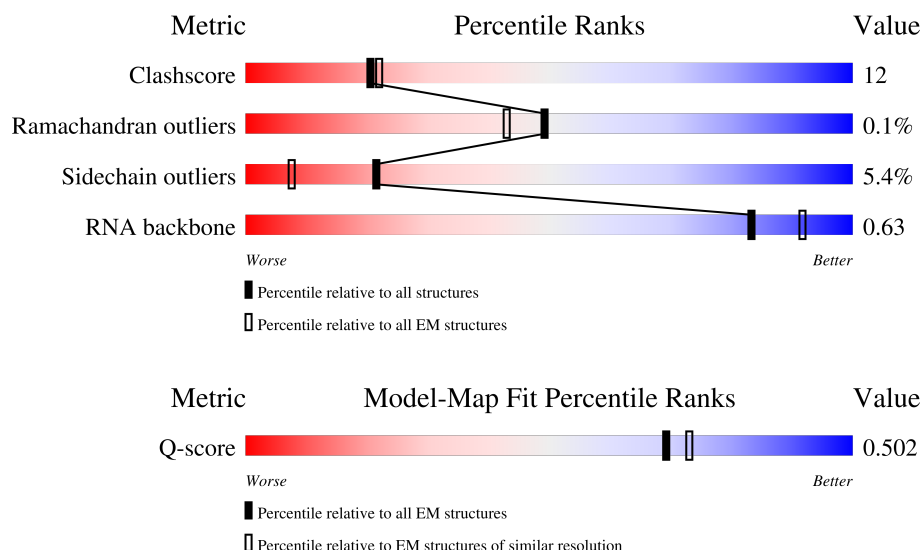
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	A	314	
1	B	314	
2	C	1193	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1199	
4	F	67	
5	T	19	
6	R	8	
7	N	10	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22367 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	A	224	Total	C	N	O	0	0
			1688	1068	288	332		
1	B	224	Total	C	N	O	0	0
			1663	1055	284	324		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1117	Total	C	N	O	S	0	0
			8688	5460	1515	1680	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1176	Total	C	N	O	S	0	0
			9085	5742	1602	1698	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	61	Total	C	N	O	S	0	0
			478	302	83	89	4		

- Molecule 5 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*GP*GP*GP*CP*GP*TP*CP*CP*GP*CP*GP*CP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	19	Total	C	N	O	P	0	0
			385	182	70	115	18		

- Molecule 6 is a RNA chain called RNA (5'-R(P*GP*GP*CP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	8	Total	C	N	O	P	0	0
			175	77	34	56	8		

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*CP*GP*CP*CP*CP*GP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	10	Total	C	N	O	P	0	0
			202	95	40	57	10		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

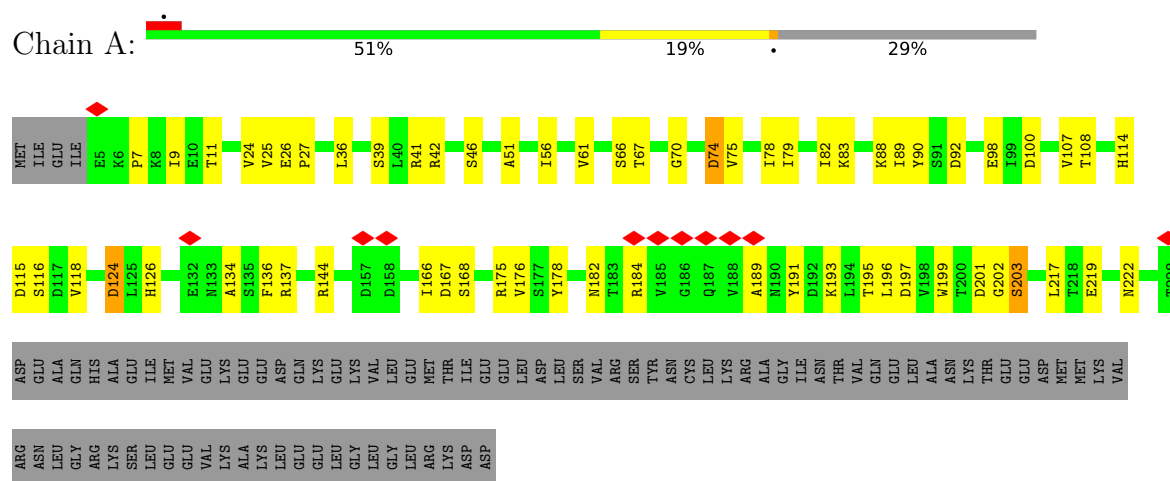
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

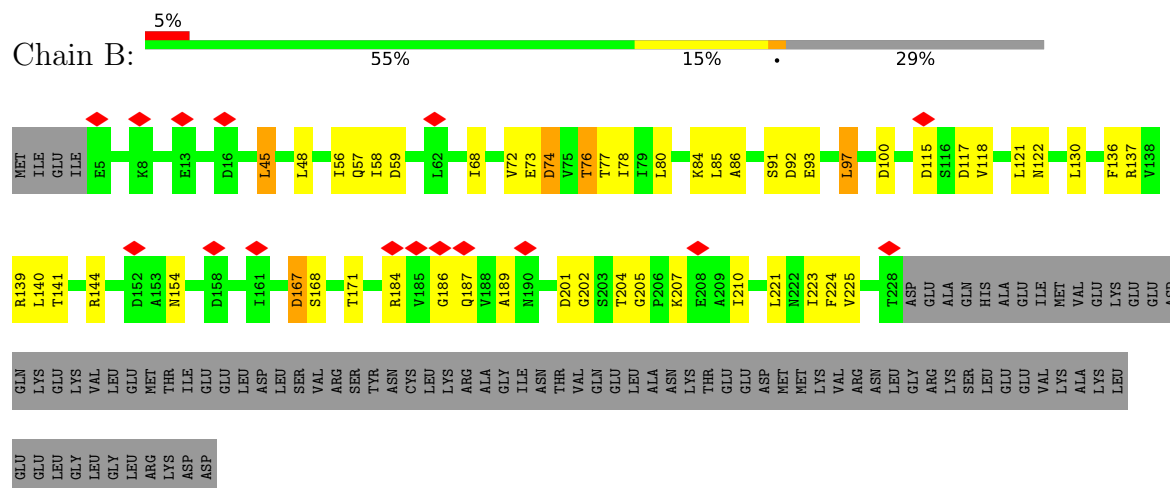
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

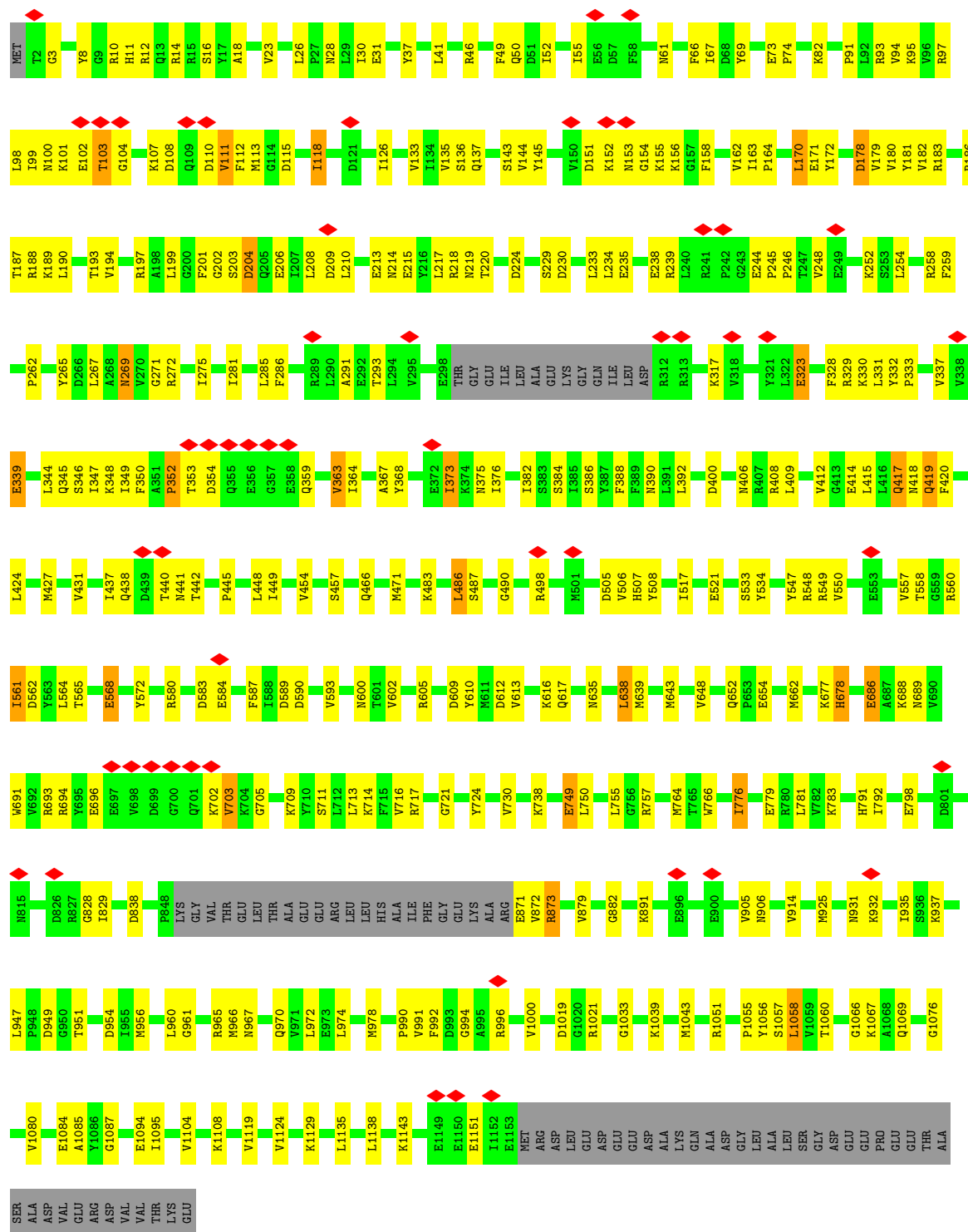


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



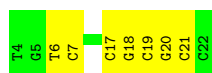


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 67% 29%



Chain T:  63% 37%



- Molecule 6: RNA (5'-R(P*GP*GP*CP*GP*CP*GP*CP*G)-3')

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: DNA (5'-D(P*AP*CP*GP*CP*CP*CP*GP*AP*CP*A)-3')

Chain N:  10% 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58854	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 ($e^-/\text{\AA}^2$)	52.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	59500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.356	Depositor
Minimum map value	-5.764	Depositor
Average map value	-0.026	Depositor
Map value standard deviation	0.774	Depositor
Recommended contour level	1.55	Depositor
Map size (Å)	157.92, 144.48, 139.44	wwPDB
Map dimensions	166, 172, 188	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84000003	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: 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	A	0.23	0/1714	0.42	0/2336
1	B	0.29	0/1688	0.55	0/2303
2	C	0.26	0/8843	0.51	1/11971 (0.0%)
3	D	0.21	0/9233	0.43	1/12488 (0.0%)
4	F	0.21	0/483	0.53	0/646
5	T	0.20	0/430	0.30	0/662
6	R	0.15	0/195	0.17	0/303
7	N	0.22	0/226	0.31	0/345
All	All	0.24	0/22812	0.47	2/31054 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	339	GLU	CA-C-O	6.67	121.81	117.94
3	D	1140	GLN	CB-CA-C	-6.31	109.31	116.63

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	A	1688	0	1693	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1663	0	1664	32	0
2	C	8688	0	8529	219	0
3	D	9085	0	9181	244	0
4	F	478	0	499	18	0
5	T	385	0	214	5	0
6	R	175	0	89	0	0
7	N	202	0	111	3	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	22367	0	21980	530	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 12.

