



Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 09:49 AM EDT

PDB ID : 8EOS
EMDB ID : EMD-28466
Title : M. tuberculosis RNAP elongation complex with NusG and CMPCPP
Authors : Vishwakarma, R.K.; Murakami, K.S.
Deposited on : 2022-10-04
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

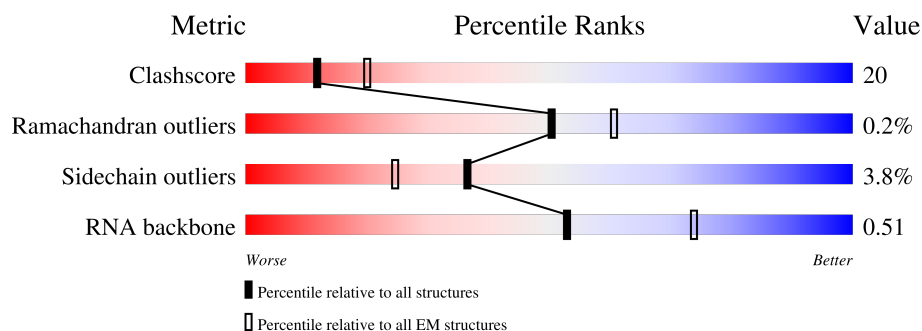
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	347	
1	B	347	
2	C	1178	
3	D	1316	
4	E	110	
5	G	238	
6	T	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	N	40	
8	R	20	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25620 atoms, of which 14 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	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1123	Total	C	N	O	S	0	0
			8686	5431	1529	1687	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1276	Total	C	N	O	S	0	0
			9982	6248	1817	1876	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	124	Total	C	N	O	S	0	0
			968	614	170	183	1		

- Molecule 6 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	38	Total	C	N	O	P	0	0
			774	366	141	229	38		

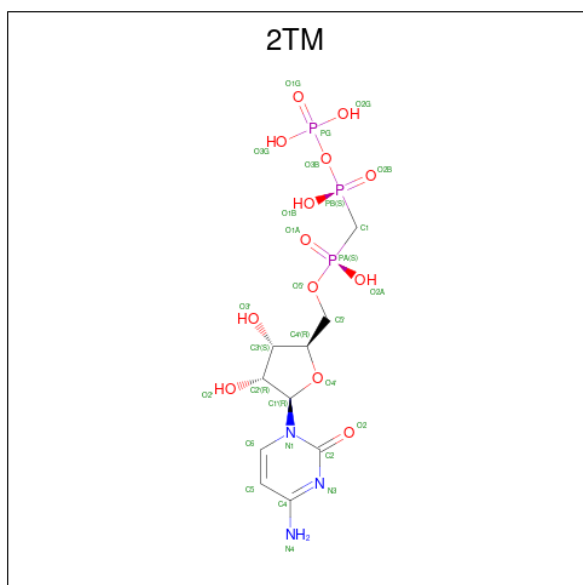
- Molecule 7 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	36	Total	C	N	O	P	0	0
			737	348	138	215	36		

- Molecule 8 is a RNA chain called RNA (5'-R(P*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	13	Total	C	N	O	P	0	0
			288	128	60	87	13		

- Molecule 9 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	H	N	O	P
			43	10	14	3	13	3

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Mg	0
			2	2	

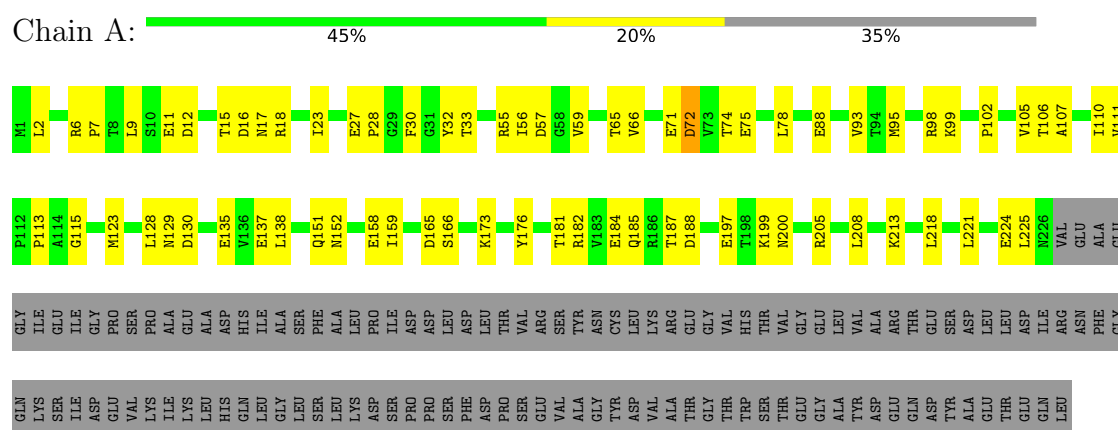
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

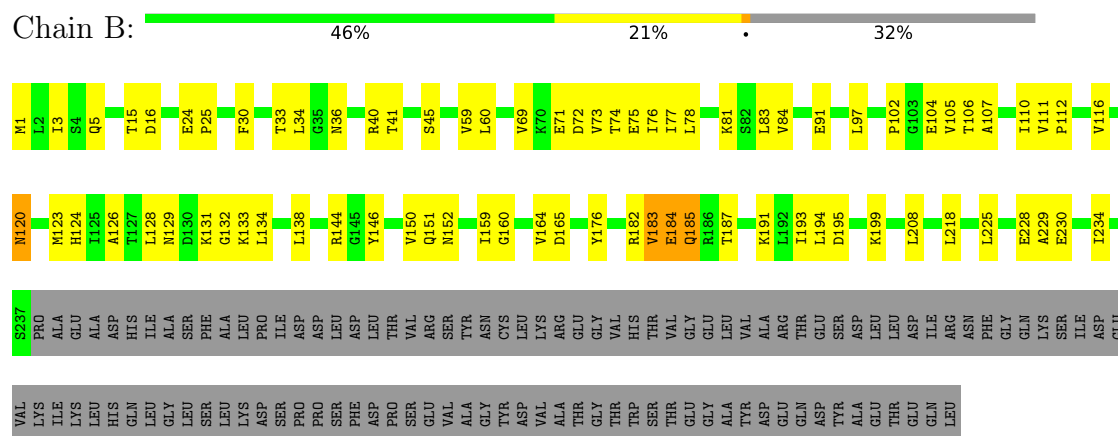
3 Residue-property plots

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

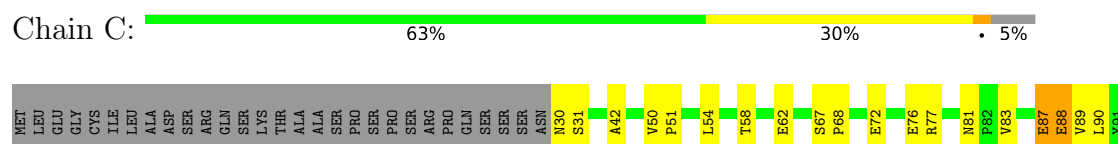
• Molecule 1: DNA-directed RNA polymerase subunit alpha

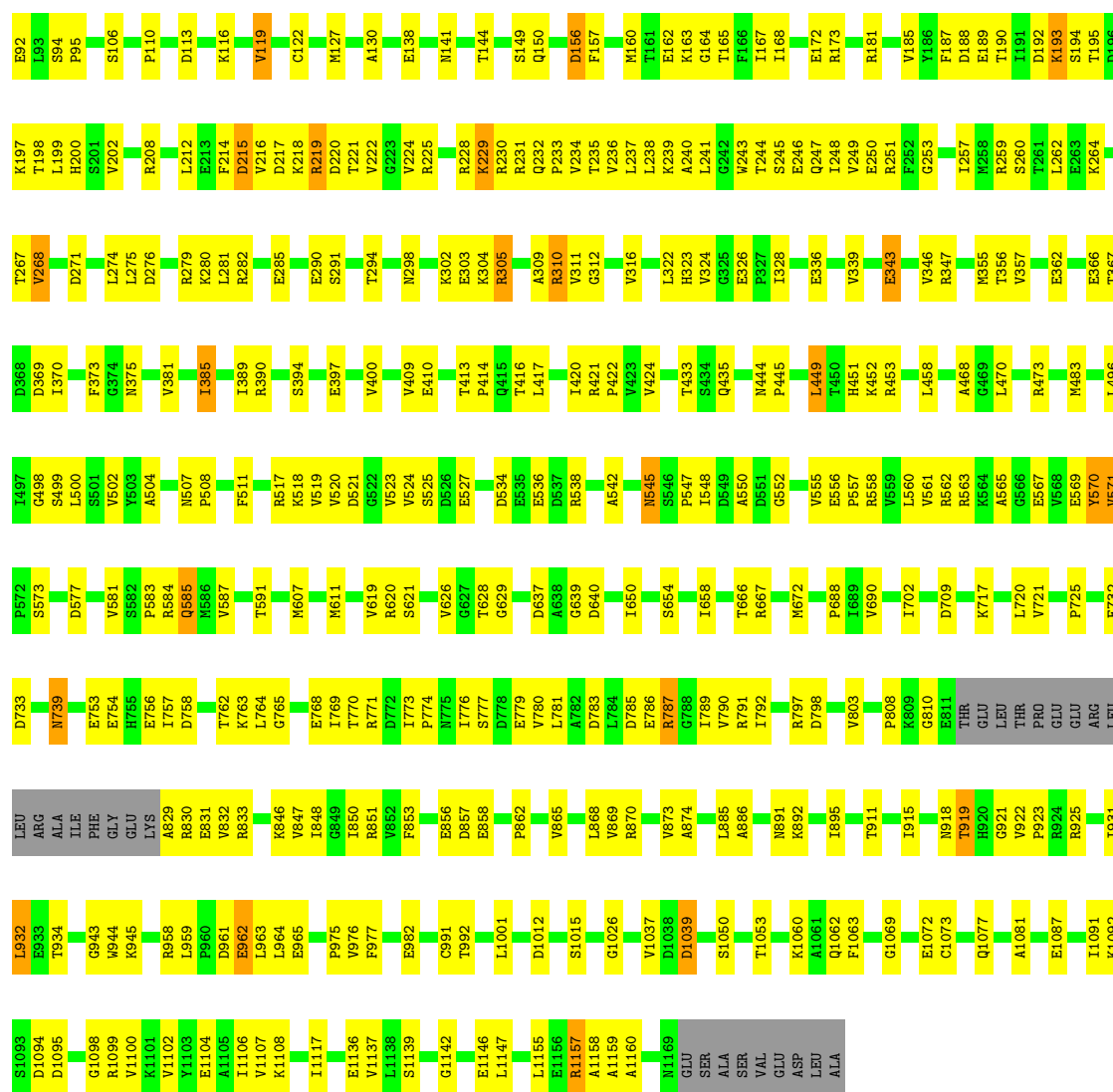


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

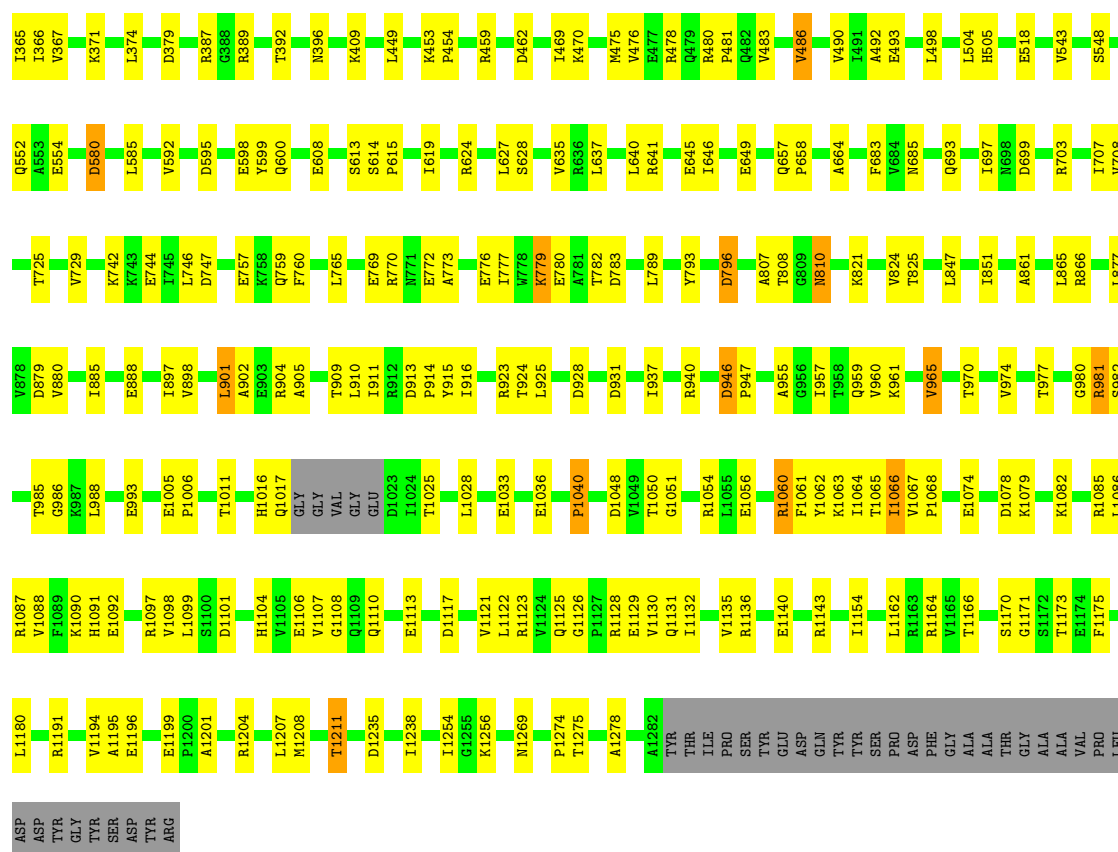




• Molecule 3: DNA-directed RNA polymerase subunit beta'

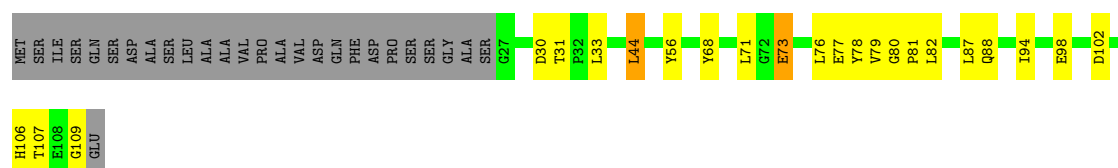
Chain D: 67% 29%





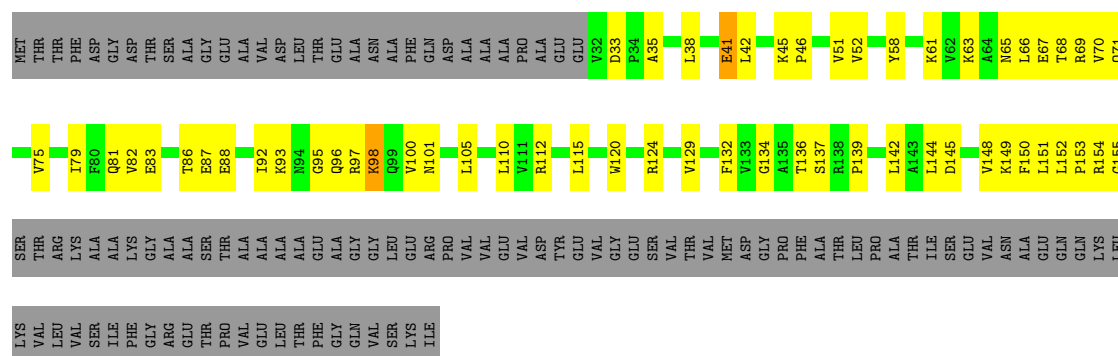
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 55% 19% 25%

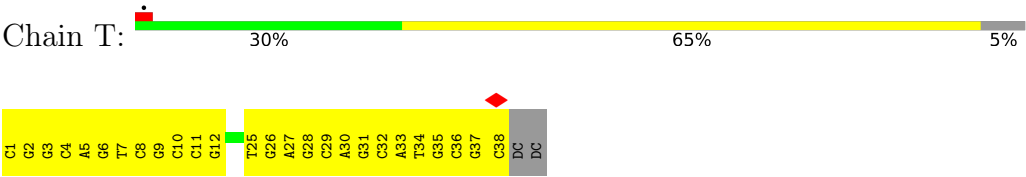


• Molecule 5: Transcription termination/antitermination protein NusG

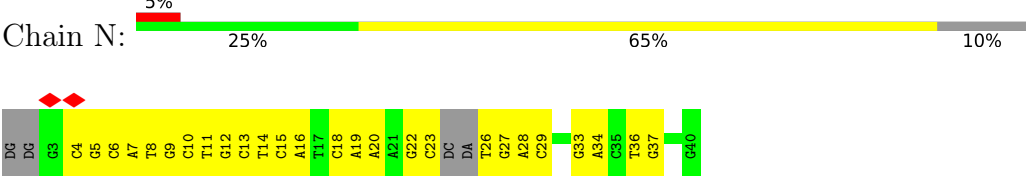
Chain G: 28% 24% 48%



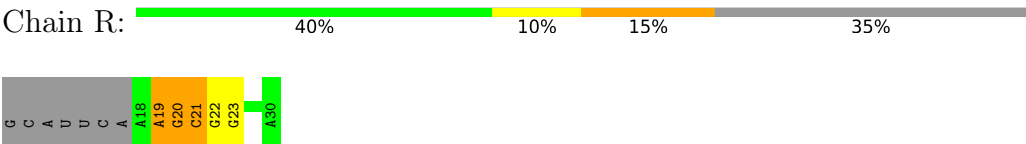
● Molecule 6: DNA (38-MER)



● Molecule 7: DNA (36-MER)



● Molecule 8: RNA (5'-R(P*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129716	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.964	Depositor
Minimum map value	-0.734	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2TM, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1750	0.53	0/2380
1	B	0.27	0/1792	0.51	0/2442
2	C	0.29	0/8842	0.52	0/11987
3	D	0.28	0/10149	0.52	0/13718
4	E	0.29	0/662	0.50	0/901
5	G	0.24	0/987	0.46	0/1343
6	T	0.60	0/866	0.89	0/1333
7	N	0.50	0/825	0.87	0/1268
8	R	0.42	0/324	0.78	0/505
All	All	0.31	0/26197	0.55	0/35877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1724	0	1768	60	0
1	B	1765	0	1794	86	0
2	C	8686	0	8606	357	0
3	D	9982	0	10040	370	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	649	0	645	17	0
5	G	968	0	973	55	0
6	T	774	0	426	35	0
7	N	737	0	404	44	0
8	R	288	0	142	4	0
9	C	29	14	14	0	0
10	D	2	0	0	0	0
11	D	2	0	0	0	0
All	All	25606	14	24812	988	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 20.