All (530) 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)
3:D:1167:ILE:HD11	3:D:1169:LYS:HD3	1.66	0.78
3:D:596:LEU:HD21	3:D:605:VAL:HG11	1.67	0.77
2:C:183:ARG:HH12	2:C:186:ARG:HA	1.50	0.76
2:C:639:MET:HE1	2:C:932:LYS:HE2	1.69	0.74
3:D:103:HIS:HD2	3:D:105:TRP:H	1.35	0.73
2:C:438:GLN:HE22	2:C:441:ASN:HB2	1.54	0.72
3:D:989:GLN:HE22	3:D:1006:TYR:HA	1.54	0.72
1:A:184:ARG:HA	1:A:189:ALA:HA	1.72	0.70
1:A:70:GLY:HA3	1:A:134:ALA:HB2	1.73	0.70
1:A:88:LYS:NZ	1:A:203:SER:O	2.25	0.70
3:D:536:ARG:NH2	3:D:609:GLN:O	2.25	0.70
3:D:837:GLU:OE1	3:D:1056:ARG:NH2	2.25	0.69
2:C:400:ASP:O	2:C:406:ASN:ND2	2.24	0.69
3:D:759:ILE:HG22	3:D:761:LEU:H	1.56	0.69
3:D:1161:LEU:HD23	3:D:1171:VAL:HB	1.73	0.69
2:C:93:ARG:HG2	2:C:112:PHE:HA	1.74	0.68
2:C:702:LYS:NZ	2:C:703:VAL:O	2.25	0.68
2:C:143:SER:OG	2:C:144:VAL:N	2.27	0.68
3:D:264:ARG:HG3	3:D:287:MET:HE3	1.75	0.67
2:C:424:LEU:HA	2:C:427:MET:HG2	1.75	0.67
3:D:50:ARG:HA	3:D:80:VAL:HB	1.77	0.66
3:D:987:LYS:O	3:D:989:GLN:NE2	2.28	0.66
2:C:234:LEU:HD22	2:C:246:PRO:HB2	1.78	0.66
1:B:45:LEU:HD23	3:D:527:GLN:HG3	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:GLU:HA	2:C:217:LEU:HD23	1.79	0.65
2:C:151:ASP:OD1	2:C:155:LYS:N	2.30	0.65
3:D:1183:VAL:O	4:F:25:ARG:NH1	2.30	0.65
3:D:388:ARG:HH21	3:D:389:LYS:HG3	1.61	0.65
2:C:291:ALA:HB3	2:C:348:LYS:HG3	1.79	0.65
3:D:513:GLY:HA3	3:D:603:LYS:HG3	1.79	0.65
3:D:962:ALA:O	3:D:1032:LYS:NZ	2.30	0.65
4:F:7:ASP:OD1	4:F:7:ASP:N	2.30	0.64
2:C:419:GLN:O	2:C:457:SER:OG	2.15	0.64
2:C:931:ASN:ND2	2:C:970:GLN:OE1	2.31	0.64
1:A:92:ASP:HA	1:A:144:ARG:HD2	1.79	0.64
1:A:115:ASP:OD1	1:A:116:SER:N	2.31	0.64
3:D:968:GLN:HE21	3:D:1030:ASP:HB2	1.63	0.64
1:B:48:LEU:HB2	1:B:171:THR:HG23	1.80	0.63
3:D:373:GLU:HG3	3:D:404:VAL:HG22	1.80	0.63
1:B:84:LYS:HG2	3:D:517:LYS:HD2	1.79	0.63
1:A:175:ARG:NH2	2:C:949:ASP:O	2.31	0.62
3:D:9:TYR:HD1	3:D:1157:GLU:HG3	1.64	0.62
3:D:838:ARG:NH1	3:D:840:GLU:OE1	2.32	0.62
2:C:254:LEU:HD11	2:C:258:ARG:HH21	1.63	0.62
3:D:540:ALA:O	3:D:543:SER:OG	2.16	0.62
2:C:766:TRP:O	3:D:652:THR:OG1	2.12	0.62
3:D:988:GLN:HE22	3:D:1006:TYR:HD2	1.48	0.62
2:C:549:ARG:HE	2:C:560:ARG:HH12	1.47	0.62
3:D:935:THR:O	3:D:1058:GLN:NE2	2.33	0.62
1:A:51:ALA:HA	1:A:144:ARG:HA	1.81	0.62
3:D:1083:ALA:O	3:D:1086:THR:OG1	2.18	0.62
2:C:871:GLU:HG2	2:C:872:VAL:HG13	1.82	0.61
1:B:187:GLN:HE21	3:D:395:PRO:HB2	1.65	0.61
2:C:420:PHE:HE1	2:C:454:VAL:HG13	1.66	0.61
3:D:75:CYS:HB3	3:D:78:CYS:HB2	1.83	0.61
3:D:289:GLN:NE2	3:D:293:ASP:OD1	2.33	0.61
2:C:97:ARG:HG3	2:C:99:ILE:HD11	1.82	0.60
3:D:156:ARG:HA	3:D:156:ARG:NH1	2.15	0.60
2:C:91:PRO:HA	2:C:115:ASP:HA	1.83	0.60
3:D:553:GLN:NE2	3:D:592:ASP:OD1	2.34	0.60
2:C:197:ARG:NH2	2:C:202:GLY:O	2.35	0.59
4:F:28:ARG:O	4:F:32:ILE:HG13	2.03	0.59
3:D:207:ILE:HG13	3:D:208:LYS:HD3	1.84	0.59
3:D:697:ARG:NH2	3:D:760:GLU:OE1	2.36	0.59
4:F:26:ARG:NH2	4:F:29:GLU:OE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:VAL:HG22	2:C:162:VAL:HG22	1.84	0.59
3:D:395:PRO:HA	3:D:398:TRP:HD1	1.68	0.59
1:A:39:SER:OG	1:A:217:LEU:HD11	2.02	0.59
2:C:408:ARG:NH2	2:C:414:GLU:OE2	2.36	0.59
5:T:6:DT:H2"	5:T:7:DC:H5"	1.85	0.59
2:C:67:ILE:HB	2:C:95:LYS:HG3	1.85	0.58
2:C:925:MET:HG3	2:C:935:ILE:HD11	1.85	0.58
2:C:187:THR:HG22	2:C:188:ARG:H	1.68	0.58
3:D:627:ILE:HD12	3:D:639:MET:HE3	1.84	0.58
3:D:1185:PRO:HB2	4:F:58:LEU:HD11	1.84	0.58
2:C:1119:VAL:O	4:F:28:ARG:NH2	2.27	0.58
3:D:532:HIS:CD2	3:D:533:LEU:H	2.22	0.58
2:C:587:PHE:O	2:C:605:ARG:NH1	2.37	0.58
2:C:779:GLU:OE2	2:C:783:LYS:NZ	2.36	0.58
3:D:986:ASP:O	3:D:988:GLN:NE2	2.37	0.58
3:D:560:THR:OG1	3:D:561:THR:N	2.37	0.58
3:D:1079:ARG:HH22	3:D:1117:ARG:HH11	1.52	0.58
2:C:170:LEU:HD12	2:C:259:PHE:HE1	1.69	0.57
3:D:796:ASP:OD2	3:D:957:GLN:NE2	2.37	0.57
2:C:1057:SER:OG	2:C:1058:LEU:N	2.36	0.57
3:D:184:LEU:O	3:D:188:VAL:HG23	2.04	0.57
3:D:961:GLU:O	3:D:963:ARG:N	2.37	0.57
1:A:108:THR:HG22	1:A:126:HIS:HA	1.87	0.57
2:C:23:VAL:HG21	2:C:548:ARG:HD2	1.85	0.57
2:C:203:SER:N	2:C:206:GLU:OE2	2.36	0.57
3:D:936:MET:HE3	3:D:937:ARG:H	1.70	0.57
3:D:1158:LEU:HD13	3:D:1167:ILE:HD13	1.86	0.57
1:B:184:ARG:HA	1:B:189:ALA:HA	1.86	0.57
2:C:652:GLN:OE1	2:C:757:ARG:NH1	2.37	0.57
2:C:1051:ARG:NH2	2:C:1055:PRO:O	2.38	0.57
3:D:670:GLN:O	3:D:674:GLU:HG2	2.05	0.57
2:C:333:PRO:HG2	2:C:344:LEU:HB2	1.86	0.56
3:D:113:ARG:HD2	3:D:1151:ILE:HD12	1.87	0.56
3:D:667:ASP:OD1	3:D:667:ASP:N	2.38	0.56
3:D:1053:LYS:O	3:D:1057:MET:HG2	2.05	0.56
3:D:1077:LYS:NZ	3:D:1095:ASP:OD2	2.38	0.56
1:A:201:ASP:OD1	1:A:203:SER:N	2.34	0.56
2:C:419:GLN:OE1	2:C:457:SER:OG	2.18	0.56
2:C:639:MET:O	2:C:643:MET:HG2	2.06	0.56
3:D:482:PRO:HB3	3:D:908:ALA:HB2	1.88	0.56
1:B:154:ASN:HD21	1:B:168:SER:HB3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:379:LEU:HB3	3:D:389:LYS:HZ3	1.71	0.56
3:D:62:CYS:HB3	3:D:78:CYS:SG	2.45	0.56
3:D:204:THR:O	3:D:208:LYS:HG2	2.06	0.56
2:C:331:LEU:HD22	2:C:367:ALA:HB1	1.88	0.55
3:D:33:THR:HG23	3:D:259:ARG:HH12	1.70	0.55
2:C:61:ASN:O	2:C:100:ASN:ND2	2.39	0.55
2:C:204:ASP:OD1	2:C:204:ASP:N	2.40	0.55
3:D:464:GLU:O	3:D:468:GLU:HG3	2.06	0.55
3:D:298:ASN:OD1	3:D:299:GLY:N	2.40	0.55
3:D:464:GLU:HG3	4:F:24:ALA:HB1	1.89	0.55
3:D:693:THR:HG23	3:D:695:GLU:H	1.71	0.54
2:C:652:GLN:O	2:C:757:ARG:NH1	2.40	0.54
2:C:1080:VAL:O	2:C:1084:GLU:HG3	2.07	0.54
3:D:570:ILE:O	3:D:642:ARG:NH2	2.40	0.54
3:D:700:ARG:O	3:D:704:ILE:HG13	2.07	0.54
2:C:1060:THR:HG21	3:D:330:ASN:ND2	2.23	0.54
3:D:145:GLU:HB3	3:D:148:GLN:HB2	1.88	0.54
3:D:948:ASP:OD2	3:D:1007:ASN:ND2	2.41	0.54
2:C:26:LEU:HD23	2:C:534:TYR:CE2	2.42	0.54
3:D:870:GLU:O	3:D:874:LEU:HG	2.08	0.54
2:C:271:GLY:O	2:C:275:ILE:HG13	2.08	0.54
2:C:693:ARG:NH2	2:C:705:GLY:O	2.40	0.54
1:B:91:SER:O	1:B:144:ARG:NH2	2.28	0.54
2:C:285:LEU:HD11	2:C:347:ILE:HG13	1.91	0.53
3:D:872:LYS:HA	3:D:875:GLU:HG2	1.90	0.53
3:D:1029:ILE:HG21	3:D:1034:LEU:HD22	1.90	0.53
1:A:7:PRO:HB2	1:B:223:ILE:HG12	1.89	0.53
3:D:110:ILE:HB	3:D:111:PRO:HD3	1.89	0.53
3:D:305:VAL:HG12	3:D:313:LEU:HD12	1.91	0.53
3:D:1039:ASP:OD2	3:D:1040:LEU:N	2.41	0.53
3:D:1064:ASP:O	3:D:1068:GLU:HG3	2.08	0.53
1:B:204:THR:OG1	1:B:205:GLY:N	2.40	0.53
3:D:1052:GLN:OE1	3:D:1056:ARG:NH1	2.42	0.53
2:C:654:GLU:HG2	2:C:757:ARG:HD2	1.89	0.53
2:C:966:MET:HG2	3:D:744:LEU:HD11	1.89	0.53
2:C:332:TYR:HB2	2:C:333:PRO:HD3	1.91	0.53
3:D:169:SER:OG	3:D:170:MET:N	2.41	0.53
2:C:776:ILE:HG22	2:C:937:LYS:HB3	1.89	0.52
2:C:210:LEU:HD11	2:C:382:ILE:HG21	1.91	0.52
2:C:691:TRP:NE1	2:C:709:LYS:HG3	2.24	0.52
3:D:60:CYS:HB3	3:D:65:TYR:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:HB3	1:A:196:LEU:HD12	1.91	0.52
3:D:1055:TYR:HB3	3:D:1060:VAL:HG23	1.92	0.52
3:D:1064:ASP:OD2	3:D:1064:ASP:N	2.36	0.52
2:C:590:ASP:OD1	2:C:605:ARG:NE	2.41	0.52
2:C:61:ASN:ND2	2:C:102:GLU:OE2	2.43	0.52
2:C:713:LEU:HD23	2:C:716:VAL:HG21	1.91	0.52
3:D:889:ALA:O	3:D:1072:ARG:HD2	2.10	0.52
3:D:1097:HIS:O	3:D:1101:GLU:HG2	2.10	0.52
3:D:35:ASN:O	3:D:37:ARG:N	2.42	0.52
1:A:24:VAL:HG22	1:A:195:THR:HG23	1.90	0.51
2:C:10:ARG:HG3	2:C:11:HIS:ND1	2.25	0.51
3:D:9:TYR:CD1	3:D:1157:GLU:HG3	2.44	0.51
2:C:93:ARG:HD2	2:C:110:ASP:OD2	2.10	0.51
3:D:1178:MET:O	3:D:1182:LYS:HG2	2.11	0.51
3:D:52:PHE:CD1	3:D:236:PRO:HD3	2.44	0.51
3:D:118:LEU:O	3:D:120:MET:N	2.43	0.51
2:C:466:GLN:OE1	2:C:490:GLY:HA2	2.11	0.51
1:A:27:PRO:HB2	1:A:191:TYR:CD2	2.46	0.51
1:B:221:LEU:O	1:B:225:VAL:HG23	2.10	0.51
3:D:253:ASP:OD2	3:D:314:LYS:N	2.36	0.51
3:D:748:ARG:HD3	3:D:771:LEU:HD21	1.92	0.51
2:C:330:LYS:HB3	2:C:332:TYR:CE1	2.46	0.51
3:D:396:GLU:H	3:D:396:GLU:CD	2.19	0.51
2:C:328:PHE:HD2	2:C:330:LYS:HE2	1.74	0.51
2:C:217:LEU:HA	2:C:220:THR:HG22	1.93	0.51
2:C:431:VAL:HG13	2:C:448:LEU:HD13	1.92	0.51
3:D:820:THR:HG22	3:D:822:ARG:H	1.75	0.50
2:C:181:TYR:CG	2:C:189:LYS:HE3	2.46	0.50
2:C:215:GLU:O	2:C:217:LEU:N	2.37	0.50
2:C:215:GLU:C	2:C:217:LEU:H	2.19	0.50
3:D:1038:THR:HG22	3:D:1039:ASP:H	1.77	0.50
2:C:145:TYR:CD2	2:C:163:ILE:HD12	2.47	0.50
2:C:717:ARG:HH11	2:C:721:GLY:HA2	1.77	0.50
2:C:420:PHE:CE1	2:C:454:VAL:HG13	2.46	0.50
3:D:395:PRO:HA	3:D:398:TRP:CD1	2.47	0.50
3:D:722:GLU:HG3	3:D:723:LEU:HD22	1.94	0.50
2:C:95:LYS:NZ	2:C:107:LYS:HD2	2.26	0.50
3:D:379:LEU:HB3	3:D:389:LYS:NZ	2.26	0.50
3:D:669:LYS:NZ	3:D:764:LYS:O	2.33	0.50
2:C:323:GLU:N	2:C:323:GLU:OE1	2.45	0.49
3:D:415:ALA:HB3	3:D:416:PRO:HD3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:851:GLN:HG2	3:D:864:GLU:H	1.76	0.49
1:A:88:LYS:HD3	1:A:90:TYR:CE1	2.47	0.49
2:C:689:ASN:HD22	2:C:711:SER:HA	1.76	0.49
7:N:6:DC:H2'	7:N:7:DC:C6	2.46	0.49
1:B:86:ALA:H	1:B:122:ASN:ND2	2.10	0.49
2:C:93:ARG:NH1	2:C:93:ARG:HB2	2.28	0.49
1:B:115:ASP:OD1	1:B:115:ASP:N	2.42	0.49
2:C:94:VAL:HG21	2:C:113:MET:HE2	1.94	0.49
3:D:903:TYR:HD1	3:D:913:VAL:HG11	1.78	0.49
3:D:1107:LEU:HA	3:D:1113:PRO:HD3	1.95	0.49
3:D:64:LYS:HB2	3:D:77:ARG:NH2	2.27	0.49
3:D:123:ARG:HA	3:D:126:GLU:OE2	2.13	0.49
3:D:705:TRP:CE2	3:D:762:PRO:HG3	2.48	0.49
3:D:974:ILE:HD13	3:D:1000:ARG:NH2	2.28	0.49
1:B:73:GLU:HB3	1:B:77:THR:HB	1.94	0.48
2:C:871:GLU:O	2:C:873:ARG:NH2	2.45	0.48
2:C:201:PHE:HB3	2:C:206:GLU:HG3	1.95	0.48
2:C:37:TYR:HE2	2:C:118:ILE:HD12	1.78	0.48
3:D:737:ASN:N	3:D:737:ASN:OD1	2.45	0.48
3:D:1185:PRO:HB3	4:F:22:VAL:HG13	1.95	0.48
1:A:74:ASP:OD2	1:A:74:ASP:N	2.45	0.48
3:D:190:MET:O	3:D:193:GLU:HG3	2.14	0.48
2:C:41:LEU:O	2:C:69:TYR:OH	2.31	0.48
2:C:291:ALA:HA	2:C:350:PHE:CZ	2.48	0.48
2:C:688:LYS:O	2:C:689:ASN:ND2	2.46	0.48
3:D:67:ARG:HB2	3:D:70:TYR:HE2	1.79	0.48
3:D:373:GLU:HA	3:D:376:GLU:HG2	1.95	0.48
3:D:639:MET:HE2	3:D:643:MET:HE3	1.95	0.48
3:D:895:PRO:HB3	3:D:1097:HIS:CD2	2.49	0.48
2:C:108:ASP:HB2	2:C:445:PRO:HD2	1.94	0.48
3:D:965:PRO:HG2	3:D:968:GLN:HG2	1.96	0.48
2:C:978:MET:HB2	2:C:1033:GLY:HA2	1.95	0.48
3:D:241:MET:HB3	3:D:251:THR:HG22	1.95	0.48
3:D:707:ALA:HA	3:D:710:ASP:OD2	2.12	0.48
2:C:281:ILE:O	2:C:285:LEU:HG	2.13	0.48
2:C:1056:TYR:OH	3:D:337:ASP:OD1	2.22	0.48
2:C:1066:GLY:N	2:C:1069:GLN:OE1	2.39	0.48
3:D:634:THR:O	3:D:638:LYS:HG3	2.14	0.48
3:D:918:ALA:O	3:D:922:ILE:HG12	2.14	0.48
2:C:95:LYS:HZ1	2:C:107:LYS:HD2	1.78	0.47
1:A:124:ASP:OD1	1:A:124:ASP:N	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:VAL:HG23	2:C:111:VAL:HG13	1.96	0.47
2:C:136:SER:OG	2:C:137:GLN:N	2.47	0.47
3:D:359:LYS:HB2	3:D:398:TRP:HZ3	1.80	0.47
3:D:837:GLU:HG2	3:D:842:ARG:HG2	1.97	0.47
2:C:172:TYR:HB2	2:C:388:PHE:CE2	2.49	0.47
2:C:549:ARG:NE	2:C:560:ARG:HH12	2.12	0.47
2:C:10:ARG:HE	2:C:11:HIS:CE1	2.32	0.47
2:C:550:VAL:HG22	2:C:557:VAL:HG22	1.96	0.47
2:C:1104:VAL:HG22	2:C:1108:LYS:HD3	1.97	0.47
3:D:185:VAL:HG12	3:D:217:ARG:HD2	1.96	0.47
3:D:359:LYS:HB2	3:D:398:TRP:CZ3	2.49	0.47
1:B:137:ARG:CZ	1:B:137:ARG:HB3	2.45	0.47
3:D:971:ILE:HD11	3:D:1033:GLU:HG2	1.97	0.47
2:C:46:ARG:O	2:C:50:GLN:HG2	2.15	0.47
1:B:74:ASP:O	1:B:78:ILE:HG12	2.15	0.47
3:D:200:GLY:O	3:D:204:THR:HG23	2.15	0.47
3:D:389:LYS:HG2	3:D:394:GLN:OE1	2.14	0.47
3:D:1161:LEU:O	3:D:1165:VAL:HG23	2.15	0.47
3:D:875:GLU:HA	3:D:878:GLU:HG3	1.97	0.46
3:D:965:PRO:HB2	3:D:1028:SER:HB2	1.96	0.46
2:C:235:GLU:HA	2:C:238:GLU:HG2	1.97	0.46
2:C:561:ILE:HG13	2:C:561:ILE:O	2.15	0.46
2:C:635:ASN:O	2:C:639:MET:HG3	2.15	0.46
2:C:8:TYR:HE1	2:C:14:ARG:HB2	1.81	0.46
3:D:367:LYS:O	3:D:371:MET:HG2	2.15	0.46
3:D:1040:LEU:O	3:D:1044:GLN:HG2	2.15	0.46
3:D:1186:VAL:HG22	4:F:59:LEU:H	1.79	0.46
1:B:91:SER:OG	1:B:92:ASP:N	2.46	0.46
1:B:201:ASP:OD1	1:B:202:GLY:N	2.48	0.46
2:C:12:ARG:HH21	2:C:12:ARG:HG3	1.80	0.46
2:C:328:PHE:C	2:C:329:ARG:HE	2.23	0.46
3:D:111:PRO:HG2	3:D:113:ARG:HH12	1.80	0.46
3:D:979:VAL:HG23	3:D:994:GLN:NE2	2.30	0.46
3:D:1164:ASN:HD22	3:D:1169:LYS:HE3	1.80	0.46
2:C:61:ASN:OD1	2:C:101:LYS:N	2.49	0.46
2:C:498:ARG:HG2	7:N:3:DA:H5'	1.98	0.46
3:D:618:GLY:O	3:D:622:LYS:HG3	2.15	0.46
3:D:1134:LEU:HD23	3:D:1134:LEU:HA	1.80	0.46
4:F:1:MET:HG2	4:F:3:ASP:H	1.80	0.46
5:T:20:DG:H2'	5:T:21:DC:C6	2.50	0.46
2:C:213:GLU:OE1	2:C:218:ARG:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:GLU:CD	2:C:245:PRO:HD2	2.40	0.46
2:C:1067:LYS:HB2	2:C:1067:LYS:HE2	1.70	0.46
3:D:78:CYS:HB3	3:D:80:VAL:HG12	1.98	0.46
2:C:346:SER:O	2:C:347:ILE:HD13	2.16	0.46
2:C:272:ARG:HD3	2:C:373:ILE:HD11	1.96	0.46
2:C:792:ILE:HG12	2:C:914:VAL:HG23	1.98	0.46
2:C:960:LEU:HD13	3:D:729:MET:SD	2.56	0.46
3:D:145:GLU:HG2	3:D:146:LYS:N	2.31	0.46
3:D:735:ARG:HG3	3:D:735:ARG:HH11	1.81	0.46
3:D:1000:ARG:HG2	3:D:1001:SER:H	1.81	0.46
4:F:16:LYS:HA	4:F:19:LEU:HB2	1.97	0.46
3:D:439:HIS:ND1	3:D:440:PRO:HD2	2.31	0.46
1:B:57:GLN:HB3	1:B:139:ARG:HG3	1.97	0.45
1:B:100:ASP:HA	1:B:136:PHE:O	2.16	0.45
3:D:979:VAL:HG23	3:D:994:GLN:HE22	1.81	0.45
2:C:193:THR:HG21	2:C:224:ASP:HB2	1.97	0.45
2:C:409:LEU:HD21	2:C:486:LEU:HD22	1.99	0.45
3:D:1101:GLU:O	3:D:1105:LYS:HG2	2.15	0.45
2:C:11:HIS:HB3	2:C:750:LEU:HD13	1.98	0.45
2:C:190:LEU:HD12	2:C:194:VAL:HG11	1.98	0.45
2:C:262:PRO:HG3	2:C:375:ASN:ND2	2.31	0.45
3:D:822:ARG:HG3	3:D:822:ARG:HH11	1.81	0.45
2:C:269:ASN:OD1	2:C:269:ASN:N	2.41	0.45
2:C:691:TRP:CZ2	2:C:709:LYS:HE2	2.52	0.45
3:D:838:ARG:N	3:D:841:GLU:OE2	2.42	0.45
2:C:28:ASN:HB3	2:C:31:GLU:HB3	1.98	0.45
3:D:204:THR:OG1	3:D:205:ARG:N	2.49	0.45
3:D:604:ALA:O	3:D:608:GLN:HG2	2.16	0.45
1:B:74:ASP:OD2	1:B:74:ASP:N	2.49	0.45
2:C:208:LEU:HB2	2:C:213:GLU:HG3	1.99	0.45
2:C:764:MET:HE3	2:C:956:MET:HE3	1.99	0.45
3:D:814:ARG:NH1	3:D:896:HIS:O	2.49	0.45
1:B:207:LYS:HE3	1:B:207:LYS:HB2	1.80	0.45
3:D:686:GLN:NE2	3:D:691:LEU:HD12	2.32	0.45
3:D:983:GLU:OE2	3:D:985:ARG:NH1	2.50	0.45
2:C:103:THR:HG22	2:C:104:GLY:H	1.82	0.45
2:C:209:ASP:OD1	2:C:209:ASP:N	2.50	0.45
3:D:190:MET:HE3	3:D:194:GLU:HB2	1.98	0.45
3:D:1030:ASP:HB3	3:D:1033:GLU:HB3	1.98	0.45
3:D:1155:ARG:NH1	3:D:1157:GLU:OE2	2.50	0.45
1:B:59:ASP:OD2	1:B:59:ASP:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ALA:HB2	2:C:990:PRO:HG2	1.99	0.45
2:C:113:MET:HG3	2:C:454:VAL:HG11	1.99	0.45
3:D:934:LEU:HA	3:D:1058:GLN:HG2	1.99	0.45
1:A:98:GLU:OE2	1:A:137:ARG:NH2	2.50	0.44
2:C:891:LYS:HB3	2:C:891:LYS:HE3	1.74	0.44
3:D:70:TYR:HB3	3:D:73:VAL:HG12	1.97	0.44
1:B:76:THR:O	1:B:80:LEU:HD23	2.18	0.44
2:C:179:VAL:HG13	2:C:181:TYR:CE1	2.52	0.44
2:C:197:ARG:HA	2:C:201:PHE:O	2.18	0.44
3:D:752:ALA:HA	3:D:758:ILE:HA	1.99	0.44
4:F:3:ASP:OD2	4:F:42:ILE:HD12	2.18	0.44
1:A:75:VAL:O	1:A:79:ILE:HG12	2.17	0.44
2:C:137:GLN:HA	2:C:487:SER:O	2.17	0.44
2:C:991:VAL:HG13	2:C:992:PHE:HD1	1.83	0.44
1:A:175:ARG:HG3	1:A:199:TRP:CE3	2.53	0.44
2:C:199:LEU:H	2:C:233:LEU:HD21	1.81	0.44
3:D:252:SER:OG	3:D:255:ASN:OD1	2.29	0.44
3:D:509:ALA:HB3	3:D:535:THR:HB	1.99	0.44
7:N:9:DG:H2'	7:N:10:DA:C8	2.52	0.44
1:A:9:ILE:HB	1:A:25:VAL:HG22	1.98	0.44
2:C:961:GLY:O	2:C:965:ARG:HD2	2.17	0.44
2:C:1138:LEU:HD13	3:D:105:TRP:CH2	2.53	0.44
3:D:1078:VAL:HG23	3:D:1117:ARG:C	2.42	0.44
1:A:193:LYS:HB3	1:A:193:LYS:HE3	1.82	0.44
2:C:133:VAL:HG23	2:C:471:MET:HB3	1.99	0.44
2:C:293:THR:HA	2:C:317:LYS:H	1.81	0.44
3:D:12:ILE:HG23	3:D:1150:ALA:HA	1.99	0.44
3:D:1157:GLU:O	3:D:1159:LEU:N	2.48	0.44
5:T:20:DG:H2'	5:T:21:DC:H6	1.83	0.44
1:A:201:ASP:OD1	1:A:202:GLY:N	2.51	0.44
2:C:593:VAL:HA	2:C:602:VAL:HA	1.99	0.44
2:C:612:ASP:OD1	2:C:613:VAL:N	2.47	0.44
3:D:693:THR:HG22	3:D:696:GLU:OE1	2.17	0.44
3:D:959:LEU:HD11	3:D:1050:GLU:HB3	2.00	0.44
4:F:18:THR:O	4:F:22:VAL:HG23	2.17	0.44
1:B:56:ILE:HD12	1:B:58:ILE:HG13	2.00	0.44
2:C:994:GLY:H	2:C:996:ARG:NH1	2.16	0.44
3:D:162:TYR:HB2	3:D:166:PHE:HE2	1.82	0.44
3:D:803:ARG:NH1	3:D:961:GLU:OE1	2.48	0.44
5:T:17:DC:H2'	5:T:18:DG:H8	1.82	0.44
5:T:19:DC:H2'	5:T:20:DG:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:PRO:C	2:C:353:THR:HG1	2.23	0.43
2:C:583:ASP:OD1	2:C:584:GLU:N	2.50	0.43
2:C:716:VAL:HG23	2:C:724:TYR:HB3	2.00	0.43
3:D:156:ARG:HA	3:D:156:ARG:HH11	1.81	0.43
3:D:897:GLY:O	3:D:1072:ARG:NH2	2.51	0.43
3:D:1020:ARG:NH1	3:D:1037:VAL:O	2.50	0.43
1:A:36:LEU:HD13	1:B:224:PHE:HE2	1.81	0.43
2:C:3:GLY:HA3	2:C:16:SER:O	2.18	0.43
2:C:333:PRO:HD2	2:C:345:GLN:H	1.83	0.43
2:C:572:TYR:HB3	2:C:609:ASP:HB2	1.99	0.43
2:C:871:GLU:N	2:C:871:GLU:OE1	2.51	0.43
3:D:84:ARG:HD2	3:D:86:LYS:HG2	1.99	0.43
1:A:83:LYS:HG3	1:A:166:ILE:HD12	2.00	0.43