All (988) 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:177:LEU:HD21	3:D:201:GLY:HA3	1.36	1.06
4:E:76:LEU:HD23	4:E:78:TYR:H	1.26	0.99
2:C:224:VAL:HG13	2:C:234:VAL:HG12	1.45	0.98
2:C:248:ILE:HD13	2:C:262:LEU:HD11	1.44	0.98
3:D:123:LYS:NZ	7:N:36:DT:OP2	1.97	0.96
2:C:764:LEU:HD13	2:C:808:PRO:HB2	1.47	0.95
3:D:281:ILE:HA	3:D:289:LYS:HE3	1.47	0.94
3:D:1036:GLU:OE2	3:D:1211:THR:OG1	1.85	0.93
3:D:1050:THR:HG23	3:D:1107:VAL:HG23	1.52	0.92
5:G:70:VAL:HG13	5:G:75:VAL:HG23	1.49	0.91
3:D:1088:VAL:HG12	3:D:1098:VAL:HG22	1.52	0.89
1:B:128:LEU:HD11	1:B:134:LEU:HD23	1.55	0.87
3:D:120:LEU:HB3	3:D:125:LEU:HD21	1.57	0.87
3:D:166:ARG:HH21	3:D:209:ARG:HB2	1.38	0.87
3:D:637:LEU:HD23	3:D:640:LEU:HD12	1.56	0.87
3:D:281:ILE:HD12	3:D:293:LEU:HD12	1.58	0.85
2:C:92:GLU:OE2	2:C:390:ARG:NH1	2.09	0.85
3:D:901:LEU:HD23	3:D:916:ILE:HD11	1.58	0.85
3:D:60:CYS:SG	3:D:61:TYR:N	2.50	0.84
1:A:98:ARG:NH1	1:A:135:GLU:OE2	2.10	0.84
3:D:273:GLU:OE2	3:D:295:ARG:NH2	2.12	0.83
2:C:165:THR:OG1	2:C:172:GLU:OE2	1.96	0.82
2:C:789:ILE:HD12	2:C:789:ILE:H	1.43	0.82
1:B:69:VAL:HG22	1:B:128:LEU:HD21	1.62	0.82
2:C:253:GLY:HA2	2:C:259:ARG:HH12	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1050:THR:HG22	3:D:1106:GLU:HA	1.60	0.80
2:C:557:PRO:O	2:C:573:SER:N	2.14	0.80
3:D:1170:SER:OG	3:D:1175:PHE:O	1.99	0.80
3:D:126:GLU:OE2	3:D:387:ARG:NH1	2.15	0.80
3:D:320:ILE:O	3:D:325:ARG:NH1	2.14	0.80
3:D:1129:GLU:N	3:D:1129:GLU:OE1	2.14	0.79
3:D:1090:LYS:NZ	3:D:1091:HIS:O	2.15	0.79
7:N:28:DA:H4'	7:N:29:DC:OP1	1.83	0.79
1:B:41:THR:O	1:B:45:SER:OG	2.01	0.79
3:D:166:ARG:HE	3:D:209:ARG:HA	1.46	0.79
1:A:99:LYS:HG3	1:A:105:VAL:HG22	1.65	0.79
1:A:15:THR:HG22	1:A:16:ASP:H	1.46	0.78
2:C:757:ILE:HG21	2:C:803:VAL:HG21	1.63	0.78
3:D:211:ARG:O	3:D:214:ARG:HG2	1.84	0.78
6:T:4:DC:H2''	6:T:5:DA:C8	2.18	0.78
2:C:336:GLU:N	2:C:336:GLU:OE1	2.16	0.78
3:D:744:GLU:OE1	3:D:744:GLU:N	2.17	0.78
3:D:365:ILE:HD11	5:G:134:GLY:HA2	1.66	0.77
2:C:248:ILE:HD12	2:C:249:VAL:N	2.00	0.77
7:N:22:DG:H2''	7:N:23:DC:H5'	1.65	0.77
2:C:758:ASP:OD1	2:C:868:LEU:HD23	1.84	0.77
3:D:121:ALA:HB1	3:D:123:LYS:HZ1	1.50	0.77
2:C:221:THR:O	2:C:231:ARG:NH2	2.18	0.77
3:D:240:LEU:HD23	3:D:244:LEU:HD13	1.65	0.77
1:A:9:LEU:HD12	1:A:23:ILE:HG12	1.67	0.77
2:C:856:GLU:OE1	2:C:856:GLU:N	2.17	0.77
5:G:93:LYS:HG3	5:G:96:GLN:HB2	1.67	0.77
2:C:523:VAL:HA	2:C:552:GLY:O	1.86	0.76
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.68	0.76
5:G:132:PHE:HB3	5:G:139:PRO:HB3	1.67	0.76
7:N:13:DC:C6	7:N:14:DT:H72	2.21	0.75
3:D:150:THR:O	3:D:154:GLU:HG2	1.87	0.75
2:C:328:ILE:O	2:C:328:ILE:HD12	1.87	0.74
3:D:1054:ARG:HB3	3:D:1056:GLU:OE2	1.87	0.74
3:D:1173:THR:HG21	3:D:1201:ALA:HB2	1.67	0.74
2:C:248:ILE:HD12	2:C:249:VAL:H	1.52	0.74
5:G:115:LEU:HD11	5:G:120:TRP:HD1	1.51	0.74
7:N:18:DC:H4'	7:N:19:DA:H5'	1.68	0.74
3:D:271:ASP:O	3:D:275:GLU:HG2	1.87	0.74
2:C:547:PRO:HB2	2:C:555:VAL:HB	1.69	0.74
3:D:181:LEU:HG	3:D:198:ARG:HD3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:219:ARG:HG2	2:C:221:THR:HG23	1.70	0.74
3:D:285:LYS:O	3:D:288:LYS:NZ	2.16	0.73
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.68	0.73
2:C:768:GLU:OE1	2:C:768:GLU:N	2.20	0.73
3:D:277:LEU:O	3:D:281:ILE:HG12	1.88	0.73
3:D:657:GLN:N	3:D:658:PRO:HD2	2.03	0.73
2:C:773:ILE:HG21	2:C:776:ILE:HD13	1.69	0.73
2:C:1050:SER:HB3	2:C:1053:THR:O	1.89	0.73
3:D:194:ARG:O	3:D:197:VAL:HG22	1.87	0.73
2:C:192:ASP:HB3	2:C:197:LYS:H	1.54	0.73
2:C:787:ARG:HG2	2:C:787:ARG:O	1.87	0.72
3:D:204:GLU:O	3:D:207:GLN:HG3	1.88	0.72
5:G:87:GLU:OE2	5:G:154:ARG:HB2	1.89	0.72
2:C:192:ASP:OD1	2:C:193:LYS:HD3	1.89	0.72
3:D:196:LYS:HA	3:D:199:ASP:OD2	1.89	0.72
2:C:381:VAL:O	2:C:385:ILE:HG22	1.88	0.72
3:D:200:GLY:O	3:D:203:ARG:HG3	1.89	0.72
3:D:1033:GLU:OE2	3:D:1040:PRO:HA	1.90	0.72
2:C:189:GLU:OE1	2:C:200:HIS:NE2	2.23	0.71
2:C:1117:ILE:HD12	3:D:2:LEU:HD13	1.71	0.71
3:D:121:ALA:HB1	3:D:123:LYS:NZ	2.04	0.71
3:D:866:ARG:HG3	3:D:1025:THR:HG22	1.70	0.71
2:C:248:ILE:HD12	2:C:249:VAL:HG23	1.73	0.71
2:C:518:LYS:O	2:C:525:SER:OG	2.08	0.71
2:C:658:ILE:HG13	2:C:672:MET:HE3	1.71	0.71
2:C:1062:GLN:OE1	2:C:1062:GLN:N	2.22	0.71
2:C:1095:ASP:O	2:C:1099:ARG:HG3	1.90	0.71
2:C:449:LEU:O	2:C:449:LEU:HD22	1.91	0.71
3:D:166:ARG:HG3	3:D:212:ALA:HB2	1.72	0.71
1:B:69:VAL:HG22	1:B:128:LEU:CD2	2.20	0.70
6:T:26:DG:H2"	6:T:27:DA:C8	2.26	0.70
3:D:459:ARG:NH1	3:D:462:ASP:OD2	2.23	0.70
3:D:243:GLU:O	3:D:247:ARG:HG2	1.92	0.70
6:T:25:DT:H2"	6:T:26:DG:C8	2.27	0.70
3:D:172:ALA:O	3:D:175:GLN:HG3	1.91	0.70
1:A:218:LEU:CD2	1:B:34:LEU:HD11	2.21	0.70
3:D:769:GLU:O	3:D:772:GLU:HG3	1.90	0.70
6:T:27:DA:H2"	6:T:28:DG:H8	1.56	0.70
2:C:780:VAL:HG23	2:C:781:LEU:HD22	1.74	0.69
1:B:84:VAL:HG22	1:B:199:LYS:HD2	1.73	0.69
3:D:904:ARG:HA	3:D:910:LEU:HD23	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:303:GLU:O	2:C:304:LYS:HD3	1.92	0.69
2:C:945:LYS:NZ	2:C:965:GLU:OE2	2.26	0.69
2:C:1157:ARG:HH11	2:C:1158:ALA:HA	1.58	0.69
3:D:904:ARG:HD2	3:D:910:LEU:HD21	1.75	0.69
3:D:1191:ARG:O	3:D:1194:VAL:HG12	1.91	0.69
3:D:281:ILE:CD1	3:D:293:LEU:HD12	2.23	0.69
2:C:253:GLY:HA2	2:C:259:ARG:HH22	1.57	0.68
4:E:76:LEU:HD23	4:E:78:TYR:N	2.06	0.68
2:C:192:ASP:OD1	2:C:193:LYS:N	2.26	0.68
2:C:777:SER:OG	2:C:779:GLU:HG2	1.93	0.68
3:D:1060:ARG:O	3:D:1082:LYS:HG2	1.94	0.68
1:A:221:LEU:O	1:A:224:GLU:HG3	1.92	0.68
7:N:26:DT:H4'	7:N:27:DG:OP2	1.93	0.68
3:D:65:TYR:CE1	3:D:73:ILE:HD11	2.28	0.68
3:D:167:ASP:O	3:D:171:GLU:HG2	1.94	0.68
2:C:773:ILE:HG23	2:C:774:PRO:HD2	1.76	0.68
6:T:5:DA:H2''	6:T:6:DG:C8	2.28	0.68
2:C:1012:ASP:OD2	2:C:1015:SER:OG	2.12	0.68
3:D:4:VAL:HG12	3:D:1256:LYS:HD3	1.74	0.68
3:D:211:ARG:HA	3:D:214:ARG:NE	2.09	0.68
2:C:356:THR:HB	2:C:362:GLU:OE1	1.94	0.68
1:B:71:GLU:N	1:B:71:GLU:OE1	2.26	0.68
2:C:248:ILE:HD13	2:C:262:LEU:CD1	2.20	0.68
2:C:560:LEU:HD13	3:D:847:LEU:HD11	1.76	0.67
3:D:86:LYS:O	3:D:89:ARG:HG2	1.95	0.67
2:C:347:ARG:HD2	2:C:355:MET:HG3	1.76	0.67
1:B:60:LEU:HD21	1:B:159:ILE:CD1	2.25	0.67
3:D:1067:VAL:HA	3:D:1074:GLU:OE1	1.94	0.67
5:G:152:LEU:HG	5:G:153:PRO:HD2	1.76	0.67
3:D:149:SER:O	3:D:152:GLU:HG3	1.94	0.67
3:D:338:SER:OG	3:D:341:ASN:OD1	2.10	0.67
2:C:1147:LEU:HA	3:D:2:LEU:HD11	1.77	0.67
1:B:128:LEU:HD21	1:B:134:LEU:CD2	2.25	0.67
3:D:166:ARG:HH12	3:D:170:LEU:HB2	1.59	0.67
3:D:268:PHE:CE2	3:D:270:ILE:HD13	2.30	0.67
3:D:866:ARG:HB2	3:D:1011:THR:HG23	1.76	0.66
1:A:27:GLU:OE2	1:B:144:ARG:HD2	1.95	0.66
2:C:192:ASP:OD2	2:C:218:LYS:HE2	1.95	0.66
1:A:182:ARG:HD3	1:A:188:ASP:OD2	1.96	0.66
3:D:498:LEU:CD2	3:D:543:VAL:HG22	2.25	0.66
3:D:779:LYS:O	3:D:782:THR:HG22	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:PRO:O	2:C:236:VAL:HG22	1.95	0.66
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.28	0.66
7:N:8:DT:H2"	7:N:9:DG:C8	2.31	0.66
3:D:344:TYR:O	3:D:348:ILE:HG12	1.96	0.66
3:D:120:LEU:HB3	3:D:125:LEU:CD2	2.26	0.65
1:A:218:LEU:HD23	1:B:34:LEU:HD11	1.78	0.65
3:D:699:ASP:OD1	3:D:703:ARG:HD3	1.96	0.65
2:C:309:ALA:O	2:C:311:VAL:N	2.29	0.65
2:C:468:ALA:HB3	2:C:473:ARG:HH21	1.62	0.65
2:C:1069:GLY:N	2:C:1072:GLU:OE1	2.29	0.65
3:D:866:ARG:HB2	3:D:1011:THR:CG2	2.25	0.65
2:C:922:VAL:HB	2:C:923:PRO:HD3	1.79	0.65
2:C:253:GLY:HA2	2:C:259:ARG:NH1	2.12	0.65
2:C:369:ASP:O	2:C:375:ASN:ND2	2.29	0.65
3:D:1048:ASP:O	3:D:1107:VAL:HG13	1.97	0.65
3:D:1254:ILE:HD11	3:D:1256:LYS:HE3	1.79	0.65
2:C:789:ILE:HG21	2:C:850:ILE:HG21	1.79	0.64
1:B:191:LYS:HE3	1:B:193:ILE:HD11	1.79	0.64
2:C:232:GLN:OE1	2:C:232:GLN:N	2.30	0.64
2:C:366:GLU:HG3	2:C:367:THR:O	1.97	0.64
3:D:1087:ARG:HH11	3:D:1110:GLN:HE21	1.44	0.64
2:C:244:THR:HG23	2:C:247:GLN:H	1.63	0.64
2:C:397:GLU:O	2:C:400:VAL:HG12	1.98	0.64
2:C:628:THR:HG22	2:C:629:GLY:H	1.63	0.64
2:C:518:LYS:NZ	2:C:527:GLU:OE1	2.22	0.64
3:D:365:ILE:HD11	5:G:134:GLY:CA	2.27	0.64
1:B:97:LEU:HD12	1:B:110:ILE:CD1	2.27	0.64
2:C:193:LYS:HD3	2:C:193:LYS:H	1.61	0.64
3:D:707:ILE:HD12	3:D:708:VAL:N	2.12	0.64
1:B:182:ARG:HA	1:B:187:THR:HA	1.80	0.64
3:D:67:ARG:HA	3:D:67:ARG:HH11	1.63	0.63
3:D:946:ASP:HB2	3:D:947:PRO:HD3	1.78	0.63
1:A:55:ARG:NH1	1:A:158:GLU:OE1	2.27	0.63
3:D:1108:GLY:HA3	3:D:1125:GLN:HE21	1.62	0.63
2:C:584:ARG:O	2:C:584:ARG:HG3	1.97	0.63
1:A:102:PRO:HB3	1:A:129:ASN:O	1.98	0.63
2:C:224:VAL:CG1	2:C:234:VAL:HG12	2.23	0.63
1:A:129:ASN:OD1	1:A:130:ASP:N	2.27	0.63
3:D:166:ARG:NH2	3:D:209:ARG:HB2	2.14	0.63
3:D:336:ALA:O	3:D:337:THR:OG1	2.09	0.63
3:D:866:ARG:HG3	3:D:1025:THR:CG2	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:707:ILE:HD12	3:D:708:VAL:H	1.64	0.63
7:N:7:DA:H2"	7:N:8:DT:C6	2.34	0.63
2:C:885:LEU:HG	2:C:895:ILE:HD11	1.79	0.62
4:E:87:LEU:HD23	4:E:88:GLN:H	1.62	0.62
6:T:36:DC:H2"	6:T:37:DG:C8	2.34	0.62
2:C:1159:ALA:HB1	3:D:470:LYS:NZ	2.15	0.62
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.81	0.62
5:G:45:LYS:HG3	5:G:46:PRO:HD2	1.81	0.62
2:C:187:PHE:CD2	2:C:202:VAL:HG22	2.34	0.62
6:T:29:DC:H2"	6:T:30:DA:C8	2.33	0.62
2:C:246:GLU:O	2:C:250:GLU:HG2	2.00	0.62
2:C:569:GLU:HG3	2:C:571:VAL:CG1	2.30	0.62
3:D:65:TYR:O	3:D:66:LYS:HD3	1.98	0.62
3:D:744:GLU:HA	3:D:747:ASP:OD2	1.98	0.62
2:C:189:GLU:OE2	2:C:198:THR:HB	2.00	0.62
3:D:281:ILE:HD12	3:D:293:LEU:CD1	2.30	0.62
1:B:102:PRO:HG3	1:B:131:LYS:NZ	2.15	0.62
1:B:3:ILE:CD1	1:B:234:ILE:HG22	2.29	0.62
3:D:204:GLU:O	3:D:208:ILE:HG13	1.99	0.62
3:D:238:GLU:OE1	3:D:238:GLU:N	2.32	0.62
6:T:27:DA:H2"	6:T:28:DG:C8	2.35	0.62
7:N:7:DA:H2"	7:N:8:DT:H71	1.82	0.62
3:D:757:GLU:OE1	3:D:770:ARG:HD2	2.00	0.61
5:G:51:VAL:HG12	5:G:110:LEU:CD2	2.30	0.61
2:C:776:ILE:HD11	2:C:781:LEU:HD21	1.81	0.61
3:D:270:ILE:CG2	3:D:303:GLN:HB2	2.30	0.61
2:C:470:LEU:HD21	3:D:865:LEU:HD12	1.82	0.61
3:D:904:ARG:HD2	3:D:910:LEU:CD2	2.29	0.61
3:D:270:ILE:HG21	3:D:303:GLN:HB2	1.82	0.61
7:N:4:DC:H2"	7:N:5:DG:C8	2.34	0.61
3:D:330:LEU:O	3:D:333:GLY:N	2.30	0.61
2:C:1147:LEU:HD23	2:C:1147:LEU:O	2.01	0.61
3:D:169:GLU:OE1	3:D:211:ARG:NH2	2.16	0.61
3:D:281:ILE:HA	3:D:289:LYS:CE	2.25	0.61
6:T:32:DC:H2"	6:T:33:DA:C8	2.35	0.61
2:C:763:LYS:N	2:C:763:LYS:HE2	2.15	0.61
2:C:831:GLU:O	2:C:831:GLU:HG2	2.00	0.61
6:T:34:DT:H2"	6:T:35:DG:C8	2.35	0.61
2:C:225:ARG:HD3	2:C:228:ARG:HA	1.82	0.61
3:D:888:GLU:OE2	3:D:970:THR:HG22	2.00	0.61
5:G:38:LEU:O	5:G:42:LEU:HD13	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:ILE:HG12	3:D:211:ARG:NH1	2.15	0.61
1:A:2:LEU:HD22	1:B:144:ARG:HH21	1.66	0.61
2:C:312:GLY:O	2:C:316:VAL:HG23	2.00	0.61
5:G:63:LYS:HG3	5:G:82:VAL:CG1	2.31	0.61
7:N:36:DT:H2''	7:N:37:DG:C8	2.36	0.61
3:D:360:LEU:HD23	3:D:360:LEU:O	1.99	0.60
3:D:924:THR:HG21	3:D:977:THR:O	2.01	0.60
5:G:33:ASP:OD2	5:G:35:ALA:HB3	2.01	0.60
6:T:7:DT:H2''	6:T:8:DC:C6	2.36	0.60
2:C:545:ASN:O	2:C:545:ASN:ND2	2.32	0.60
3:D:128:ILE:HD13	3:D:135:VAL:HG21	1.83	0.60
5:G:145:ASP:O	5:G:149:LYS:HG3	2.00	0.60
2:C:251:ARG:HH22	2:C:357:VAL:HG23	1.65	0.60
3:D:364:GLU:O	3:D:367:VAL:HG22	2.02	0.60
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.81	0.60
2:C:248:ILE:CD1	2:C:249:VAL:HG23	2.29	0.60
2:C:452:LYS:O	2:C:453:ARG:HB2	2.01	0.60
2:C:547:PRO:O	2:C:555:VAL:HG23	2.01	0.60
2:C:1107:VAL:HG11	3:D:469:ILE:HD13	1.83	0.60
3:D:166:ARG:NH1	3:D:170:LEU:HB2	2.16	0.60
3:D:1126:GLY:O	3:D:1130:VAL:HG23	2.01	0.60
7:N:19:DA:H1'	7:N:20:DA:N7	2.17	0.60
3:D:91:ARG:O	3:D:321:PRO:HG3	2.02	0.60
8:R:20:G:H1'	8:R:21:C:C4	2.37	0.60
3:D:159:ARG:NE	3:D:216:LEU:HD22	2.17	0.60
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.83	0.60
3:D:789:LEU:HD11	3:D:793:TYR:HE1	1.67	0.60
2:C:215:ASP:OD1	2:C:215:ASP:N	2.35	0.59
2:C:240:ALA:O	2:C:274:LEU:HD21	2.02	0.59
1:A:184:GLU:OE1	1:A:185:GLN:HG3	2.02	0.59
2:C:1157:ARG:NH1	2:C:1158:ALA:HA	2.16	0.59
2:C:628:THR:HG22	2:C:629:GLY:N	2.17	0.59
2:C:776:ILE:CD1	2:C:781:LEU:HD21	2.32	0.59
5:G:93:LYS:CG	5:G:96:GLN:HB2	2.32	0.59
5:G:144:LEU:HD12	5:G:144:LEU:H	1.66	0.59
2:C:212:LEU:HD12	2:C:212:LEU:O	2.02	0.59
3:D:1166:THR:HG22	3:D:1180:LEU:CD2	2.32	0.59
2:C:119:VAL:HG23	2:C:167:ILE:CD1	2.33	0.59
2:C:961:ASP:OD1	2:C:962:GLU:N	2.30	0.59
5:G:51:VAL:HG12	5:G:110:LEU:HD22	1.84	0.59
5:G:83:GLU:OE2	5:G:151:LEU:HD11	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:ARG:HH12	3:D:170:LEU:HD22	1.66	0.59
2:C:1146:GLU:OE1	2:C:1146:GLU:N	2.36	0.59
3:D:268:PHE:HE2	3:D:270:ILE:HD13	1.67	0.59
2:C:556:GLU:CD	2:C:557:PRO:HD2	2.23	0.59
2:C:853:PHE:HD2	2:C:868:LEU:HD12	1.67	0.59
3:D:289:LYS:O	3:D:293:LEU:HD13	2.02	0.59
3:D:1079:LYS:HE2	3:D:1079:LYS:HA	1.85	0.59
2:C:298:ASN:HD21	2:C:302:LYS:HD2	1.67	0.59
3:D:1173:THR:HG21	3:D:1201:ALA:CB	2.32	0.59
7:N:5:DG:H2''	7:N:6:DC:C6	2.37	0.59
2:C:197:LYS:NZ	2:C:218:LYS:O	2.30	0.58
3:D:170:LEU:HD11	3:D:205:MET:HE3	1.85	0.58
2:C:830:ARG:NH1	2:C:832:VAL:HG22	2.19	0.58
2:C:934:THR:CG2	2:C:1026:GLY:HA3	2.33	0.58
1:A:225:LEU:HD22	1:B:208:LEU:HD23	1.84	0.58
1:B:72:ASP:O	1:B:76:ILE:HG12	2.04	0.58
3:D:181:LEU:HD21	3:D:198:ARG:HE	1.67	0.58
3:D:209:ARG:HD2	3:D:213:GLN:HE21	1.68	0.58
3:D:67:ARG:HA	3:D:67:ARG:NH1	2.18	0.58
5:G:52:VAL:CG1	5:G:129:VAL:HG13	2.34	0.58
5:G:70:VAL:HG22	5:G:79:ILE:HD12	1.85	0.58
6:T:6:DG:H2''	6:T:7:DT:C6	2.37	0.58
2:C:225:ARG:CD	2:C:228:ARG:HA	2.33	0.58
3:D:346:ARG:NH1	7:N:18:DC:OP2	2.36	0.58
6:T:35:DG:H2''	6:T:36:DC:C6	2.37	0.58
2:C:116:LYS:HE2	2:C:156:ASP:OD2	2.03	0.58
3:D:209:ARG:O	3:D:213:GLN:HG3	2.03	0.58
2:C:239:LYS:HE2	2:C:239:LYS:HA	1.86	0.58
2:C:934:THR:HG23	2:C:1026:GLY:HA3	1.85	0.58
3:D:153:ALA:O	3:D:157:VAL:HG23	2.04	0.58
3:D:208:ILE:HG12	3:D:211:ARG:HH12	1.69	0.58
2:C:756:GLU:CG	2:C:870:ARG:HG2	2.34	0.58
3:D:215:GLU:O	3:D:219:LEU:HD13	2.04	0.58
5:G:65:ASN:O	5:G:69:ARG:HG3	2.04	0.58
2:C:141:ASN:HD21	2:C:144:THR:HB	1.67	0.58
2:C:229:LYS:HD2	2:C:281:LEU:HD23	1.85	0.58
2:C:245:SER:O	2:C:248:ILE:HD11	2.04	0.58
2:C:271:ASP:O	2:C:275:LEU:HG	2.04	0.58
3:D:209:ARG:O	3:D:209:ARG:HD3	2.04	0.57
1:B:106:THR:HG22	1:B:107:ALA:H	1.68	0.57
2:C:298:ASN:ND2	2:C:302:LYS:HD2	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:ILE:O	2:C:420:ILE:HG22	2.04	0.57
2:C:650:ILE:HD13	2:C:690:VAL:HG21	1.86	0.57
1:B:102:PRO:HG3	1:B:131:LYS:HZ3	1.69	0.57
2:C:658:ILE:HD12	2:C:702:ILE:CG2	2.34	0.57
3:D:637:LEU:CD2	3:D:640:LEU:HD12	2.31	0.57
6:T:4:DC:H2"	6:T:5:DA:N7	2.19	0.57
3:D:861:ALA:O	3:D:865:LEU:HG	2.04	0.57
1:B:25:PRO:CB	1:B:183:VAL:HG21	2.35	0.57
2:C:230:ARG:HG3	2:C:231:ARG:H	1.69	0.57
2:C:1087:GLU:OE2	2:C:1092:LYS:NZ	2.36	0.57
3:D:599:TYR:OH	3:D:608:GLU:OE1	2.23	0.57
2:C:232:GLN:HE22	2:C:280:LYS:HE3	1.68	0.57
2:C:944:TRP:HB2	2:C:991:CYS:O	2.04	0.57
1:B:128:LEU:HD21	1:B:134:LEU:HD23	1.86	0.57
2:C:222:VAL:HG23	2:C:234:VAL:CG1	2.35	0.57
2:C:222:VAL:O	2:C:234:VAL:HG13	2.05	0.57
3:D:159:ARG:HE	3:D:216:LEU:HD22	1.69	0.57
3:D:776:GLU:O	3:D:779:LYS:HG3	2.04	0.57