1:B:59:ASP:HB3	1:B:137:ARG:HB2	1.99	0.43
2:C:30:ILE:HG21	2:C:483:LYS:HE3	2.01	0.43
2:C:337:VAL:HG23	2:C:339:GLU:H	1.82	0.43
2:C:643:MET:HE1	2:C:932:LYS:HG2	2.00	0.43
2:C:996:ARG:O	2:C:1000:VAL:HG12	2.19	0.43
3:D:825:LEU:HA	3:D:825:LEU:HD12	1.86	0.43
3:D:901:ARG:HG3	3:D:901:ARG:HH11	1.83	0.43
1:A:67:THR:HG21	2:C:714:LYS:HE2	2.01	0.43
1:B:97:LEU:HD12	1:B:140:LEU:HD12	2.01	0.43
2:C:164:PRO:HB3	2:C:265:TYR:CZ	2.53	0.43
2:C:580:ARG:HA	2:C:580:ARG:HD3	1.65	0.43
3:D:687:PHE:CD2	3:D:697:ARG:HD3	2.52	0.43
3:D:253:ASP:OD1	3:D:253:ASP:N	2.50	0.43
3:D:462:SER:O	3:D:466:GLN:HG3	2.18	0.43
3:D:983:GLU:OE2	3:D:985:ARG:HG3	2.19	0.43
1:A:136:PHE:HD1	1:A:136:PHE:HA	1.74	0.43
1:A:26:GLU:OE1	1:A:27:PRO:HB3	2.18	0.43
2:C:417:GLN:HG3	2:C:418:ASN:N	2.34	0.43
2:C:564:LEU:HD22	2:C:568:GLU:HG3	1.99	0.43
1:A:166:ILE:HG13	1:A:167:ASP:O	2.19	0.43
1:B:223:ILE:HD12	1:B:223:ILE:HA	1.84	0.43
2:C:82:LYS:HG3	2:C:126:ILE:HD13	2.00	0.43
2:C:188:ARG:HH21	2:C:239:ARG:HH22	1.66	0.43
2:C:505:ASP:OD1	3:D:785:LYS:NZ	2.52	0.43
2:C:560:ARG:NH2	2:C:562:ASP:OD2	2.51	0.43
3:D:559:ILE:HD11	3:D:596:LEU:HD11	2.00	0.43
4:F:42:ILE:HG12	4:F:52:GLU:CD	2.44	0.43
1:A:42:ARG:O	1:A:46:SER:OG	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:973:GLU:OE2	3:D:973:GLU:N	2.48	0.43
2:C:329:ARG:HA	2:C:368:TYR:HE2	1.83	0.42
2:C:440:THR:HG22	2:C:440:THR:O	2.18	0.42
2:C:1143:LYS:HB2	3:D:11:ASN:OD1	2.19	0.42
3:D:491:PRO:HG2	3:D:620:LEU:HD23	2.01	0.42
3:D:977:THR:OG1	3:D:978:VAL:N	2.52	0.42
3:D:1087:ASP:OD1	3:D:1087:ASP:N	2.52	0.42
3:D:1095:ASP:OD2	3:D:1095:ASP:N	2.52	0.42
3:D:161:LYS:HG3	3:D:162:TYR:CD1	2.54	0.42
3:D:468:GLU:HG2	4:F:20:VAL:HG11	2.02	0.42
3:D:497:LEU:HD12	3:D:497:LEU:HA	1.82	0.42
3:D:514:MET:HE2	3:D:516:PHE:CE1	2.54	0.42
3:D:531:VAL:HG22	3:D:535:THR:HG21	2.01	0.42
3:D:686:GLN:HE22	3:D:691:LEU:HD12	1.84	0.42
3:D:829:LEU:HB2	3:D:836:ILE:HB	2.00	0.42
3:D:974:ILE:HD13	3:D:1000:ARG:HH21	1.83	0.42
1:A:61:VAL:HG13	1:A:66:SER:OG	2.20	0.42
3:D:271:LEU:HD21	3:D:281:VAL:HG22	2.02	0.42
3:D:753:ASN:N	3:D:756:GLY:O	2.52	0.42
1:A:41:ARG:HG3	1:A:176:VAL:HB	2.01	0.42
2:C:155:LYS:HE3	2:C:155:LYS:HB3	1.79	0.42
2:C:178:ASP:OD2	2:C:178:ASP:N	2.52	0.42
2:C:230:ASP:OD2	2:C:248:VAL:HG11	2.19	0.42
2:C:233:LEU:CD1	2:C:252:LYS:HE2	2.50	0.42
2:C:791:HIS:CE1	2:C:1043:MET:HE1	2.55	0.42
2:C:1060:THR:HG21	3:D:330:ASN:HD21	1.85	0.42
3:D:644:LYS:HB3	3:D:644:LYS:HE2	1.87	0.42
3:D:716:LEU:HD21	3:D:745:ALA:HB3	2.01	0.42
3:D:862:VAL:HB	3:D:872:LYS:HD3	2.01	0.42
1:A:114:HIS:HB2	1:A:118:VAL:HB	2.02	0.42
2:C:648:VAL:HG12	2:C:1039:LYS:O	2.19	0.42
1:A:88:LYS:HD3	1:A:90:TYR:HE1	1.84	0.42
2:C:352:PRO:O	2:C:353:THR:OG1	2.32	0.42
2:C:691:TRP:CE2	2:C:709:LYS:HG3	2.55	0.42
3:D:664:VAL:O	3:D:664:VAL:HG23	2.20	0.42
2:C:505:ASP:OD2	2:C:506:VAL:N	2.49	0.42
2:C:600:ASN:ND2	3:D:778:ILE:HD11	2.35	0.42
3:D:152:GLU:O	3:D:156:ARG:HG2	2.20	0.42
3:D:267:ARG:HB3	3:D:284:GLU:OE2	2.20	0.42
3:D:861:LEU:HD12	3:D:875:GLU:OE2	2.20	0.42
1:A:219:GLU:O	1:A:222:ASN:ND2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:LYS:HG3	2:C:153:ASN:OD1	2.20	0.42
3:D:1078:VAL:HA	3:D:1118:PRO:HA	2.00	0.42
1:B:92:ASP:OD1	1:B:93:GLU:N	2.51	0.42
2:C:41:LEU:HD23	2:C:41:LEU:HA	1.92	0.42
2:C:73:GLU:OE2	2:C:74:PRO:HD2	2.20	0.42
2:C:534:TYR:HD1	2:C:617:GLN:HB2	1.84	0.42
2:C:702:LYS:HD2	2:C:702:LYS:HA	1.87	0.42
3:D:332:LEU:HD11	3:D:1138:SER:HB3	2.02	0.42
3:D:453:ASP:OD1	3:D:453:ASP:N	2.51	0.42
3:D:679:LYS:N	3:D:679:LYS:HD3	2.35	0.42
4:F:9:LEU:HD23	4:F:9:LEU:HA	1.81	0.42
2:C:262:PRO:HG3	2:C:375:ASN:HD22	1.85	0.41
2:C:438:GLN:NE2	2:C:442:THR:HG22	2.35	0.41
2:C:507:HIS:CE1	2:C:508:TYR:CD2	3.07	0.41
3:D:28:VAL:HG23	3:D:95:ILE:HG12	2.01	0.41
3:D:58:TRP:CD1	3:D:68:VAL:HG12	2.55	0.41
3:D:174:ALA:O	3:D:178:LEU:HD13	2.20	0.41
4:F:31:GLN:HG2	4:F:46:TYR:CD2	2.55	0.41
1:A:74:ASP:O	1:A:78:ILE:HG13	2.21	0.41
2:C:61:ASN:OD1	2:C:101:LYS:HE2	2.20	0.41
2:C:838:ASP:OD1	2:C:882:GLY:N	2.53	0.41
1:B:167:ASP:OD1	1:B:167:ASP:N	2.52	0.41
2:C:154:GLY:O	2:C:156:LYS:NZ	2.52	0.41
2:C:755:LEU:HD23	2:C:755:LEU:H	1.85	0.41
3:D:297:ASP:OD1	3:D:300:ARG:HB2	2.21	0.41
3:D:564:LYS:HE2	3:D:579:ASN:O	2.20	0.41
2:C:158:PHE:CD1	2:C:392:LEU:HD12	2.55	0.41
2:C:352:PRO:O	2:C:354:ASP:N	2.52	0.41
2:C:547:TYR:HD1	2:C:564:LEU:HD12	1.86	0.41
2:C:590:ASP:HB2	2:C:605:ARG:HH21	1.84	0.41
3:D:1022:GLN:HG2	3:D:1023:VAL:N	2.33	0.41
2:C:678:HIS:HB2	2:C:694:ARG:CD	2.51	0.41
3:D:103:HIS:CD2	3:D:105:TRP:H	2.25	0.41
3:D:221:ASN:O	3:D:222:LYS:HD2	2.21	0.41
3:D:888:SER:HB2	3:D:1068:GLU:OE1	2.20	0.41
2:C:947:LEU:HD12	2:C:951:THR:OG1	2.21	0.41
3:D:33:THR:O	3:D:42:GLU:HG2	2.21	0.41
3:D:221:ASN:HA	3:D:225:TRP:CZ3	2.55	0.41
3:D:624:ILE:HG12	3:D:639:MET:HE1	2.01	0.41
3:D:960:PHE:HB3	3:D:1123:ILE:HD13	2.03	0.41
2:C:12:ARG:NH1	2:C:750:LEU:HD12	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:ILE:HB	2:C:95:LYS:HZ2	1.85	0.41
2:C:214:ASN:HB3	2:C:359:GLN:CD	2.46	0.41
2:C:1019:ASP:C	2:C:1021:ARG:H	2.28	0.41
2:C:1085:ALA:HB1	3:D:922:ILE:HD13	2.03	0.41
3:D:494:ASP:HB2	3:D:648:PHE:HE1	1.86	0.41
3:D:539:VAL:HG21	3:D:565:LEU:HD11	2.02	0.41
3:D:854:HIS:HB3	3:D:857:THR:O	2.20	0.41
3:D:1012:VAL:HG11	3:D:1024:LEU:HD22	2.03	0.41
2:C:363:VAL:HB	2:C:390:ASN:HD21	1.84	0.41
2:C:562:ASP:HB2	2:C:610:TYR:HE2	1.86	0.41
2:C:972:LEU:HD23	2:C:972:LEU:HA	1.85	0.41
3:D:186:LYS:HD3	3:D:186:LYS:C	2.46	0.41
3:D:439:HIS:CD2	3:D:441:LEU:HB2	2.56	0.41
3:D:492:SER:HA	3:D:496:VAL:HG23	2.03	0.41
3:D:917:GLU:O	3:D:919:VAL:N	2.50	0.41
2:C:52:ILE:HG22	2:C:66:PHE:HE2	1.85	0.41
2:C:346:SER:HB2	2:C:364:ILE:HD13	2.03	0.41
2:C:616:LYS:HE2	2:C:616:LYS:HB3	1.94	0.41
2:C:696:GLU:OE2	2:C:696:GLU:N	2.49	0.41
2:C:1135:LEU:HD23	2:C:1135:LEU:HA	1.88	0.41
3:D:33:THR:OG1	3:D:34:ILE:N	2.52	0.41
3:D:173:GLU:O	3:D:177:LYS:HG2	2.21	0.41
3:D:895:PRO:HB3	3:D:1097:HIS:NE2	2.36	0.41
3:D:1164:ASN:ND2	3:D:1169:LYS:HE3	2.35	0.41
1:B:184:ARG:HH12	1:B:186:GLY:H	1.68	0.41
2:C:215:GLU:C	2:C:217:LEU:N	2.76	0.41
2:C:229:SER:O	2:C:233:LEU:HG	2.20	0.41
2:C:517:ILE:O	2:C:638:LEU:HD12	2.21	0.41
2:C:974:LEU:HG	2:C:1033:GLY:HA3	2.02	0.41
2:C:1087:GLY:O	3:D:1175:THR:HG22	2.21	0.41
4:F:15:SER:HB3	4:F:18:THR:OG1	2.20	0.41
2:C:1076:GLY:O	2:C:1080:VAL:HG13	2.21	0.40
2:C:1124:VAL:HG13	2:C:1129:LYS:HZ2	1.86	0.40
3:D:486:LYS:HB3	3:D:487:PRO:HD2	2.03	0.40
3:D:494:ASP:OD1	3:D:494:ASP:N	2.53	0.40
3:D:872:LYS:HB2	3:D:872:LYS:HE2	1.66	0.40
2:C:828:GLY:C	2:C:829:ILE:HD12	2.46	0.40
3:D:33:THR:CG2	3:D:259:ARG:HH12	2.34	0.40
3:D:216:PHE:CZ	3:D:226:MET:HE3	2.57	0.40
1:B:117:ASP:OD1	1:B:117:ASP:N	2.54	0.40
2:C:662:MET:HE2	2:C:662:MET:HB2	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:LYS:HG3	3:D:638:LYS:HZ3	1.64	0.40
3:D:668:ASP:O	3:D:672:ILE:HG22	2.22	0.40
3:D:735:ARG:HG3	3:D:735:ARG:NH1	2.36	0.40
3:D:1047:LEU:HD23	3:D:1047:LEU:HA	1.92	0.40
2:C:437:ILE:HD13	2:C:437:ILE:HA	1.96	0.40
2:C:643:MET:CE	2:C:932:LYS:HG2	2.51	0.40
2:C:677:LYS:O	2:C:738:LYS:HE2	2.21	0.40
2:C:749:GLU:O	2:C:749:GLU:HG3	2.22	0.40
3:D:365:LEU:HD23	3:D:365:LEU:HA	1.91	0.40
3:D:441:LEU:HD23	3:D:441:LEU:HA	1.89	0.40
2:C:686:GLU:O	2:C:688:LYS:N	2.55	0.40
2:C:781:LEU:HD11	2:C:954:ASP:HB3	2.03	0.40
3:D:500:TYR:HE2	3:D:728:MET:HG2	1.87	0.40
3:D:757:ARG:HE	3:D:757:ARG:HB3	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/314 (71%)	218 (98%)	4 (2%)	0	100	100
1	B	222/314 (71%)	206 (93%)	16 (7%)	0	100	100
2	C	1111/1193 (93%)	1022 (92%)	88 (8%)	1 (0%)	48	76
3	D	1172/1199 (98%)	1096 (94%)	74 (6%)	2 (0%)	43	70
4	F	59/67 (88%)	53 (90%)	6 (10%)	0	100	100
All	All	2786/3087 (90%)	2595 (93%)	188 (7%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	352	PRO
3	D	633	ILE
3	D	664	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/273 (67%)	171 (93%)	12 (7%)	15	42
1	B	177/273 (65%)	164 (93%)	13 (7%)	13	39
2	C	931/1026 (91%)	877 (94%)	54 (6%)	18	45
3	D	968/1027 (94%)	926 (96%)	42 (4%)	26	52
4	F	53/61 (87%)	50 (94%)	3 (6%)	18	46
All	All	2312/2660 (87%)	2188 (95%)	124 (5%)	21	47

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	56	ILE
1	A	74	ASP
1	A	82	ILE
1	A	89	ILE
1	A	100	ASP
1	A	107	VAL
1	A	124	ASP
1	A	168	SER
1	A	182	ASN
1	A	197	ASP
1	A	203	SER
1	B	45	LEU
1	B	68	ILE
1	B	72	VAL
1	B	74	ASP
1	B	76	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	85	LEU
1	B	97	LEU
1	B	118	VAL
1	B	121	LEU
1	B	130	LEU
1	B	141	THR
1	B	167	ASP
1	B	210	ILE
2	C	49	PHE
2	C	55	ILE
2	C	98	LEU
2	C	103	THR
2	C	111	VAL
2	C	118	ILE
2	C	135	VAL
2	C	170	LEU
2	C	171	GLU
2	C	178	ASP
2	C	180	VAL
2	C	182	VAL
2	C	204	ASP
2	C	219	ASN
2	C	267	LEU
2	C	269	ASN
2	C	286	PHE
2	C	323	GLU
2	C	349	ILE
2	C	363	VAL
2	C	373	ILE
2	C	376	ILE
2	C	384	SER
2	C	386	SER
2	C	412	VAL
2	C	415	LEU
2	C	417	GLN
2	C	419	GLN
2	C	449	ILE
2	C	486	LEU
2	C	521	GLU
2	C	533	SER
2	C	558	THR
2	C	561	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	565	THR
2	C	568	GLU
2	C	589	ASP
2	C	638	LEU
2	C	678	HIS
2	C	686	GLU
2	C	703	VAL
2	C	730	VAL
2	C	749	GLU
2	C	776	ILE
2	C	798	GLU
2	C	873	ARG
2	C	879	VAL
2	C	905	VAL
2	C	906	ASN
2	C	967	ASN
2	C	1058	LEU
2	C	1094	GLU
2	C	1095	ILE
2	C	1151	GLU
3	D	9	TYR
3	D	12	ILE
3	D	24	SER
3	D	28	VAL
3	D	57	ASP
3	D	80	VAL
3	D	102	SER
3	D	118	LEU
3	D	233	VAL
3	D	253	ASP
3	D	272	LEU
3	D	289	GLN
3	D	397	VAL
3	D	399	ASP
3	D	423	ILE
3	D	524	LEU
3	D	536	ARG
3	D	557	LEU
3	D	560	THR
3	D	593	ARG
3	D	639	MET
3	D	658	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	663	ILE
3	D	665	VAL
3	D	667	ASP
3	D	730	SER
3	D	740	ASN
3	D	744	LEU
3	D	750	LEU
3	D	792	LEU
3	D	861	LEU
3	D	978	VAL
3	D	992	VAL
3	D	993	VAL
3	D	1018	ILE
3	D	1080	VAL
3	D	1081	ILE
3	D	1108	LEU
3	D	1151	ILE
3	D	1161	LEU
3	D	1175	THR
3	D	1177	MET
4	F	5	SER
4	F	7	ASP
4	F	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
2	C	100	ASN
2	C	473	GLN
2	C	576	GLN
2	C	631	ASN
2	C	642	ASN
2	C	646	GLN
2	C	689	ASN
2	C	906	ASN
3	D	103	HIS
3	D	454	GLN
3	D	553	GLN
3	D	740	ASN
3	D	951	GLN
3	D	957	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	989	GLN
3	D	994	GLN
3	D	1007	ASN
3	D	1140	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	7/8 (87%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