1:A:208:LEU:HD23	1:B:225:LEU:CD1	2.35	0.56
2:C:547:PRO:HB2	2:C:555:VAL:CG2	2.35	0.56
2:C:720:LEU:HD12	2:C:1026:GLY:O	2.05	0.56
2:C:785:ASP:OD2	2:C:787:ARG:NH1	2.38	0.56
3:D:217:ASP:HA	3:D:220:GLU:CG	2.36	0.56
3:D:1078:ASP:OD1	3:D:1079:LYS:N	2.33	0.56
5:G:63:LYS:HG3	5:G:82:VAL:HG11	1.85	0.56
6:T:9:DG:H2"	6:T:10:DC:C6	2.39	0.56
2:C:253:GLY:CA	2:C:259:ARG:HH22	2.17	0.56
3:D:810:ASN:OD1	3:D:1017:GLN:NE2	2.38	0.56
3:D:955:ALA:HB3	3:D:957:ILE:CD1	2.35	0.56
3:D:1275:THR:HG23	3:D:1278:ALA:H	1.71	0.56
5:G:93:LYS:HG3	5:G:93:LYS:O	2.05	0.56
2:C:195:THR:OG1	2:C:197:LYS:HE2	2.05	0.56
2:C:253:GLY:HA2	2:C:259:ARG:NH2	2.20	0.56
2:C:282:ARG:HB2	2:C:285:GLU:OE2	2.06	0.56
6:T:37:DG:H2"	6:T:38:DC:C6	2.41	0.56
2:C:290:GLU:OE1	2:C:290:GLU:N	2.25	0.56
3:D:1171:GLY:HA3	3:D:1199:GLU:CD	2.26	0.56
5:G:93:LYS:HD3	5:G:98:LYS:NZ	2.21	0.56
1:B:3:ILE:HD13	1:B:234:ILE:HG22	1.88	0.56
1:B:106:THR:HG23	1:B:123:MET:O	2.06	0.56
5:G:81:GLN:OE1	5:G:112:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ASP:OD1	2:C:189:GLU:N	2.39	0.56
2:C:786:GLU:OE1	2:C:787:ARG:HB3	2.06	0.56
3:D:158:GLU:O	3:D:162:VAL:HG23	2.05	0.56
2:C:260:SER:HB3	2:C:264:LYS:NZ	2.21	0.56
3:D:159:ARG:HH12	3:D:220:GLU:HB3	1.71	0.56
3:D:475:MET:HG3	3:D:480:ARG:HG3	1.88	0.56
2:C:764:LEU:HD12	2:C:765:GLY:N	2.21	0.56
3:D:1173:THR:CG2	3:D:1201:ALA:HB2	2.37	0.56
3:D:250:GLU:N	3:D:250:GLU:OE1	2.38	0.55
3:D:366:ILE:HD12	3:D:366:ILE:H	1.71	0.55
3:D:980:GLY:O	3:D:988:LEU:HD12	2.06	0.55
2:C:291:SER:HA	2:C:294:THR:HG22	1.88	0.55
2:C:628:THR:HG23	2:C:975:PRO:HA	1.88	0.55
3:D:1088:VAL:CG1	3:D:1098:VAL:HG22	2.31	0.55
2:C:83:VAL:HB	2:C:87:GLU:OE2	2.06	0.55
2:C:88:GLU:HG3	2:C:89:VAL:N	2.21	0.55
2:C:1136:GLU:O	3:D:10:LEU:HD12	2.06	0.55
3:D:304:GLN:OE1	3:D:305:SER:OG	2.07	0.55
1:B:74:THR:CG2	3:D:608:GLU:HG3	2.37	0.55
1:B:228:GLU:OE1	1:B:228:GLU:N	2.38	0.55
2:C:302:LYS:HG2	2:C:304:LYS:HE2	1.88	0.55
3:D:200:GLY:HA2	3:D:203:ARG:HG2	1.87	0.55
7:N:23:DC:N3	7:N:26:DT:H72	2.22	0.55
3:D:365:ILE:CD1	5:G:134:GLY:HA2	2.35	0.55
3:D:759:GLN:CD	3:D:765:LEU:HD11	2.27	0.55
5:G:68:THR:HA	5:G:71:GLN:NE2	2.21	0.55
2:C:240:ALA:HB1	2:C:274:LEU:HD23	1.87	0.55
2:C:558:ARG:HB3	2:C:570:TYR:CE2	2.41	0.55
2:C:620:ARG:HB2	2:C:717:LYS:NZ	2.22	0.55
3:D:364:GLU:N	3:D:364:GLU:OE1	2.40	0.55
1:B:74:THR:HG21	3:D:608:GLU:HG3	1.89	0.55
1:B:230:GLU:HG3	1:B:230:GLU:O	2.06	0.55
2:C:507:ASN:HB2	2:C:511:PHE:O	2.07	0.55
2:C:547:PRO:HB2	2:C:555:VAL:CB	2.35	0.55
2:C:721:VAL:HG22	2:C:915:ILE:HG23	1.88	0.55
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.42	0.55
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.88	0.55
3:D:901:LEU:CD2	3:D:916:ILE:HD11	2.35	0.55
2:C:445:PRO:HG3	2:C:640:ASP:OD2	2.07	0.55
2:C:621:SER:O	2:C:709:ASP:HB2	2.06	0.54
3:D:354:LEU:HD22	3:D:354:LEU:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:4:DC:H2'	6:T:4:DC:OP2	2.07	0.54
6:T:31:DG:H2''	6:T:32:DC:C6	2.42	0.54
1:B:60:LEU:HD21	1:B:159:ILE:HD11	1.90	0.54
2:C:302:LYS:HG2	2:C:304:LYS:CE	2.38	0.54
1:A:93:VAL:CG1	1:A:113:PRO:HG2	2.37	0.54
1:A:93:VAL:HG12	1:A:113:PRO:HG2	1.88	0.54
1:B:97:LEU:HD12	1:B:110:ILE:HD13	1.89	0.54
2:C:220:ASP:HB3	2:C:257:ILE:HG13	1.90	0.54
3:D:580:ASP:OD1	3:D:580:ASP:N	2.37	0.54
1:A:111:VAL:HG23	1:A:111:VAL:O	2.07	0.54
1:B:106:THR:HG22	1:B:107:ALA:N	2.21	0.54
3:D:203:ARG:HA	3:D:206:ARG:HE	1.71	0.54
1:B:111:VAL:O	1:B:111:VAL:HG13	2.07	0.54
3:D:137:THR:HG21	3:D:263:LYS:HE3	1.90	0.54
1:A:33:THR:HG22	1:B:36:ASN:ND2	2.23	0.54
2:C:214:PHE:CD1	2:C:224:VAL:HG12	2.43	0.54
3:D:901:LEU:HD13	3:D:901:LEU:O	2.08	0.54
3:D:1117:ASP:O	3:D:1121:VAL:HG23	2.07	0.54
1:A:218:LEU:HD21	1:B:34:LEU:HD11	1.88	0.54
2:C:192:ASP:CB	2:C:197:LYS:H	2.21	0.54
3:D:338:SER:O	3:D:340:LEU:N	2.39	0.54
2:C:848:ILE:HD11	2:C:874:ALA:CB	2.38	0.54
2:C:1158:ALA:O	2:C:1160:ALA:N	2.39	0.54
5:G:105:LEU:HD21	5:G:150:PHE:CE2	2.43	0.54
6:T:8:DC:H2''	6:T:9:DG:C8	2.43	0.54
1:B:187:THR:O	1:B:187:THR:HG22	2.07	0.53
3:D:459:ARG:HB3	3:D:486:VAL:HG21	1.90	0.53
1:B:60:LEU:HD11	1:B:159:ILE:HD12	1.90	0.53
2:C:558:ARG:HB3	2:C:570:TYR:CD2	2.43	0.53
3:D:657:GLN:OE1	3:D:657:GLN:HA	2.08	0.53
5:G:88:GLU:H	5:G:155:GLY:HA3	1.73	0.53
7:N:6:DC:H2''	7:N:7:DA:C8	2.44	0.53
7:N:7:DA:C2'	7:N:8:DT:H71	2.39	0.53
7:N:11:DT:H2''	7:N:12:DG:C8	2.44	0.53
2:C:421:ARG:O	2:C:424:VAL:HG22	2.09	0.53
3:D:1131:GLN:O	3:D:1135:VAL:HG23	2.09	0.53
2:C:303:GLU:O	2:C:303:GLU:HG3	2.08	0.53
3:D:877:LEU:O	3:D:880:VAL:HG12	2.09	0.53
3:D:1068:PRO:HD3	3:D:1074:GLU:OE1	2.08	0.53
3:D:1136:ARG:O	3:D:1140:GLU:HG3	2.09	0.53
7:N:10:DC:H2'	7:N:11:DT:H71	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:63:LYS:O	5:G:67:GLU:HG3	2.09	0.53
2:C:547:PRO:CB	2:C:555:VAL:HB	2.39	0.53
1:B:73:VAL:O	1:B:77:ILE:HD13	2.09	0.53
2:C:787:ARG:O	2:C:787:ARG:CG	2.56	0.53
2:C:833:ARG:NH1	8:R:19:A:H5'	2.23	0.53
2:C:444:ASN:HB2	2:C:445:PRO:HD2	1.90	0.52
3:D:365:ILE:HG23	3:D:366:ILE:HD12	1.90	0.52
2:C:520:VAL:HG23	2:C:521:ASP:OD1	2.08	0.52
3:D:239:ASN:O	3:D:242:ARG:HG2	2.10	0.52
2:C:276:ASP:O	2:C:279:ARG:HG2	2.09	0.52
2:C:520:VAL:O	2:C:523:VAL:HG12	2.10	0.52
2:C:583:PRO:O	2:C:584:ARG:HG2	2.08	0.52
3:D:208:ILE:HG23	3:D:211:ARG:NH2	2.24	0.52
3:D:1050:THR:HG22	3:D:1106:GLU:CA	2.34	0.52
1:A:32:TYR:HD1	1:A:176:TYR:HE1	1.56	0.52
1:B:182:ARG:HG2	1:B:187:THR:HA	1.92	0.52
2:C:483:MET:CE	2:C:498:GLY:HA3	2.40	0.52
2:C:921:GLY:O	2:C:925:ARG:HG3	2.10	0.52
2:C:943:GLY:O	2:C:992:THR:HG23	2.09	0.52
3:D:613:SER:O	3:D:614:SER:OG	2.22	0.52
7:N:19:DA:H1'	7:N:20:DA:C8	2.45	0.52
2:C:336:GLU:O	2:C:339:VAL:HG22	2.10	0.52
3:D:156:ALA:O	3:D:160:LYS:HG3	2.10	0.52
3:D:166:ARG:HH21	3:D:209:ARG:CB	2.18	0.52
2:C:868:LEU:HD22	2:C:869:VAL:N	2.24	0.52
2:C:931:ILE:HD12	2:C:932:LEU:HD13	1.91	0.52
3:D:498:LEU:HD23	3:D:543:VAL:HG22	1.91	0.52
3:D:1064:ILE:N	3:D:1064:ILE:HD12	2.25	0.52
5:G:92:ILE:HG22	5:G:95:GLY:H	1.75	0.52
7:N:12:DG:H2''	7:N:13:DC:H6	1.75	0.52
3:D:847:LEU:O	3:D:851:ILE:HG23	2.09	0.52
6:T:6:DG:H2''	6:T:7:DT:H6	1.74	0.52
7:N:14:DT:H2''	7:N:15:DC:C5	2.45	0.52
1:B:105:VAL:CG1	1:B:126:ALA:HB3	2.40	0.51
2:C:30:ASN:O	2:C:31:SER:OG	2.24	0.51
3:D:1051:GLY:O	3:D:1104:HIS:ND1	2.43	0.51
3:D:1060:ARG:HG2	3:D:1061:PHE:CD1	2.46	0.51
3:D:645:GLU:HG2	3:D:646:ILE:N	2.25	0.51
1:B:129:ASN:O	1:B:131:LYS:HE2	2.10	0.51
2:C:222:VAL:HG23	2:C:234:VAL:HG13	1.92	0.51
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:ASP:HA	3:D:220:GLU:HG3	1.92	0.51
3:D:1171:GLY:HA3	3:D:1199:GLU:OE1	2.11	0.51
6:T:2:DG:H2"	6:T:3:DG:C8	2.46	0.51
1:A:11:GLU:OE1	1:A:205:ARG:NH2	2.44	0.51
2:C:163:LYS:HE2	2:C:639:GLY:HA3	1.91	0.51
2:C:235:THR:O	2:C:239:LYS:HG2	2.10	0.51
3:D:141:GLU:OE1	3:D:141:GLU:N	2.38	0.51
3:D:240:LEU:O	3:D:244:LEU:HD13	2.11	0.51
2:C:857:ASP:O	2:C:858:GLU:HG2	2.10	0.51
3:D:201:GLY:O	3:D:205:MET:HG3	2.10	0.51
1:B:112:PRO:CB	1:B:116:VAL:HG23	2.41	0.51
2:C:507:ASN:OD1	2:C:508:PRO:HD2	2.10	0.51
3:D:1091:HIS:CG	3:D:1092:GLU:H	2.29	0.51
2:C:444:ASN:HB2	2:C:445:PRO:CD	2.40	0.51
3:D:911:ILE:O	3:D:911:ILE:HG13	2.10	0.51
3:D:217:ASP:O	3:D:220:GLU:HG3	2.11	0.51
3:D:1088:VAL:HG12	3:D:1098:VAL:CG2	2.32	0.51
1:A:71:GLU:HB3	1:A:75:GLU:HG3	1.93	0.50
1:B:69:VAL:CG2	1:B:134:LEU:HD21	2.41	0.50
2:C:239:LYS:HE2	2:C:239:LYS:CA	2.41	0.50
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.27	0.50
2:C:620:ARG:HB2	2:C:717:LYS:HZ1	1.75	0.50
2:C:763:LYS:HE2	2:C:763:LYS:CA	2.41	0.50
7:N:13:DC:H2"	7:N:14:DT:OP2	2.10	0.50
2:C:62:GLU:OE1	2:C:67:SER:OG	2.13	0.50
4:E:94:ILE:O	4:E:98:GLU:HG3	2.10	0.50
1:A:15:THR:HG22	1:A:16:ASP:N	2.21	0.50
3:D:82:VAL:O	3:D:82:VAL:HG13	2.11	0.50
3:D:901:LEU:O	3:D:902:ALA:HB3	2.11	0.50
5:G:86:THR:HG21	5:G:101:ASN:HB3	1.94	0.50
5:G:98:LYS:HD3	5:G:100:VAL:HG22	1.92	0.50
2:C:773:ILE:HG21	2:C:776:ILE:CD1	2.41	0.50
3:D:32:GLU:HB3	3:D:42:GLU:HG3	1.93	0.50
4:E:44:LEU:O	4:E:44:LEU:HD23	2.11	0.50
5:G:66:LEU:O	5:G:70:VAL:HG23	2.11	0.50
2:C:326:GLU:OE1	2:C:326:GLU:N	2.31	0.50
2:C:500:LEU:HD22	2:C:504:ALA:HB3	1.93	0.50
2:C:790:VAL:HG22	2:C:791:ARG:N	2.26	0.50
2:C:895:ILE:N	2:C:895:ILE:HD12	2.26	0.50
3:D:281:ILE:CA	3:D:289:LYS:HE3	2.33	0.50
3:D:343:LEU:O	3:D:347:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1164:ARG:HG3	3:D:1208:MET:SD	2.52	0.50
2:C:409:VAL:HG12	2:C:410:GLU:H	1.75	0.50
3:D:170:LEU:HD11	3:D:205:MET:CE	2.42	0.50
7:N:15:DC:H2''	7:N:16:DA:C8	2.46	0.50
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.39	0.50
1:A:165:ASP:OD1	1:A:166:SER:N	2.45	0.50
2:C:964:LEU:O	2:C:965:GLU:HG2	2.11	0.50
3:D:409:LYS:O	3:D:409:LYS:HG2	2.11	0.50
3:D:657:GLN:N	3:D:658:PRO:CD	2.74	0.50
3:D:1016:HIS:O	3:D:1017:GLN:HG3	2.12	0.50
6:T:26:DG:H2''	6:T:27:DA:H8	1.76	0.50
1:A:173:LYS:CE	2:C:911:THR:HG22	2.42	0.50
3:D:160:LYS:O	3:D:163:GLU:HG3	2.12	0.50
1:B:3:ILE:HD11	1:B:234:ILE:HA	1.93	0.50
1:B:30:PHE:O	1:B:34:LEU:HD13	2.12	0.50
2:C:347:ARG:HD2	2:C:355:MET:HB2	1.93	0.50
2:C:786:GLU:CD	2:C:787:ARG:HB3	2.33	0.50
2:C:739:ASN:O	2:C:739:ASN:ND2	2.39	0.49
1:B:128:LEU:HD21	1:B:134:LEU:HD21	1.94	0.49
2:C:106:SER:OG	2:C:138:GLU:HG2	2.12	0.49
2:C:524:VAL:HG21	2:C:548:ILE:HD11	1.92	0.49
3:D:14:LEU:HD21	3:D:106:TYR:OH	2.12	0.49
3:D:885:ILE:HG23	3:D:993:GLU:O	2.11	0.49
2:C:721:VAL:HG22	2:C:915:ILE:CG2	2.42	0.49
2:C:1157:ARG:HH11	2:C:1158:ALA:CA	2.22	0.49
3:D:330:LEU:HB2	3:D:334:ARG:O	2.12	0.49
3:D:1064:ILE:HG22	3:D:1066:ILE:HG13	1.94	0.49
2:C:756:GLU:HG2	2:C:870:ARG:HG2	1.93	0.49
6:T:7:DT:H2''	6:T:8:DC:C5	2.48	0.49
7:N:9:DG:H2''	7:N:10:DC:C5	2.48	0.49
7:N:10:DC:H1'	7:N:11:DT:H5'	1.94	0.49
1:B:15:THR:HG22	1:B:16:ASP:N	2.28	0.49
1:B:228:GLU:O	1:B:228:GLU:HG2	2.13	0.49
3:D:64:LYS:HE3	3:D:65:TYR:CE2	2.48	0.49
3:D:1166:THR:HG22	3:D:1180:LEU:HD23	1.93	0.49
3:D:1195:ALA:C	3:D:1196:GLU:HG3	2.32	0.49
5:G:83:GLU:CD	5:G:151:LEU:HD21	2.33	0.49
7:N:28:DA:H2''	7:N:29:DC:O5'	2.13	0.49
1:B:5:GLN:HA	1:B:5:GLN:OE1	2.12	0.49
2:C:168:ILE:HG12	2:C:173:ARG:HD2	1.95	0.49
2:C:560:LEU:CD1	3:D:847:LEU:HD11	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:20:G:H1'	8:R:21:C:C5	2.48	0.49
3:D:1091:HIS:HE1	3:D:1104:HIS:H	1.60	0.49
2:C:168:ILE:CG1	2:C:173:ARG:HD2	2.42	0.49
2:C:786:GLU:OE2	2:C:787:ARG:HD2	2.13	0.49
3:D:190:LYS:O	3:D:194:ARG:HG2	2.13	0.49
3:D:1088:VAL:O	3:D:1088:VAL:HG23	2.12	0.49
6:T:2:DG:H2''	6:T:3:DG:H8	1.78	0.49
2:C:162:GLU:C	2:C:163:LYS:HD2	2.33	0.48
7:N:7:DA:H2''	7:N:8:DT:C5	2.47	0.48
2:C:244:THR:CG2	2:C:247:GLN:HG3	2.43	0.48
2:C:607:MET:HE1	2:C:892:LYS:HD3	1.95	0.48
3:D:742:LYS:HE3	3:D:746:LEU:HD11	1.96	0.48
4:E:33:LEU:HD23	4:E:33:LEU:H	1.76	0.48
7:N:4:DC:H2''	7:N:5:DG:H8	1.76	0.48
2:C:141:ASN:ND2	2:C:144:THR:H	2.12	0.48
2:C:846:LYS:O	2:C:873:VAL:HG13	2.13	0.48
2:C:1159:ALA:HB1	3:D:470:LYS:HZ3	1.78	0.48
3:D:31:PRO:HB3	3:D:345:ARG:HG3	1.95	0.48
3:D:98:ALA:HB3	3:D:354:LEU:HD12	1.96	0.48
5:G:70:VAL:HG13	5:G:75:VAL:CG2	2.32	0.48
3:D:208:ILE:HG12	3:D:211:ARG:NH2	2.29	0.48
3:D:1122:LEU:HB2	3:D:1130:VAL:HG21	1.95	0.48
5:G:92:ILE:CD1	5:G:97:ARG:HG2	2.43	0.48
5:G:98:LYS:HG3	5:G:100:VAL:HG23	1.96	0.48
2:C:770:THR:OG1	2:C:771:ARG:N	2.47	0.48
2:C:1098:GLY:O	2:C:1102:VAL:HG23	2.14	0.48
3:D:242:ARG:HA	3:D:245:VAL:HG12	1.95	0.48
5:G:58:TYR:CD2	5:G:61:LYS:HE3	2.49	0.48
1:B:25:PRO:HB3	1:B:183:VAL:HG21	1.95	0.48
2:C:416:THR:HG22	2:C:416:THR:O	2.12	0.48
2:C:789:ILE:HG21	2:C:850:ILE:CG2	2.43	0.48
3:D:136:ILE:HD12	3:D:229:LEU:HD22	1.95	0.48
3:D:211:ARG:HA	3:D:214:ARG:HE	1.79	0.48
6:T:3:DG:H2''	6:T:4:DC:H6	1.78	0.48
1:A:98:ARG:HG2	1:A:135:GLU:OE1	2.13	0.48
2:C:1106:ILE:HG21	3:D:454:PRO:HB2	1.95	0.48
2:C:1157:ARG:HG2	2:C:1158:ALA:H	1.79	0.48
3:D:73:ILE:O	3:D:82:VAL:HG12	2.14	0.48
3:D:113:ARG:HG2	3:D:1238:ILE:CD1	2.44	0.48
3:D:615:PRO:O	3:D:619:ILE:HG13	2.14	0.48
1:B:120:ASN:H	1:B:120:ASN:HD22	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:CD1	1:B:134:LEU:HD23	2.37	0.48
2:C:810:GLY:H	2:C:831:GLU:CG	2.27	0.48
2:C:918:ASN:OD1	2:C:919:THR:N	2.47	0.48
3:D:155:MET:HA	3:D:158:GLU:OE1	2.13	0.48
3:D:1054:ARG:HA	3:D:1101:ASP:OD1	2.14	0.48
3:D:1269:ASN:O	4:E:109:GLY:HA3	2.13	0.48
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.96	0.47
2:C:119:VAL:HG23	2:C:167:ILE:HD12	1.95	0.47
3:D:76:GLU:OE1	3:D:76:GLU:N	2.46	0.47
3:D:320:ILE:CG2	3:D:325:ARG:HD3	2.44	0.47
3:D:374:LEU:HD23	3:D:374:LEU:C	2.35	0.47
3:D:449:LEU:HD21	3:D:483:VAL:CG1	2.44	0.47
3:D:905:ALA:N	3:D:909:THR:O	2.42	0.47
3:D:1056:GLU:HB2	3:D:1063:LYS:HE3	1.96	0.47
3:D:1062:TYR:HE2	3:D:1086:LEU:HD11	1.79	0.47
1:A:72:ASP:OD1	1:A:72:ASP:N	2.23	0.47
2:C:1155:LEU:HD12	2:C:1155:LEU:O	2.14	0.47
2:C:585:GLN:O	2:C:585:GLN:HG3	2.13	0.47
3:D:824:VAL:HG12	3:D:825:THR:N	2.30	0.47
3:D:1085:ARG:HB2	3:D:1113:GLU:HG3	1.95	0.47
2:C:791:ARG:O	2:C:847:VAL:HG11	2.14	0.47
2:C:310:ARG:NH1	2:C:328:ILE:HD11	2.29	0.47
3:D:504:LEU:HB3	3:D:1005:GLU:HG2	1.96	0.47
2:C:483:MET:HE2	2:C:498:GLY:HA3	1.97	0.47
2:C:777:SER:O	2:C:780:VAL:HG22	2.14	0.47
3:D:208:ILE:HG12	3:D:211:ARG:CZ	2.45	0.47
3:D:238:GLU:H	3:D:238:GLU:CD	2.17	0.47
3:D:492:ALA:O	3:D:493:GLU:HB2	2.14	0.47
3:D:957:ILE:N	3:D:957:ILE:HD12	2.30	0.47
3:D:1128:ARG:O	3:D:1132:ILE:HG13	2.13	0.47
2:C:122:CYS:HA	2:C:127:MET:HG3	1.96	0.47
2:C:298:ASN:CB	2:C:305:ARG:HH22	2.27	0.47
2:C:650:ILE:HD13	2:C:690:VAL:CG2	2.43	0.47
3:D:123:LYS:H	3:D:123:LYS:HD3	1.79	0.47
3:D:128:ILE:CG2	3:D:135:VAL:HG21	2.45	0.47
6:T:9:DG:H2'	6:T:10:DC:H6	1.80	0.47
6:T:6:DG:C8	6:T:7:DT:H72	2.50	0.47
7:N:26:DT:C2'	7:N:26:DT:O2	2.63	0.47
1:A:105:VAL:HG23	1:A:128:LEU:HD13	1.95	0.47
3:D:181:LEU:HA	3:D:185:GLU:HB3	1.97	0.47
3:D:304:GLN:OE1	3:D:305:SER:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:898:VAL:HG11	3:D:959:GLN:NE2	2.30	0.47
2:C:138:GLU:HB2	2:C:149:SER:OG	2.15	0.47
2:C:298:ASN:CA	2:C:305:ARG:HH22	2.28	0.47
2:C:853:PHE:CD2	2:C:868:LEU:HD12	2.50	0.47
3:D:389:ARG:NE	3:D:389:ARG:HA	2.30	0.47
1:B:138:LEU:N	1:B:138:LEU:HD12	2.30	0.46
2:C:94:SER:HB2	2:C:95:PRO:HA	1.96	0.46
2:C:1157:ARG:O	2:C:1158:ALA:HB3	2.15	0.46
3:D:342:ASP:O	3:D:346:ARG:HG3	2.15	0.46
2:C:654:SER:O	2:C:688:PRO:HG3	2.15	0.46
2:C:792:ILE:HA	2:C:847:VAL:HG13	1.96	0.46
5:G:124:ARG:O	5:G:124:ARG:NH1	2.48	0.46
6:T:3:DG:H2''	6:T:4:DC:C6	2.50	0.46
2:C:611:MET:CE	2:C:886:ALA:HB1	2.45	0.46
3:D:184:LEU:CB	3:D:190:LYS:HE2	2.45	0.46
3:D:1097:ARG:CZ	3:D:1097:ARG:HB3	2.45	0.46
5:G:41:GLU:HG3	5:G:42:LEU:HD12	1.97	0.46
7:N:14:DT:H2''	7:N:15:DC:C6	2.50	0.46
2:C:216:VAL:HG22	2:C:222:VAL:HG12	1.97	0.46
2:C:369:ASP:OD1	2:C:370:ILE:N	2.48	0.46
3:D:151:LEU:HB3	3:D:223:TRP:HZ3	1.78	0.46
3:D:693:GLN:O	3:D:697:ILE:HG12	2.16	0.46
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.97	0.46
5:G:51:VAL:HG13	5:G:142:LEU:HD11	1.96	0.46
7:N:12:DG:H2''	7:N:13:DC:C6	2.51	0.46
1:B:3:ILE:HD11	1:B:234:ILE:HG22	1.97	0.46
2:C:304:LYS:HB3	2:C:305:ARG:HD3	1.97	0.46
2:C:400:VAL:HG23	2:C:417:LEU:O	2.15	0.46
1:A:95:MET:HE2	1:A:110:ILE:HG21	1.98	0.46
1:B:112:PRO:HB3	1:B:116:VAL:HG23	1.98	0.46
2:C:76:GLU:OE1	2:C:77:ARG:N	2.49	0.46
3:D:187:GLU:OE1	3:D:189:ALA:HB3	2.15	0.46
3:D:363:PRO:HD2	3:D:366:ILE:HD13	1.97	0.46
7:N:7:DA:H2''	7:N:8:DT:C7	2.45	0.46
1:A:9:LEU:CD1	1:A:23:ILE:HG12	2.43	0.46
1:A:213:LYS:HE2	1:B:229:ALA:HB3	1.96	0.46
2:C:225:ARG:HG2	2:C:228:ARG:HA	1.97	0.46
2:C:253:GLY:CA	2:C:259:ARG:HH12	2.23	0.46
2:C:538:ARG:O	2:C:538:ARG:HG3	2.16	0.46
3:D:155:MET:O	3:D:159:ARG:HG2	2.15	0.46
3:D:179:ALA:O	3:D:183:GLU:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:HD22	1:B:120:ASN:N	2.14	0.46
1:B:183:VAL:O	1:B:184:GLU:CB	2.64	0.46
2:C:591:THR:HG22	2:C:591:THR:O	2.16	0.46
3:D:1079:LYS:HE2	3:D:1079:LYS:CA	2.45	0.46
3:D:1086:LEU:HD23	3:D:1099:LEU:O	2.15	0.46
3:D:1195:ALA:O	3:D:1196:GLU:HG3	2.15	0.46
5:G:152:LEU:HD23	5:G:153:PRO:O	2.16	0.46
1:A:88:GLU:OE2	1:A:115:GLY:HA2	2.16	0.46
2:C:829:ALA:O	2:C:830:ARG:HB3	2.15	0.46
2:C:919:THR:O	2:C:919:THR:OG1	2.34	0.46
3:D:913:ASP:OD1	3:D:914:PRO:HD2	2.16	0.46
2:C:58:THR:O	2:C:62:GLU:HG2	2.15	0.46
2:C:192:ASP:OD2	2:C:195:THR:OG1	2.34	0.46
2:C:322:LEU:O	2:C:324:VAL:HG13	2.16	0.46
3:D:897:ILE:HD11	3:D:923:ARG:NH1	2.30	0.46
1:B:5:GLN:HE21	1:B:183:VAL:HG13	1.81	0.45
2:C:141:ASN:HD21	2:C:144:THR:CB	2.29	0.45
2:C:310:ARG:CZ	2:C:328:ILE:HD11	2.46	0.45
7:N:22:DG:C2'	7:N:23:DC:H5'	2.42	0.45
1:A:106:THR:HB	1:A:123:MET:O	2.16	0.45
1:A:138:LEU:HD12	1:A:138:LEU:N	2.30	0.45
3:D:348:ILE:HG12	3:D:348:ILE:H	1.59	0.45
3:D:350:ARG:NH2	7:N:18:DC:OP1	2.49	0.45
3:D:1087:ARG:HH11	3:D:1110:GLN:NE2	2.13	0.45
6:T:11:DC:H2'	6:T:12:DG:C8	2.51	0.45
2:C:773:ILE:HG23	2:C:774:PRO:CD	2.45	0.45
3:D:285:LYS:HA	3:D:289:LYS:CG	2.46	0.45
2:C:54:LEU:HD21	2:C:449:LEU:HD23	1.99	0.45
2:C:268:VAL:HG13	2:C:268:VAL:O	2.17	0.45
2:C:732:GLU:O	2:C:733:ASP:HB2	2.17	0.45
1:A:56:ILE:HG22	1:A:57:ASP:H	1.81	0.45
1:B:132:GLY:C	1:B:133:LYS:HD2	2.37	0.45
2:C:160:MET:SD	2:C:164:GLY:HA2	2.56	0.45
2:C:217:ASP:OD1	2:C:219:ARG:HD2	2.15	0.45
2:C:248:ILE:H	2:C:248:ILE:HG13	1.61	0.45
4:E:107:THR:HG23	4:E:107:THR:O	2.17	0.45
5:G:51:VAL:CG1	5:G:142:LEU:HD11	2.46	0.45
7:N:15:DC:H2''	7:N:16:DA:N7	2.31	0.45
1:B:91:GLU:HA	1:B:91:GLU:OE1	2.17	0.45
1:B:97:LEU:C	1:B:97:LEU:HD23	2.37	0.45
3:D:131:PHE:HB3	3:D:256:MET:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:81:PRO:HB3	4:E:94:ILE:HG21	1.98	0.45
6:T:8:DC:H2"	6:T:9:DG:H8	1.80	0.45
7:N:14:DT:C2	7:N:15:DC:C4	3.05	0.45
1:B:104:GLU:OE2	1:B:124:HIS:ND1	2.50	0.45
2:C:199:LEU:HD12	2:C:199:LEU:N	2.32	0.45
2:C:239:LYS:NZ	2:C:244:THR:O	2.50	0.45
2:C:783:ASP:O	2:C:791:ARG:HG3	2.16	0.45
5:G:68:THR:O	5:G:71:GLN:HG2	2.16	0.45
2:C:298:ASN:OD1	2:C:302:LYS:NZ	2.30	0.45
3:D:4:VAL:CG1	3:D:1256:LYS:HD3	2.42	0.45
3:D:66:LYS:O	3:D:67:ARG:HD2	2.17	0.45
3:D:160:LYS:HA	3:D:163:GLU:CG	2.46	0.45
1:A:56:ILE:HG22	1:A:57:ASP:N	2.32	0.45
2:C:232:GLN:NE2	2:C:280:LYS:HE3	2.32	0.45
2:C:569:GLU:HG3	2:C:571:VAL:HG12	1.99	0.45
2:C:619:VAL:HG12	2:C:619:VAL:O	2.17	0.45
3:D:242:ARG:O	3:D:245:VAL:HG12	2.17	0.45
2:C:370:ILE:HG12	2:C:370:ILE:O	2.17	0.45
2:C:976:VAL:HG13	2:C:977:PHE:CD2	2.52	0.45
3:D:320:ILE:HG12	3:D:321:PRO:HD2	1.99	0.45
3:D:773:ALA:O	3:D:777:ILE:HD13	2.16	0.45
3:D:796:ASP:OD1	3:D:796:ASP:N	2.49	0.45
3:D:931:ASP:OD2	3:D:937:ILE:HG12	2.17	0.45
3:D:965:VAL:CG2	3:D:974:VAL:HG11	2.47	0.45
5:G:87:GLU:OE1	5:G:155:GLY:N	2.50	0.45
2:C:298:ASN:O	2:C:305:ARG:NH2	2.50	0.44
2:C:1157:ARG:HH12	3:D:469:ILE:HD12	1.82	0.44
2:C:90:LEU:HD22	2:C:110:PRO:HG3	2.00	0.44
2:C:420:ILE:O	2:C:424:VAL:HG13	2.17	0.44
2:C:1037:VAL:O	2:C:1037:VAL:HG22	2.17	0.44
1:A:208:LEU:HD23	1:B:225:LEU:HD12	1.97	0.44
3:D:181:LEU:HD11	3:D:198:ARG:HE	1.82	0.44
3:D:262:GLN:O	3:D:266:GLU:HG3	2.18	0.44
3:D:287:GLN:OE1	3:D:287:GLN:N	2.39	0.44
3:D:760:PHE:CG	3:D:770:ARG:HD3	2.53	0.44
6:T:33:DA:C2'	6:T:34:DT:H72	2.48	0.44
2:C:244:THR:HG22	2:C:247:GLN:HG3	1.99	0.44
3:D:1154:ILE:HG22	3:D:1154:ILE:O	2.18	0.44
2:C:241:LEU:HD12	2:C:241:LEU:O	2.18	0.44
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.99	0.44
3:D:453:LYS:HG2	3:D:476:VAL:HG11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:PHE:CE2	2:C:389:ILE:HD11	2.52	0.44
2:C:193:LYS:HD3	2:C:194:SER:H	1.82	0.44
2:C:1100:VAL:O	2:C:1104:GLU:HG3	2.18	0.44
3:D:4:VAL:HG11	3:D:1256:LYS:HB3	2.00	0.44
3:D:548:SER:O	3:D:552:GLN:HG3	2.18	0.44
1:A:99:LYS:CG	1:A:105:VAL:HG22	2.42	0.44
2:C:797:ARG:HG2	2:C:798:ASP:H	1.83	0.44
2:C:848:ILE:HD11	2:C:874:ALA:HB2	1.99	0.44
3:D:89:ARG:HB3	3:D:323:GLU:HG3	2.00	0.44
3:D:174:ALA:O	3:D:178:GLU:HG3	2.18	0.44
4:E:79:VAL:HG22	4:E:80:GLY:N	2.33	0.44
1:B:228:GLU:H	1:B:228:GLU:CD	2.21	0.44
2:C:347:ARG:HD2	2:C:355:MET:CG	2.47	0.44
2:C:851:ARG:HD3	2:C:853:PHE:CZ	2.53	0.44
2:C:958:ARG:HD3	2:C:958:ARG:N	2.33	0.44
1:A:187:THR:HG22	1:A:187:THR:O	2.18	0.43
3:D:683:PHE:CE2	3:D:685:ASN:HB2	2.53	0.43
3:D:982:SER:HB3	3:D:985:THR:CG2	2.48	0.43
5:G:41:GLU:HG3	5:G:42:LEU:N	2.33	0.43
5:G:93:LYS:HD3	5:G:98:LYS:HZ1	1.82	0.43
2:C:130:ALA:HB1	2:C:157:PHE:O	2.18	0.43
2:C:1137:VAL:HG22	3:D:10:LEU:HD13	2.00	0.43
3:D:208:ILE:O	3:D:211:ARG:HG2	2.18	0.43
3:D:729:VAL:O	3:D:729:VAL:HG23	2.18	0.43
6:T:28:DG:H2"	6:T:29:DC:C6	2.53	0.43
7:N:15:DC:N3	7:N:16:DA:N6	2.66	0.43
2:C:208:ARG:O	2:C:208:ARG:HG3	2.18	0.43
2:C:225:ARG:CG	2:C:228:ARG:HA	2.49	0.43
3:D:396:ASN:O	3:D:396:ASN:ND2	2.51	0.43
3:D:925:LEU:HD11	3:D:960:VAL:CG1	2.48	0.43
3:D:1050:THR:CG2	3:D:1106:GLU:HA	2.40	0.43
3:D:1066:ILE:O	3:D:1066:ILE:HG22	2.19	0.43
5:G:92:ILE:HD12	5:G:97:ARG:HG2	1.99	0.43
1:A:151:GLN:HA	1:A:151:GLN:OE1	2.18	0.43
2:C:548:ILE:HG22	2:C:550:ALA:H	1.83	0.43
2:C:769:ILE:O	2:C:769:ILE:HG13	2.17	0.43
3:D:600:GLN:OE1	3:D:600:GLN:HA	2.17	0.43
3:D:1050:THR:HG23	3:D:1107:VAL:CG2	2.36	0.43
2:C:193:LYS:HD3	2:C:193:LYS:N	2.30	0.43
4:E:30:ASP:OD1	4:E:30:ASP:N	2.51	0.43
5:G:144:LEU:O	5:G:148:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1:DC:H2"	6:T:2:DG:H8	1.84	0.43
1:A:65:THR:HG22	1:A:66:VAL:N	2.34	0.43
2:C:54:LEU:HD22	2:C:452:LYS:HD2	2.01	0.43
2:C:1106:ILE:CG2	3:D:454:PRO:HB2	2.49	0.43
3:D:128:ILE:HG21	3:D:135:VAL:HG21	2.01	0.43
3:D:478:ARG:HE	3:D:480:ARG:HE	1.66	0.43
3:D:1065:THR:HB	3:D:1074:GLU:CG	2.49	0.43
2:C:141:ASN:HD22	2:C:144:THR:H	1.66	0.43
2:C:220:ASP:C	2:C:257:ILE:HG13	2.39	0.43
2:C:502:VAL:HG23	2:C:587:VAL:O	2.19	0.43
2:C:517:ARG:HD2	2:C:525:SER:O	2.18	0.43
2:C:773:ILE:HG22	2:C:774:PRO:O	2.19	0.43
2:C:1139:SER:HB2	2:C:1142:GLY:O	2.19	0.43
3:D:33:THR:HG22	3:D:46:LEU:HB2	2.01	0.43
2:C:611:MET:HE1	2:C:891:ASN:O	2.19	0.43
2:C:810:GLY:H	2:C:831:GLU:HG3	1.83	0.43
3:D:171:GLU:HA	3:D:171:GLU:OE1	2.19	0.43
3:D:982:SER:HB3	3:D:985:THR:HG22	2.01	0.43
3:D:1123:ARG:HG3	3:D:1204:ARG:HH21	1.84	0.43
4:E:31:THR:O	4:E:31:THR:HG23	2.18	0.43
1:B:69:VAL:HG21	1:B:134:LEU:HD21	2.00	0.42
1:B:112:PRO:HB2	1:B:116:VAL:HG23	2.01	0.42
2:C:122:CYS:HA	2:C:127:MET:CG	2.49	0.42
2:C:163:LYS:HE3	2:C:163:LYS:HA	2.00	0.42
2:C:725:PRO:O	3:D:725:THR:HG23	2.19	0.42
2:C:774:PRO:HG3	2:C:832:VAL:HG23	2.01	0.42
3:D:14:LEU:HD21	3:D:106:TYR:CZ	2.54	0.42
3:D:123:LYS:HD3	3:D:123:LYS:N	2.34	0.42
3:D:238:GLU:CG	3:D:242:ARG:HH21	2.32	0.42
2:C:50:VAL:HA	2:C:51:PRO:HD3	1.93	0.42
2:C:868:LEU:HD22	2:C:869:VAL:H	1.83	0.42
2:C:931:ILE:CD1	2:C:932:LEU:HD13	2.48	0.42
3:D:392:THR:HB	3:D:396:ASN:HA	2.01	0.42
2:C:563:ARG:NE	2:C:569:GLU:OE2	2.33	0.42
2:C:961:ASP:C	2:C:963:LEU:H	2.23	0.42
3:D:46:LEU:O	3:D:325:ARG:NH2	2.53	0.42
3:D:203:ARG:N	3:D:206:ARG:HH21	2.18	0.42
3:D:518:GLU:OE1	3:D:518:GLU:N	2.38	0.42
3:D:779:LYS:HD2	3:D:780:GLU:N	2.35	0.42
3:D:1056:GLU:OE1	3:D:1063:LYS:NZ	2.51	0.42
1:B:59:VAL:HG13	1:B:59:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CG	1:B:146:TYR:O	2.72	0.42
1:B:152:ASN:OD1	1:B:152:ASN:N	2.51	0.42
2:C:212:LEU:HD12	2:C:212:LEU:C	2.40	0.42
3:D:649:GLU:HA	3:D:649:GLU:OE1	2.20	0.42
1:B:72:ASP:OD1	1:B:75:GLU:HG3	2.20	0.42
2:C:244:THR:HG22	2:C:247:GLN:CG	2.49	0.42
2:C:421:ARG:HB2	2:C:422:PRO:HD3	2.01	0.42
3:D:136:ILE:HG12	3:D:252:PHE:HE1	1.84	0.42
3:D:203:ARG:HA	3:D:206:ARG:NE	2.35	0.42
3:D:592:VAL:HG23	3:D:592:VAL:O	2.19	0.42
5:G:52:VAL:HG11	5:G:129:VAL:HG13	2.01	0.42
6:T:5:DA:H2''	6:T:6:DG:H8	1.82	0.42
7:N:9:DG:H2''	7:N:10:DC:H5	1.84	0.42
1:A:27:GLU:OE1	1:A:28:PRO:HD2	2.19	0.42
3:D:240:LEU:HD23	3:D:244:LEU:CD1	2.42	0.42
7:N:5:DG:H2''	7:N:6:DC:C5	2.55	0.42
2:C:452:LYS:O	2:C:453:ARG:CB	2.66	0.42
2:C:1108:LYS:HD2	2:C:1157:ARG:NE	2.34	0.42
3:D:239:ASN:HA	3:D:242:ARG:HG2	2.02	0.42
3:D:285:LYS:HA	3:D:289:LYS:HG2	2.02	0.42
4:E:77:GLU:HG2	4:E:78:TYR:N	2.34	0.42
1:A:88:GLU:N	1:A:88:GLU:OE1	2.53	0.42
2:C:267:THR:O	2:C:268:VAL:C	2.58	0.42
2:C:298:ASN:HB3	2:C:305:ARG:HH22	1.85	0.42
3:D:229:LEU:HD23	3:D:229:LEU:HA	1.79	0.42
5:G:136:THR:HG22	5:G:137:SER:N	2.35	0.42
1:A:6:ARG:CG	1:A:7:PRO:HD2	2.50	0.42
2:C:236:VAL:HG23	2:C:237:LEU:N	2.35	0.42
2:C:753:GLU:HG3	2:C:754:GLU:N	2.35	0.42
2:C:1081:ALA:HB1	3:D:554:GLU:OE1	2.20	0.42
3:D:807:ALA:O	3:D:808:THR:HG23	2.19	0.42
3:D:1005:GLU:N	3:D:1006:PRO:HD2	2.35	0.42
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.42
1:B:110:ILE:O	1:B:111:VAL:HG12	2.20	0.42
1:B:159:ILE:HG13	1:B:160:GLY:N	2.34	0.42
2:C:385:ILE:HD12	2:C:385:ILE:O	2.20	0.42
2:C:413:THR:OG1	2:C:414:PRO:HD2	2.20	0.42
3:D:61:TYR:HB3	3:D:78:CYS:SG	2.60	0.42
3:D:120:LEU:HD12	3:D:120:LEU:HA	1.87	0.42
6:T:36:DC:H2''	6:T:37:DG:H8	1.82	0.42
1:A:17:ASN:OD1	1:A:17:ASN:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:409:VAL:HG12	2:C:410:GLU:N	2.35	0.41
2:C:658:ILE:HD12	2:C:702:ILE:HG23	2.02	0.41
2:C:667:ARG:CZ	2:C:667:ARG:HB2	2.50	0.41
3:D:340:LEU:HD23	3:D:340:LEU:HA	1.90	0.41
3:D:637:LEU:CD1	3:D:664:ALA:HB3	2.50	0.41
7:N:33:DG:H2"	7:N:34:DA:C8	2.55	0.41
1:A:199:LYS:O	1:A:200:ASN:CB	2.68	0.41
1:B:60:LEU:HD21	1:B:159:ILE:HG13	2.02	0.41
4:E:33:LEU:HD23	4:E:33:LEU:N	2.34	0.41
7:N:15:DC:C2	7:N:16:DA:C6	3.08	0.41
1:A:33:THR:HG21	1:B:40:ARG:HG3	2.02	0.41
1:A:181:THR:O	1:A:181:THR:HG22	2.21	0.41
2:C:557:PRO:HA	2:C:573:SER:HB2	2.02	0.41
1:A:11:GLU:HG2	1:A:12:ASP:N	2.35	0.41
2:C:68:PRO:O	2:C:72:GLU:HG3	2.21	0.41
2:C:762:THR:HG23	2:C:764:LEU:HD12	2.01	0.41
3:D:123:LYS:HB2	3:D:123:LYS:HE2	1.68	0.41
3:D:357:LEU:HD21	3:D:366:ILE:CG2	2.50	0.41
3:D:960:VAL:HG12	3:D:961:LYS:N	2.36	0.41
3:D:1162:LEU:HD21	3:D:1207:LEU:HD13	2.03	0.41
2:C:547:PRO:CG	2:C:555:VAL:HB	2.50	0.41
2:C:732:GLU:OE1	2:C:732:GLU:HA	2.21	0.41
2:C:847:VAL:HG13	2:C:847:VAL:O	2.20	0.41
2:C:1039:ASP:O	2:C:1060:LYS:NZ	2.54	0.41
3:D:181:LEU:HD21	3:D:198:ARG:NE	2.34	0.41
3:D:637:LEU:HD13	3:D:664:ALA:CB	2.51	0.41
5:G:105:LEU:HD21	5:G:150:PHE:HE2	1.85	0.41
1:B:81:LYS:O	1:B:81:LYS:HG2	2.20	0.41
1:B:164:VAL:HG23	1:B:165:ASP:O	2.21	0.41
2:C:150:GLN:HE21	2:C:414:PRO:HB2	1.84	0.41
2:C:343:GLU:O	2:C:346:VAL:HG12	2.20	0.41
3:D:931:ASP:HB3	3:D:957:ILE:HG13	2.02	0.41
7:N:13:DC:N1	7:N:14:DT:H72	2.34	0.41
1:A:158:GLU:OE2	1:A:159:ILE:HG22	2.20	0.41
1:B:185:GLN:H	1:B:185:GLN:NE2	2.18	0.41
2:C:241:LEU:HD11	2:C:243:TRP:CD1	2.55	0.41
2:C:523:VAL:HG13	2:C:523:VAL:O	2.20	0.41
2:C:666:THR:HG22	2:C:667:ARG:N	2.35	0.41
3:D:228:LYS:O	3:D:228:LYS:HG3	2.20	0.41
3:D:598:GLU:HG2	3:D:599:TYR:N	2.36	0.41
3:D:627:LEU:HG	3:D:628:SER:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1110:GLN:O	3:D:1110:GLN:HG3	2.20	0.41
2:C:253:GLY:HA2	2:C:259:ARG:CZ	2.50	0.41
2:C:763:LYS:HE2	2:C:763:LYS:HA	2.02	0.41
2:C:959:LEU:HD23	2:C:959:LEU:HA	1.91	0.41
3:D:39:LEU:HD22	3:D:39:LEU:N	2.35	0.41
3:D:95:ILE:HD13	3:D:348:ILE:HG23	2.02	0.41
3:D:124:ASP:O	3:D:128:ILE:HG13	2.21	0.41
3:D:357:LEU:HD12	3:D:357:LEU:HA	1.90	0.41
1:A:107:ALA:HB2	1:A:123:MET:HG2	2.03	0.41
1:B:107:ALA:O	1:B:110:ILE:HG12	2.21	0.41
2:C:792:ILE:HA	2:C:847:VAL:CG1	2.51	0.41
2:C:833:ARG:HH12	8:R:19:A:H5'	1.84	0.41
3:D:160:LYS:HA	3:D:163:GLU:HG3	2.02	0.41
3:D:212:ALA:O	3:D:216:LEU:HG	2.21	0.41
3:D:657:GLN:O	3:D:658:PRO:C	2.59	0.41
3:D:707:ILE:HD12	3:D:708:VAL:HG23	2.03	0.41
3:D:981:ARG:HD2	3:D:986:GLY:HA2	2.02	0.41
4:E:71:LEU:O	4:E:71:LEU:HD13	2.21	0.41
5:G:151:LEU:HD23	5:G:151:LEU:HA	1.92	0.41
1:A:18:ARG:HG2	1:A:197:GLU:HB2	2.03	0.41
3:D:62:CYS:SG	3:D:63:GLY:N	2.90	0.41
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.38	0.41
3:D:915:TYR:CE1	3:D:1143:ARG:HD2	2.55	0.41
3:D:928:ASP:OD1	3:D:940:ARG:HB2	2.21	0.41
1:A:128:LEU:N	1:A:128:LEU:HD12	2.35	0.40
1:B:69:VAL:HG22	1:B:134:LEU:HD21	2.03	0.40
1:B:176:TYR:HB3	1:B:194:LEU:HD12	2.03	0.40
2:C:193:LYS:H	2:C:193:LYS:CD	2.31	0.40
2:C:542:ALA:HA	2:C:561:VAL:HG12	2.02	0.40
3:D:208:ILE:HA	3:D:211:ARG:NH1	2.36	0.40
3:D:1054:ARG:NH1	3:D:1067:VAL:HG21	2.36	0.40
1:A:74:THR:O	1:A:78:LEU:HD13	2.20	0.40
2:C:77:ARG:HG3	2:C:77:ARG:O	2.20	0.40
2:C:565:ALA:HB3	2:C:567:GLU:OE1	2.21	0.40
2:C:577:ASP:OD1	2:C:577:ASP:N	2.54	0.40
4:E:73:GLU:N	4:E:73:GLU:OE1	2.54	0.40
5:G:70:VAL:CG2	5:G:79:ILE:HD12	2.50	0.40
1:A:55:ARG:HH22	1:A:158:GLU:HB3	1.87	0.40
2:C:268:VAL:O	2:C:268:VAL:HG22	2.20	0.40
2:C:298:ASN:HD22	2:C:305:ARG:NH2	2.19	0.40
2:C:556:GLU:OE1	2:C:557:PRO:HD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:MET:HE3	2:C:886:ALA:HB1	2.03	0.40
3:D:127:LYS:HE2	3:D:234:LEU:HD21	2.03	0.40
3:D:518:GLU:H	3:D:518:GLU:CD	2.23	0.40
3:D:905:ALA:HB3	3:D:909:THR:O	2.22	0.40
3:D:1085:ARG:C	3:D:1086:LEU:HD12	2.42	0.40
1:B:78:LEU:HD22	3:D:613:SER:HA	2.03	0.40
1:B:183:VAL:O	1:B:183:VAL:HG12	2.20	0.40
2:C:81:ASN:O	2:C:81:ASN:ND2	2.55	0.40
2:C:830:ARG:CG	2:C:830:ARG:O	2.70	0.40
2:C:1073:CYS:O	2:C:1077:GLN:HG3	2.21	0.40
3:D:128:ILE:HD13	3:D:135:VAL:CG2	2.50	0.40
3:D:208:ILE:HG12	3:D:211:ARG:HH22	1.86	0.40
1:A:158:GLU:CG	1:A:159:ILE:H	2.34	0.40
2:C:168:ILE:O	2:C:168:ILE:HD12	2.21	0.40
2:C:862:PRO:HG2	2:C:865:VAL:HG21	2.03	0.40
3:D:166:ARG:NH1	3:D:170:LEU:HD22	2.35	0.40
3:D:196:LYS:HA	3:D:196:LYS:HD2	1.87	0.40
3:D:367:VAL:O	3:D:371:LYS:HG3	2.22	0.40
3:D:480:ARG:HB3	3:D:481:PRO:HD2	2.04	0.40
7:N:10:DC:H2''	7:N:11:DT:O5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/347 (65%)	213 (95%)	11 (5%)	0	100	100
1	B	235/347 (68%)	216 (92%)	17 (7%)	2 (1%)	17	52
2	C	1119/1178 (95%)	1054 (94%)	63 (6%)	2 (0%)	47	79
3	D	1272/1316 (97%)	1208 (95%)	63 (5%)	1 (0%)	51	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	81/110 (74%)	80 (99%)	1 (1%)	0	100	100
5	G	122/238 (51%)	119 (98%)	3 (2%)	0	100	100
All	All	3053/3536 (86%)	2890 (95%)	158 (5%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	310	ARG
1	B	184	GLU
2	C	268	VAL
1	B	183	VAL
3	D	1066	ILE