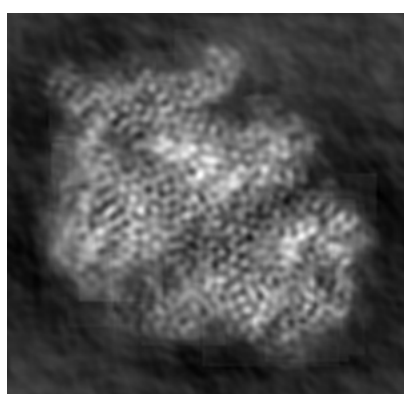
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21920. These allow visual inspection of the internal detail of the map and identification of artifacts.

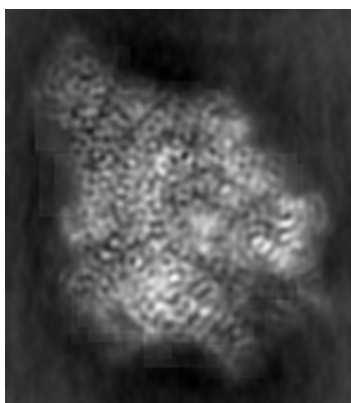
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

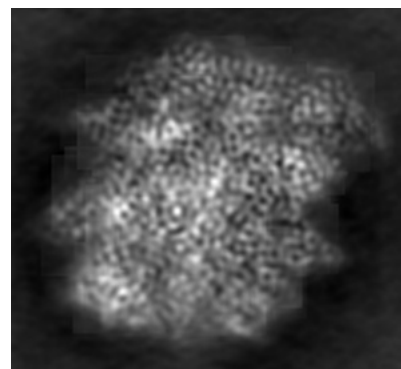
6.1.1 Primary map



X



Y

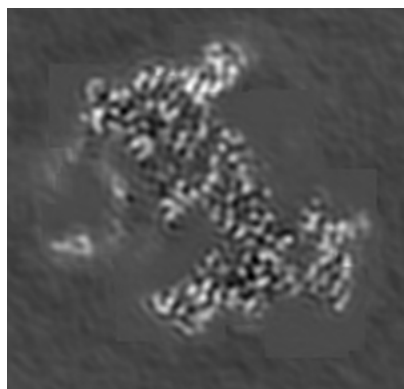


Z

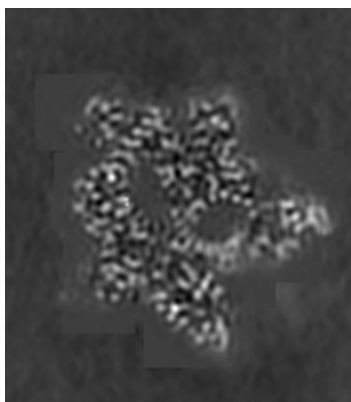
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

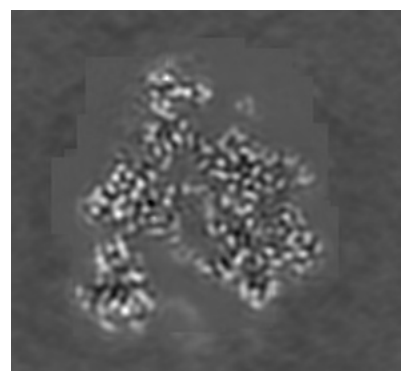
6.2.1 Primary map



X Index: 94



Y Index: 86

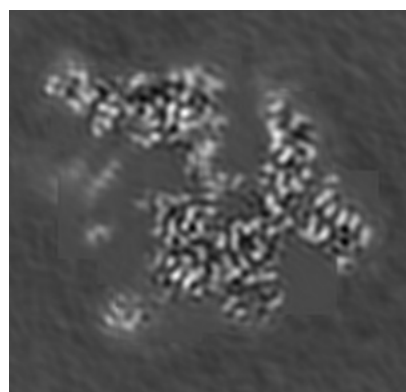


Z Index: 83

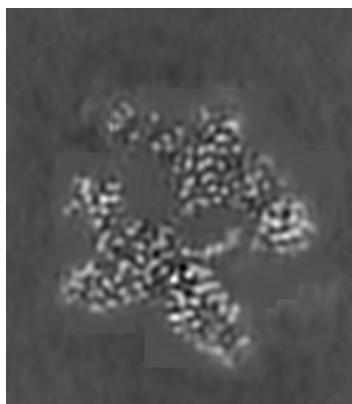
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

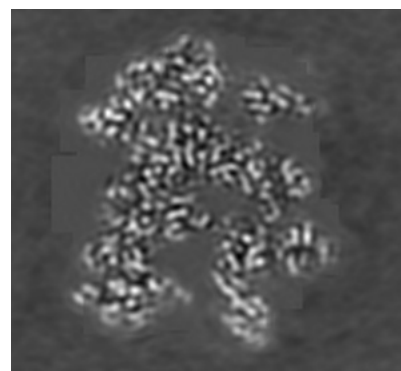
6.3.1 Primary map



X Index: 77



Y Index: 81

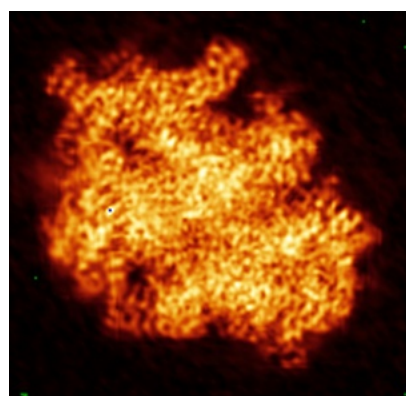


Z Index: 72

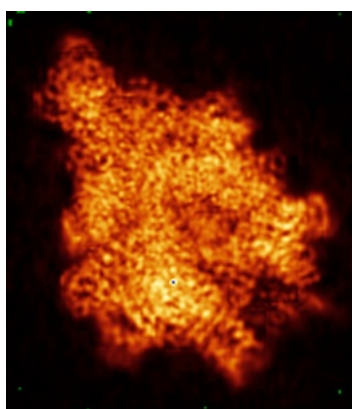
The images above show the largest variance slices of the map in three orthogonal directions.