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	A	195/297 (66%)	191 (98%)	4 (2%)	53	79
1	B	195/297 (66%)	187 (96%)	8 (4%)	30	64
2	C	944/998 (95%)	901 (95%)	43 (5%)	27	59
3	D	1057/1095 (96%)	1022 (97%)	35 (3%)	38	69
4	E	69/90 (77%)	63 (91%)	6 (9%)	10	36
5	G	104/189 (55%)	102 (98%)	2 (2%)	57	81
All	All	2564/2966 (86%)	2466 (96%)	98 (4%)	36	66

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	72	ASP
1	A	137	GLU
1	A	152	ASN
1	B	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	THR
1	B	120	ASN
1	B	150	VAL
1	B	151	GLN
1	B	185	GLN
1	B	195	ASP
1	B	218	LEU
2	C	87	GLU
2	C	88	GLU
2	C	113	ASP
2	C	119	VAL
2	C	156	ASP
2	C	181	ARG
2	C	185	VAL
2	C	193	LYS
2	C	215	ASP
2	C	219	ARG
2	C	229	LYS
2	C	238	LEU
2	C	305	ARG
2	C	323	HIS
2	C	343	GLU
2	C	373	PHE
2	C	385	ILE
2	C	394	SER
2	C	433	THR
2	C	435	GLN
2	C	449	LEU
2	C	451	HIS
2	C	499	SER
2	C	519	VAL
2	C	534	ASP
2	C	545	ASN
2	C	570	TYR
2	C	571	VAL
2	C	581	VAL
2	C	585	GLN
2	C	626	VAL
2	C	637	ASP
2	C	739	ASN
2	C	787	ARG
2	C	919	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	932	LEU
2	C	962	GLU
2	C	982	GLU
2	C	1001	LEU
2	C	1039	ASP
2	C	1063	PHE
2	C	1094	ASP
2	C	1157	ARG
3	D	28	VAL
3	D	69	ARG
3	D	80	VAL
3	D	107	PHE
3	D	166	ARG
3	D	195	ARG
3	D	246	ASP
3	D	252	PHE
3	D	285	LYS
3	D	304	GLN
3	D	325	ARG
3	D	339	ASP
3	D	348	ILE
3	D	486	VAL
3	D	490	VAL
3	D	505	HIS
3	D	580	ASP
3	D	585	LEU
3	D	595	ASP
3	D	624	ARG
3	D	635	VAL
3	D	779	LYS
3	D	783	ASP
3	D	796	ASP
3	D	810	ASN
3	D	821	LYS
3	D	879	ASP
3	D	901	LEU
3	D	946	ASP
3	D	965	VAL
3	D	981	ARG
3	D	1028	LEU
3	D	1040	PRO
3	D	1060	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1211	THR
4	E	44	LEU
4	E	56	TYR
4	E	68	TYR
4	E	73	GLU
4	E	102	ASP
4	E	106	HIS
5	G	41	GLU
5	G	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	B	120	ASN
1	B	151	GLN
1	B	185	GLN
2	C	141	ASN
2	C	150	GLN
2	C	178	GLN
2	C	386	GLN
2	C	479	HIS
2	C	610	ASN
2	C	866	ASN
2	C	1055	GLN
3	D	207	GLN
3	D	213	GLN
3	D	262	GLN
3	D	369	ASN
3	D	410	GLN
3	D	479	GLN
3	D	540	GLN
3	D	552	GLN
3	D	563	ASN
3	D	787	GLN
3	D	810	ASN
3	D	959	GLN
3	D	1017	GLN
3	D	1091	HIS
3	D	1110	GLN
3	D	1125	GLN
3	D	1239	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	71	GLN
5	G	125	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	12/20 (60%)	5 (41%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	19	A
8	R	20	G
8	R	21	C
8	R	22	G
8	R	23	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	2TM	C	1201	10	27,30,30	4.10	18 (66%)	39,47,47	1.19	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	2TM	C	1201	10	-	5/19/38/38	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	2TM	C2'-C3'	-8.50	1.30	1.53
9	C	1201	2TM	O4'-C4'	-6.70	1.30	1.45
9	C	1201	2TM	PB-O3B	6.53	1.65	1.58
9	C	1201	2TM	C6-C5	6.39	1.49	1.35
9	C	1201	2TM	C2-N3	6.07	1.48	1.36
9	C	1201	2TM	C4-N4	5.55	1.47	1.33
9	C	1201	2TM	PA-O5'	5.43	1.65	1.57
9	C	1201	2TM	C4-N3	5.27	1.45	1.34
9	C	1201	2TM	O4'-C1'	5.18	1.54	1.42
9	C	1201	2TM	C1'-N1	-4.58	1.34	1.47
9	C	1201	2TM	C2-N1	4.04	1.48	1.40
9	C	1201	2TM	C3'-C4'	3.70	1.62	1.53
9	C	1201	2TM	C6-N1	3.27	1.45	1.38
9	C	1201	2TM	O2-C2	-3.22	1.17	1.23
9	C	1201	2TM	O2'-C2'	3.00	1.50	1.43
9	C	1201	2TM	C5-C4	2.82	1.49	1.42
9	C	1201	2TM	PB-O1B	-2.14	1.51	1.56
9	C	1201	2TM	PA-O2A	-2.07	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	2TM	C3'-C2'-C1'	3.44	107.96	101.43
9	C	1201	2TM	C2'-C3'-C4'	3.22	108.90	102.64
9	C	1201	2TM	PB-O3B-PG	-2.67	123.21	132.62