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

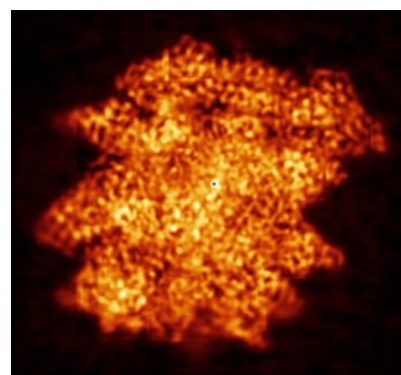
6.4.1 Primary map



X



Y

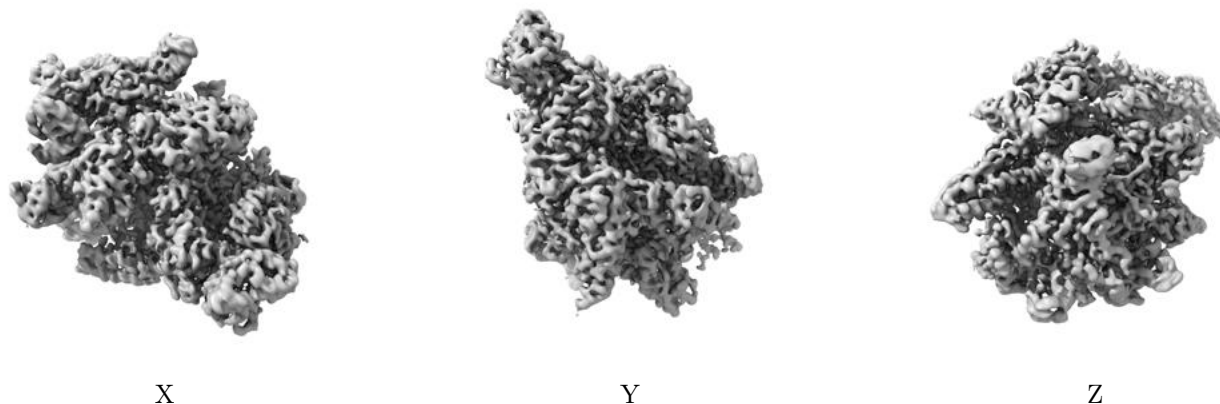


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

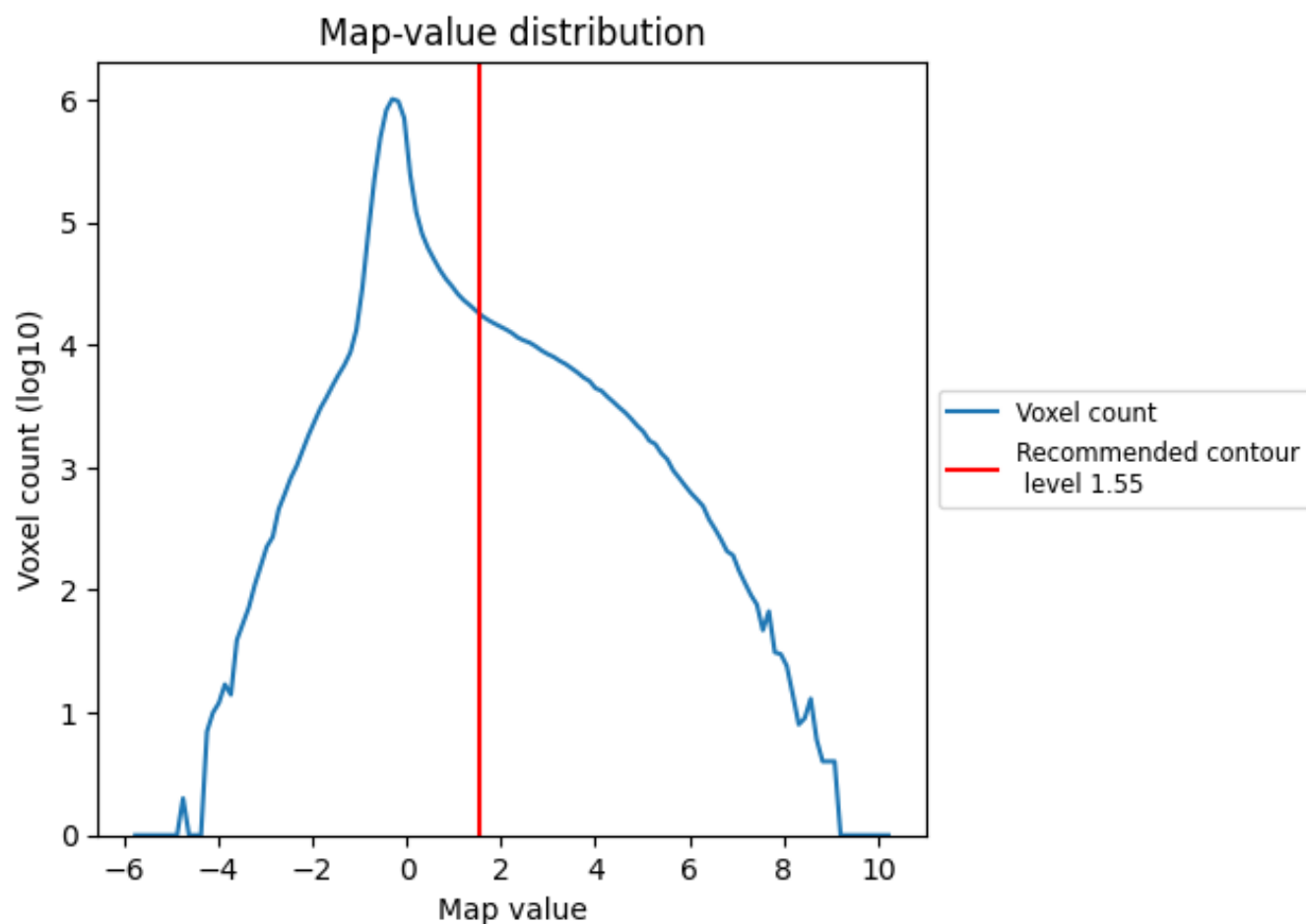
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

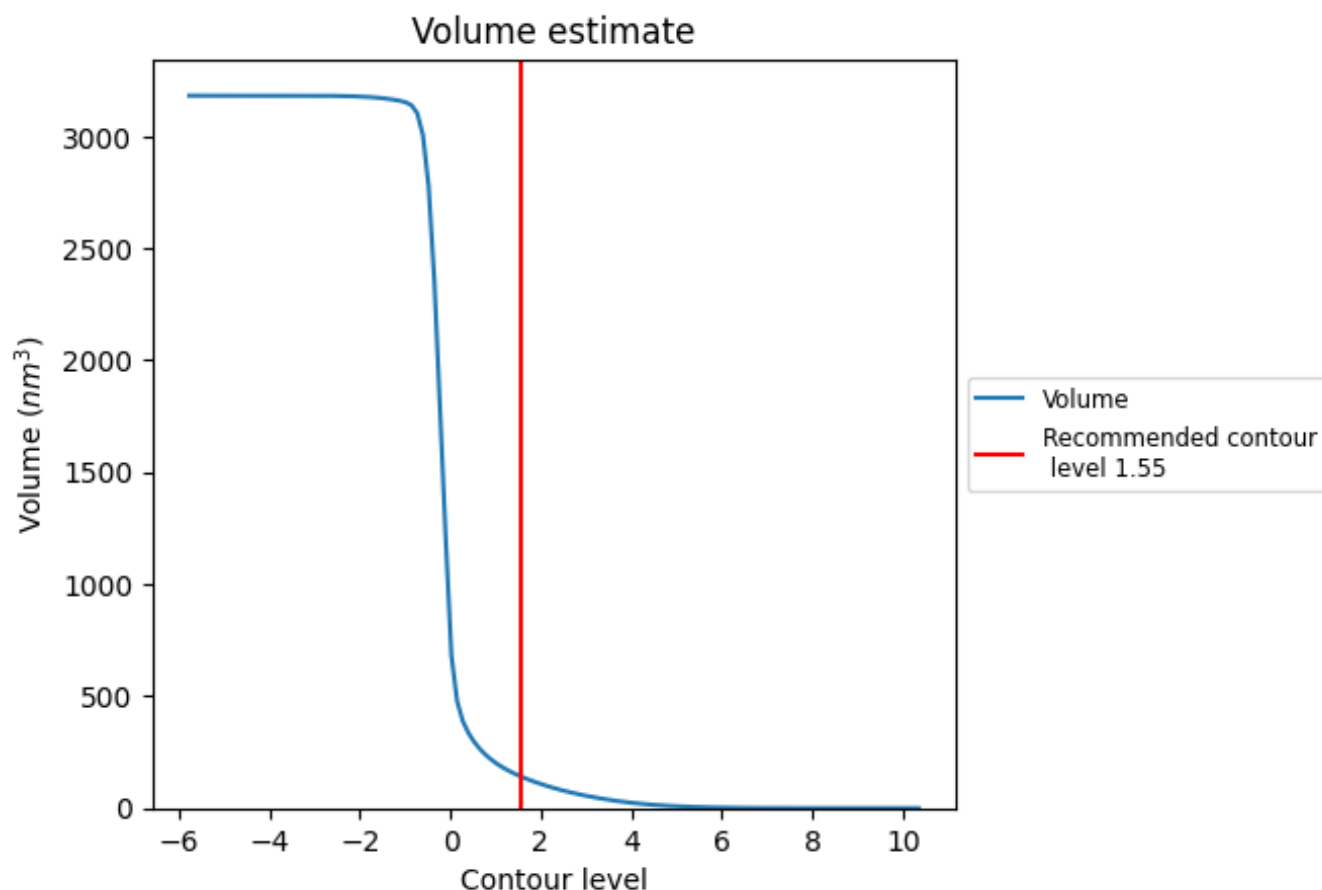
This section contains the results of statistical analysis of the map.

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 142 nm³; this corresponds to an approximate mass of 129 kDa.

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

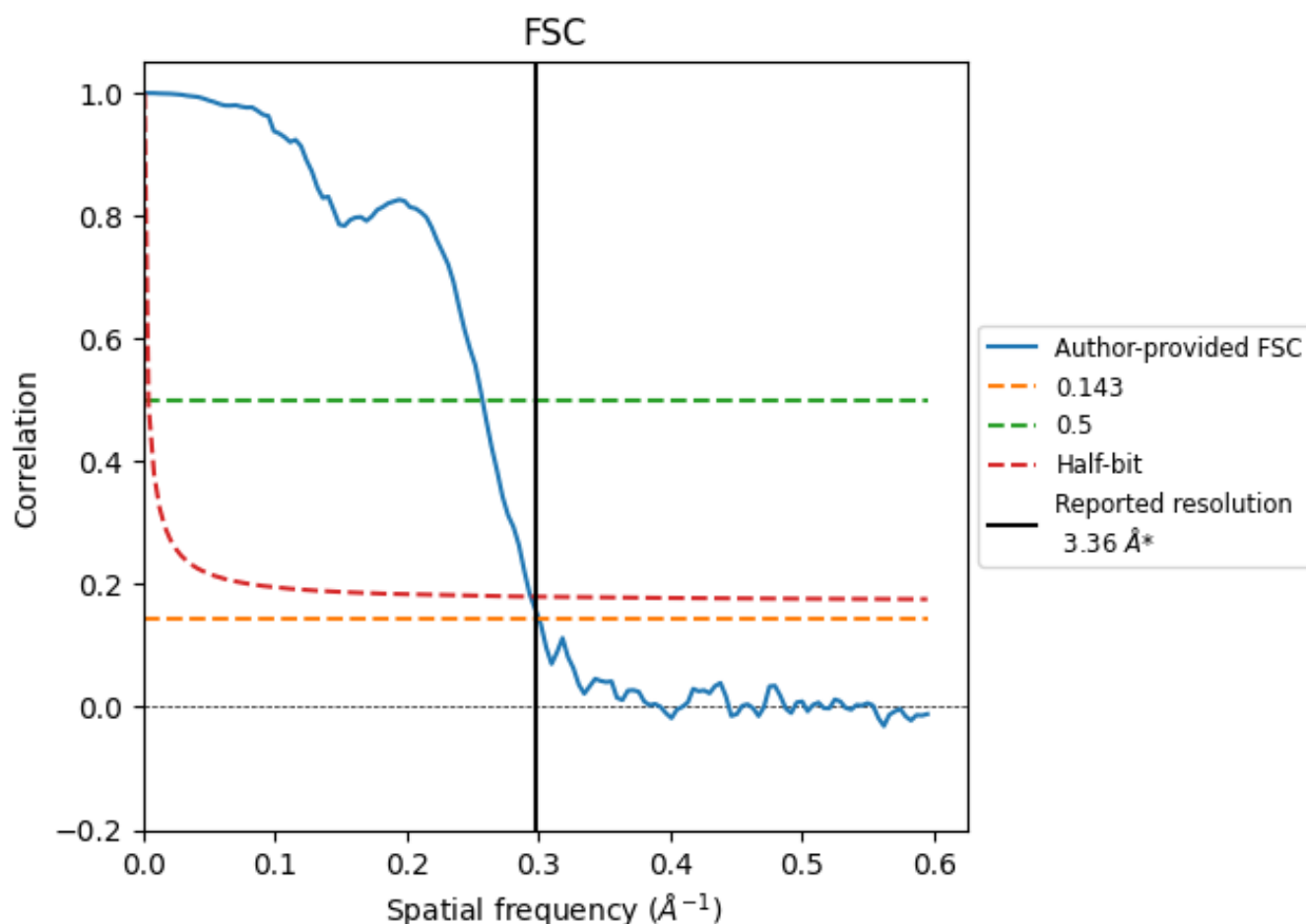
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.298 Å⁻¹