There are no chirality outliers.

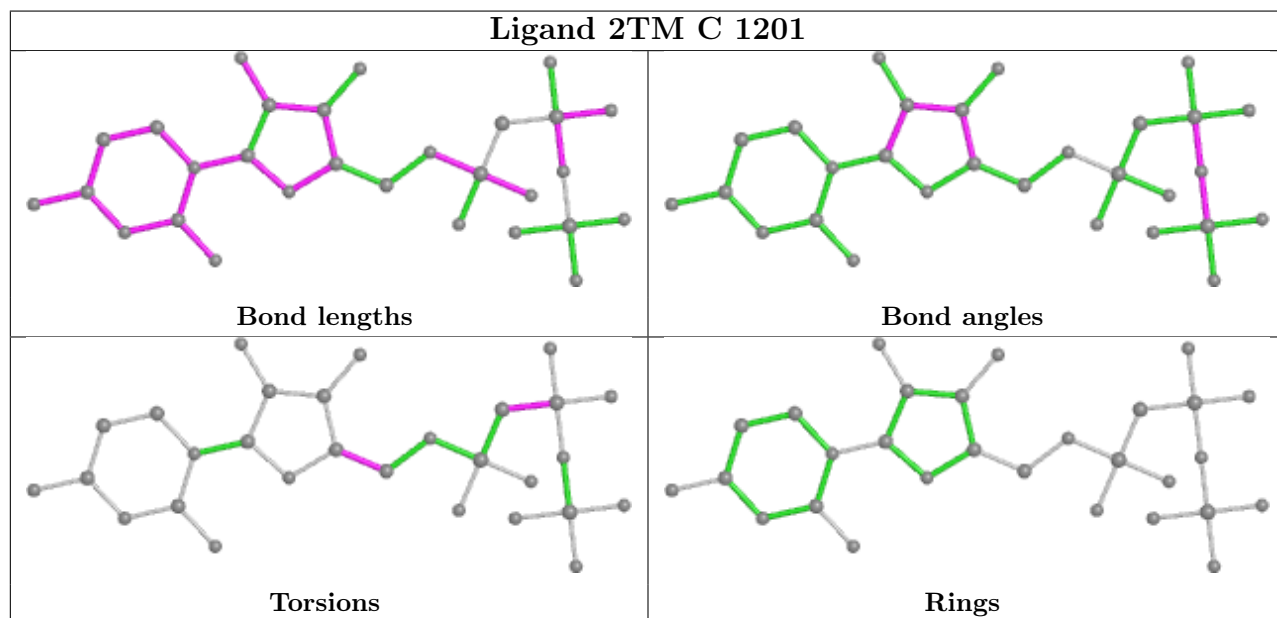
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	2TM	PA-C1-PB-O3B
9	C	1201	2TM	PA-C1-PB-O1B
9	C	1201	2TM	PA-C1-PB-O2B
9	C	1201	2TM	O4'-C4'-C5'-O5'
9	C	1201	2TM	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

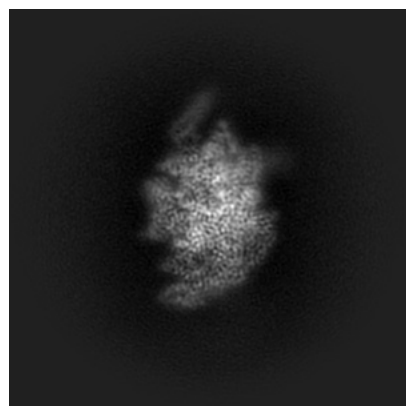
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28466. These allow visual inspection of the internal detail of the map and identification of artifacts.

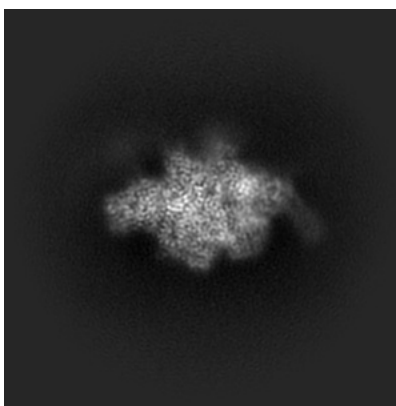
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

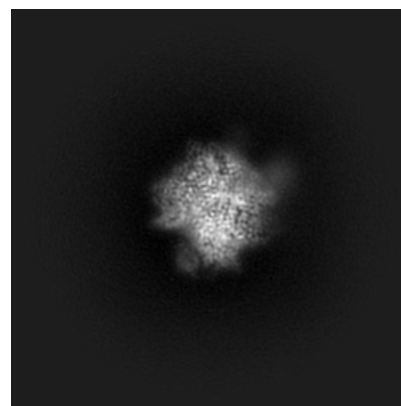
6.1.1 Primary map



X

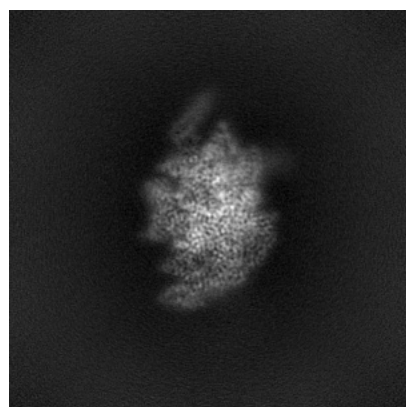


Y

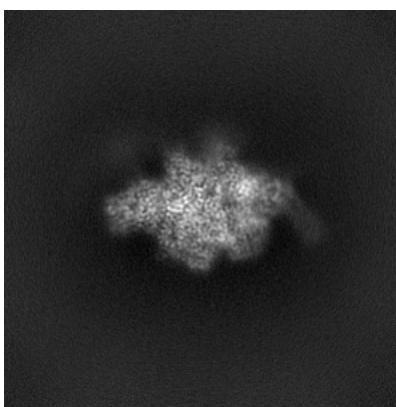


Z

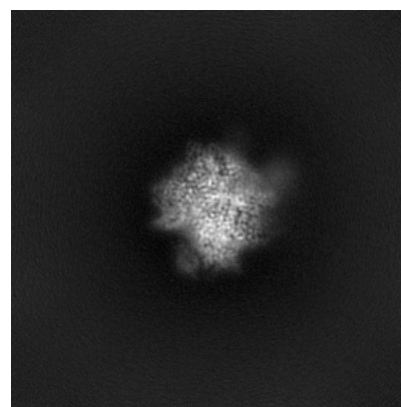
6.1.2 Raw map



X



Y

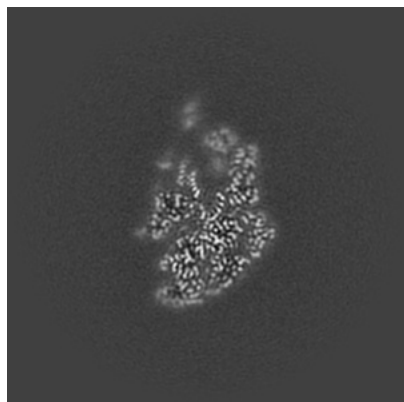


Z

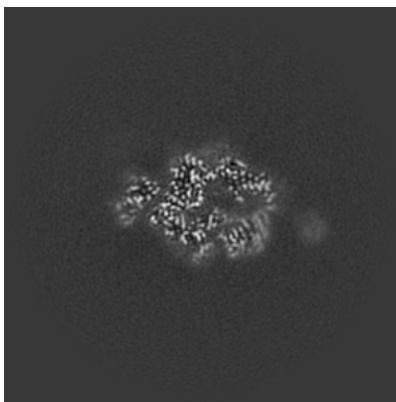
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

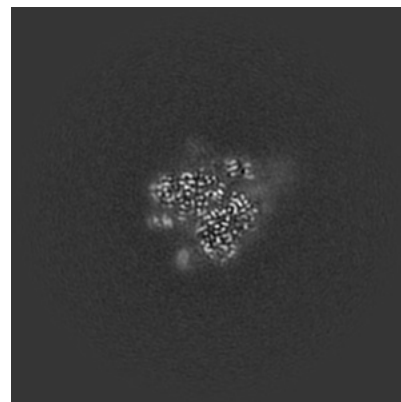
6.2.1 Primary map



X Index: 200

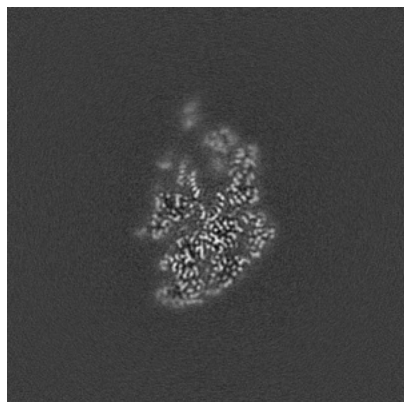


Y Index: 200

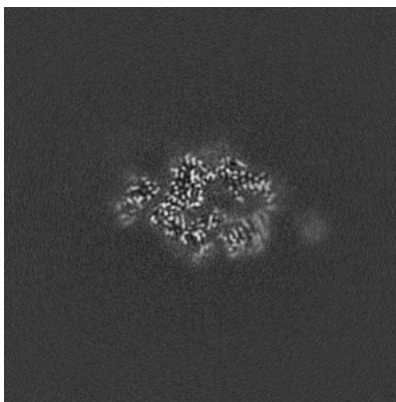


Z Index: 200

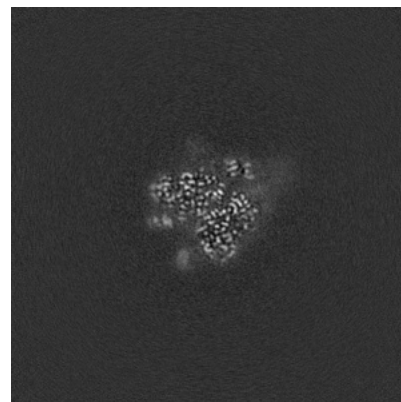
6.2.2 Raw map



X Index: 200



Y Index: 200

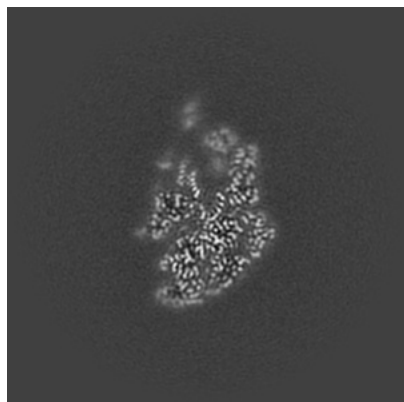


Z Index: 200

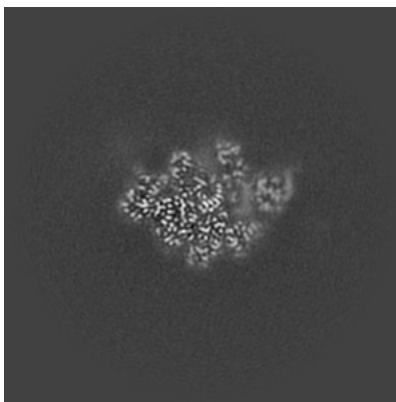
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

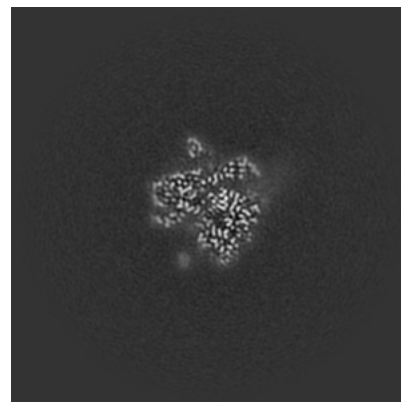
6.3.1 Primary map



X Index: 200

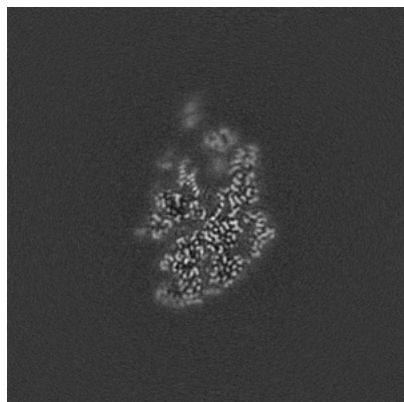


Y Index: 213

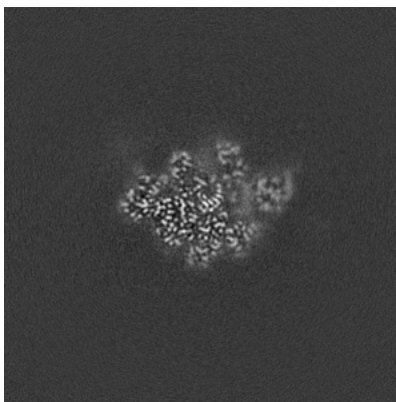


Z Index: 195

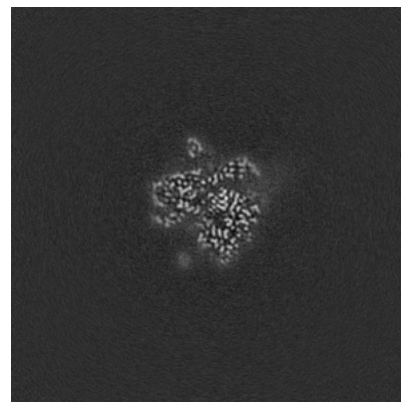
6.3.2 Raw map



X Index: 199



Y Index: 213

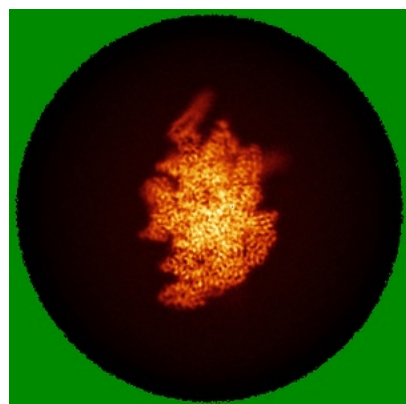


Z Index: 195

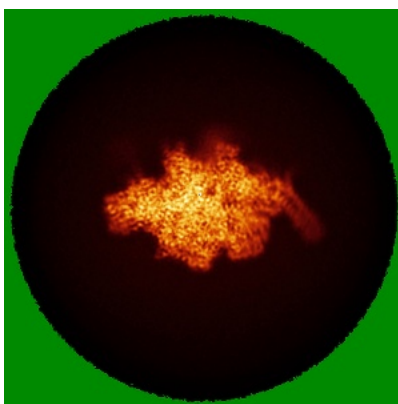
The images above show the largest variance slices of the map in three orthogonal directions.