8.2 Resolution estimates [i](#)

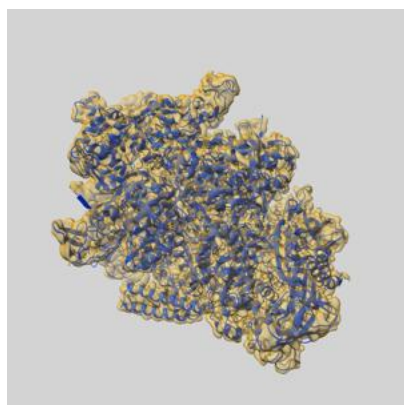
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.33	3.88	3.40
Unmasked-calculated*	-	-	-

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

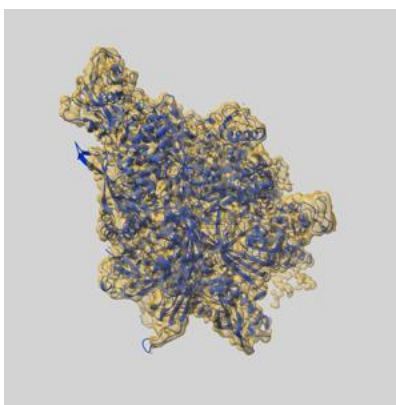
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21920 and PDB model 6WVJ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

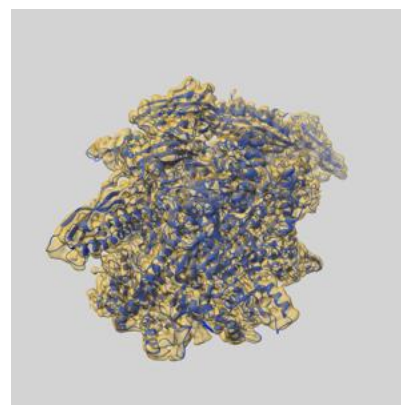
9.1 Map-model overlay [i](#)



X



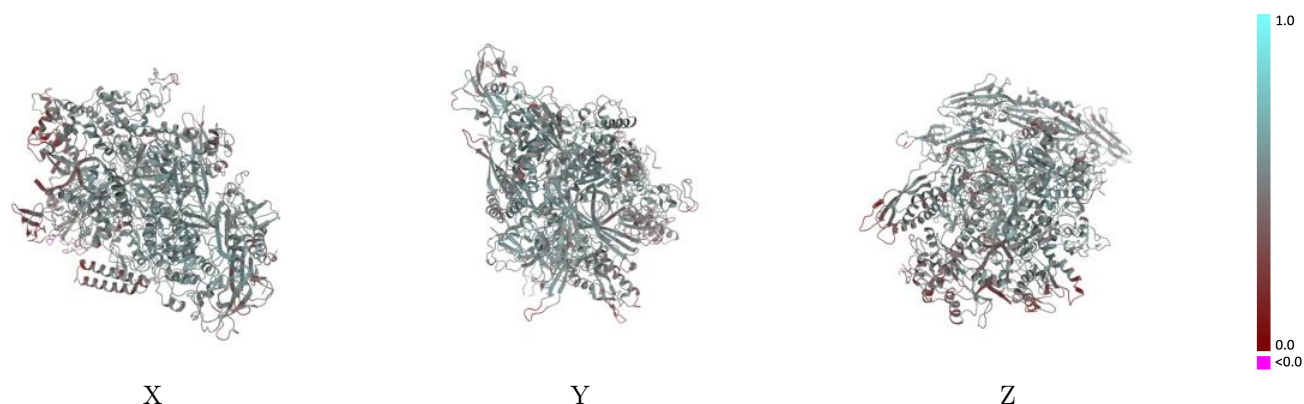
Y



Z

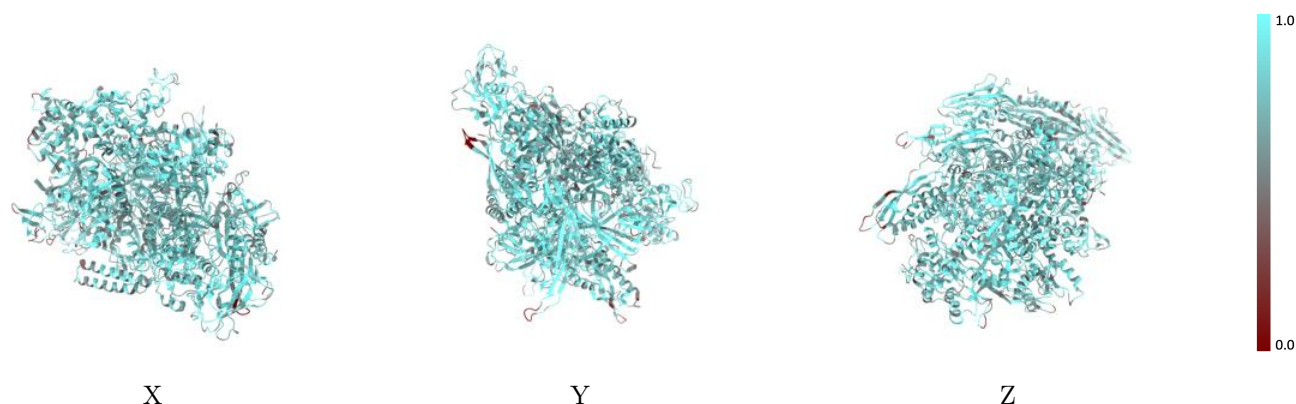
The images above show the 3D surface view of the map at the recommended contour level 1.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



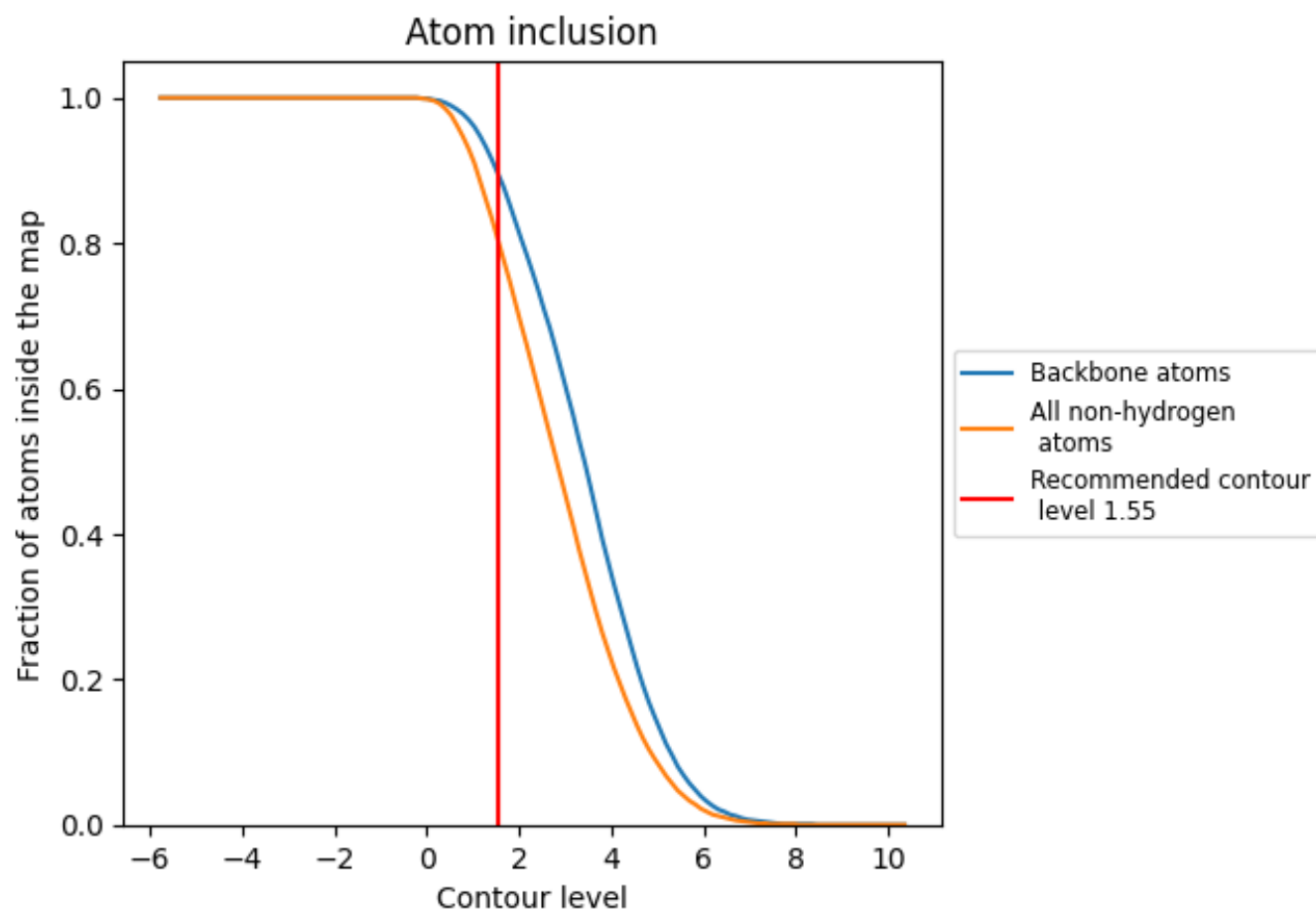
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (1.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.5020
A	0.8190	0.5170
B	0.7640	0.4990
C	0.8090	0.5050
D	0.8050	0.5030
F	0.7850	0.4950
N	0.6780	0.3580
R	0.8510	0.4850
T	0.8310	0.4480