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

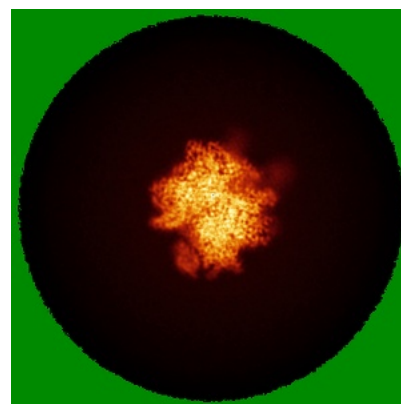
6.4.1 Primary map



X

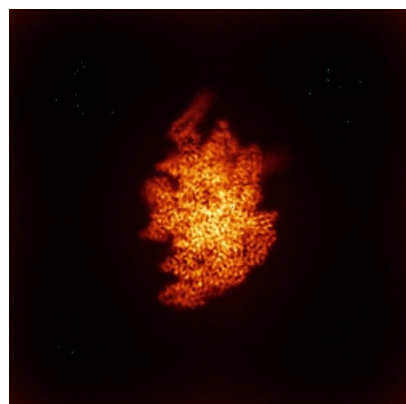


Y

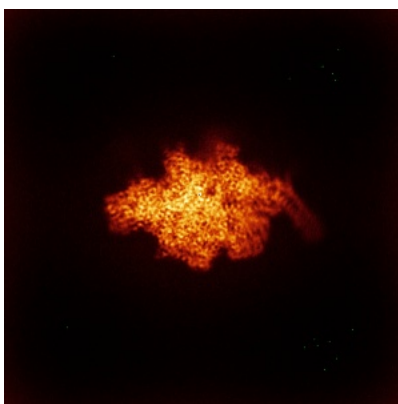


Z

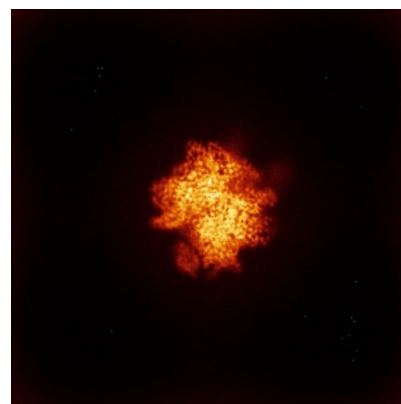
6.4.2 Raw map



X



Y

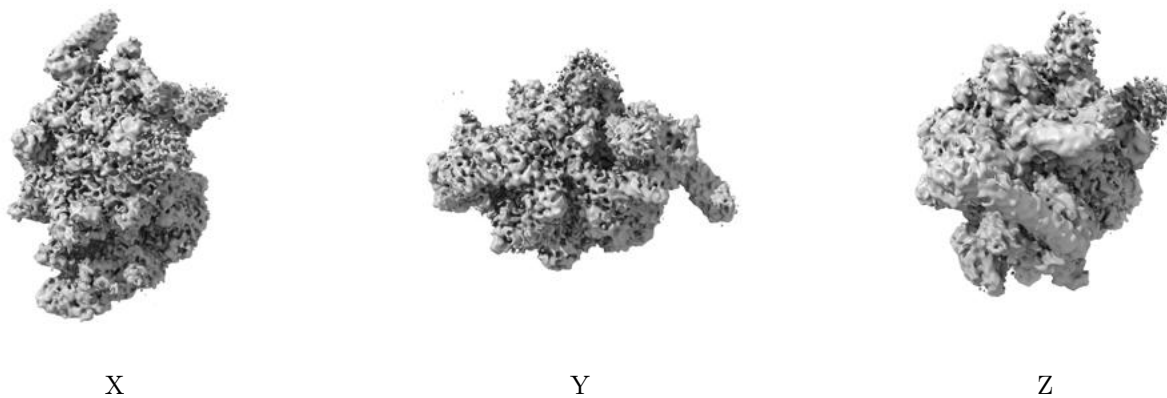


Z

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

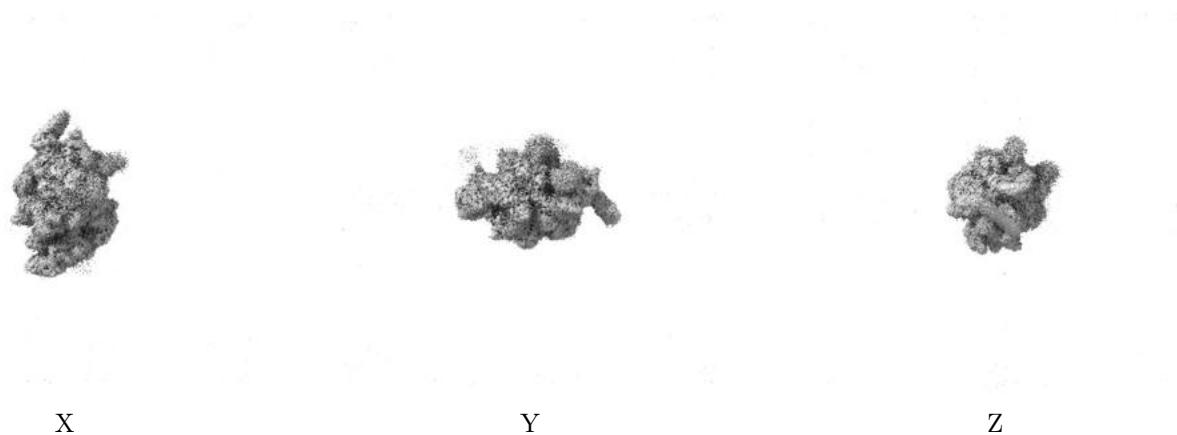
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

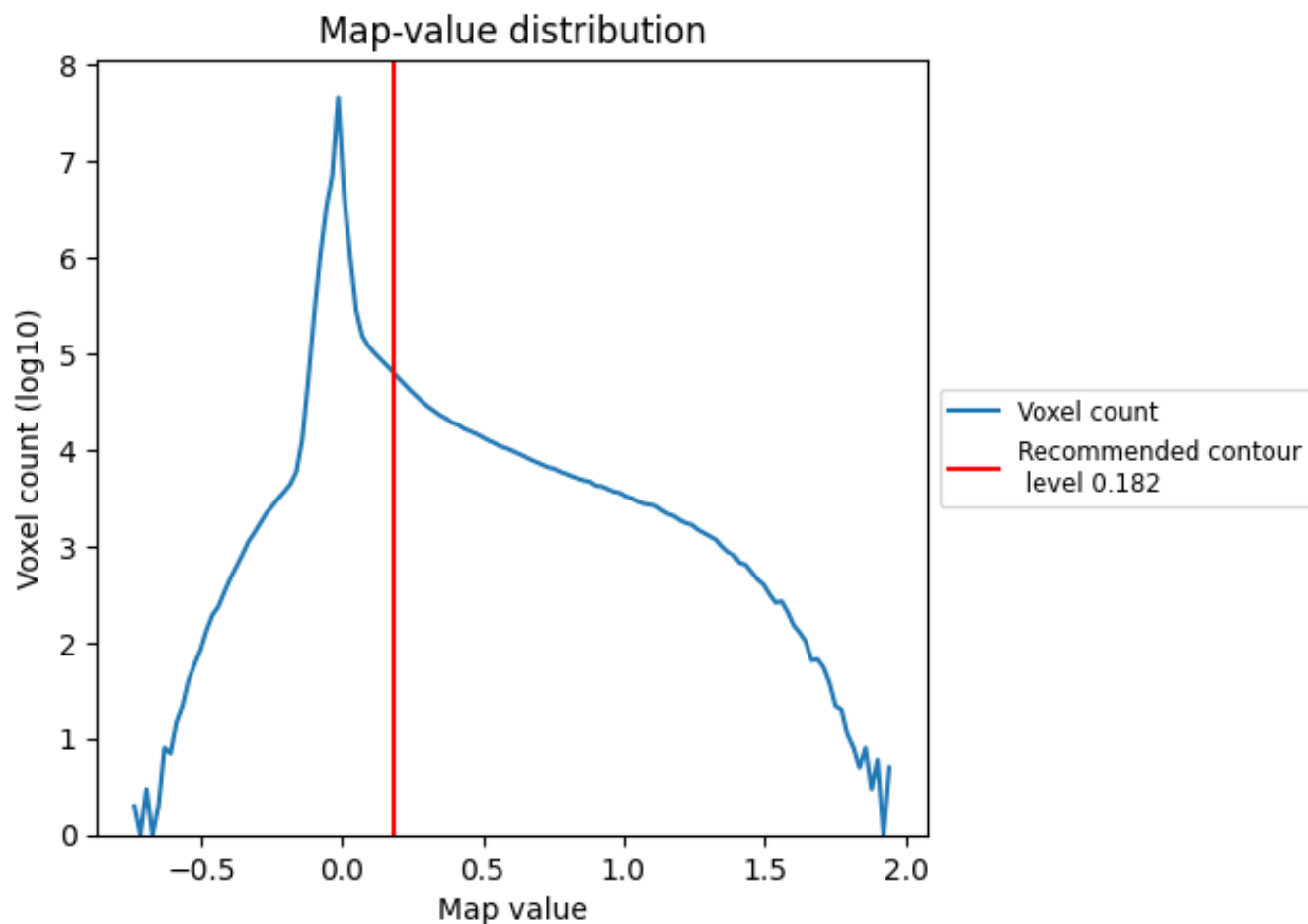
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

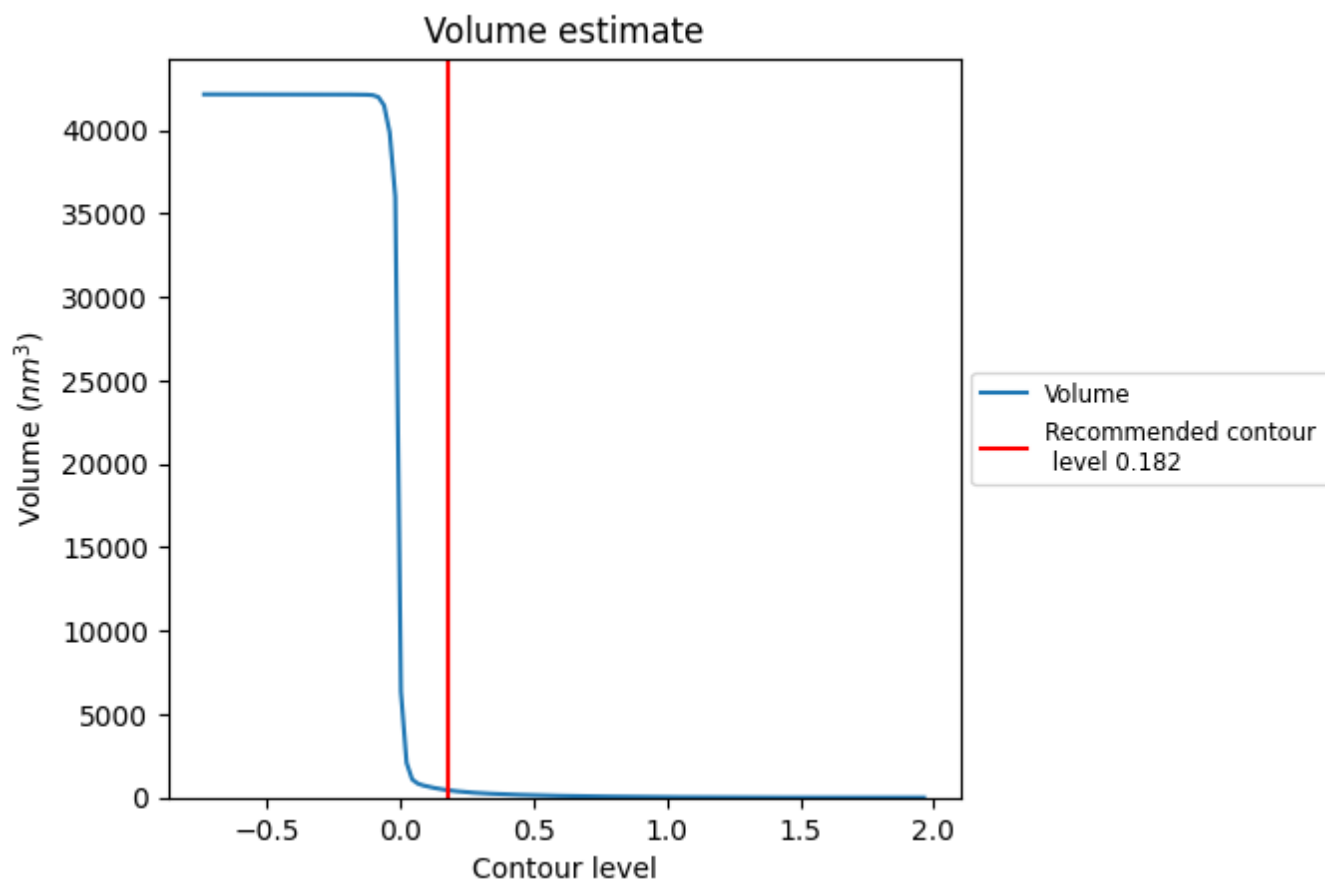
This section contains the results of statistical analysis of the map.

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.

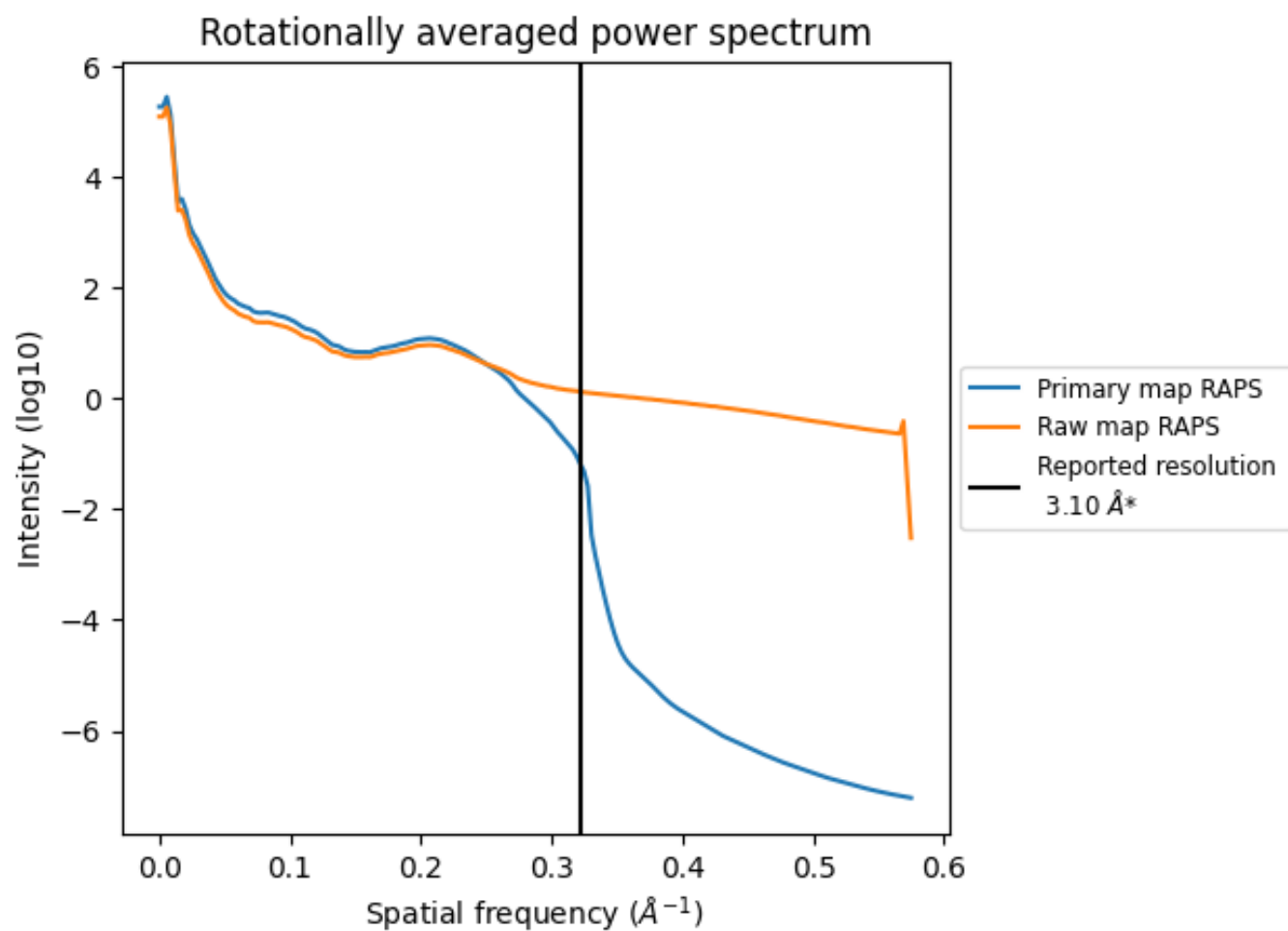
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 396 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

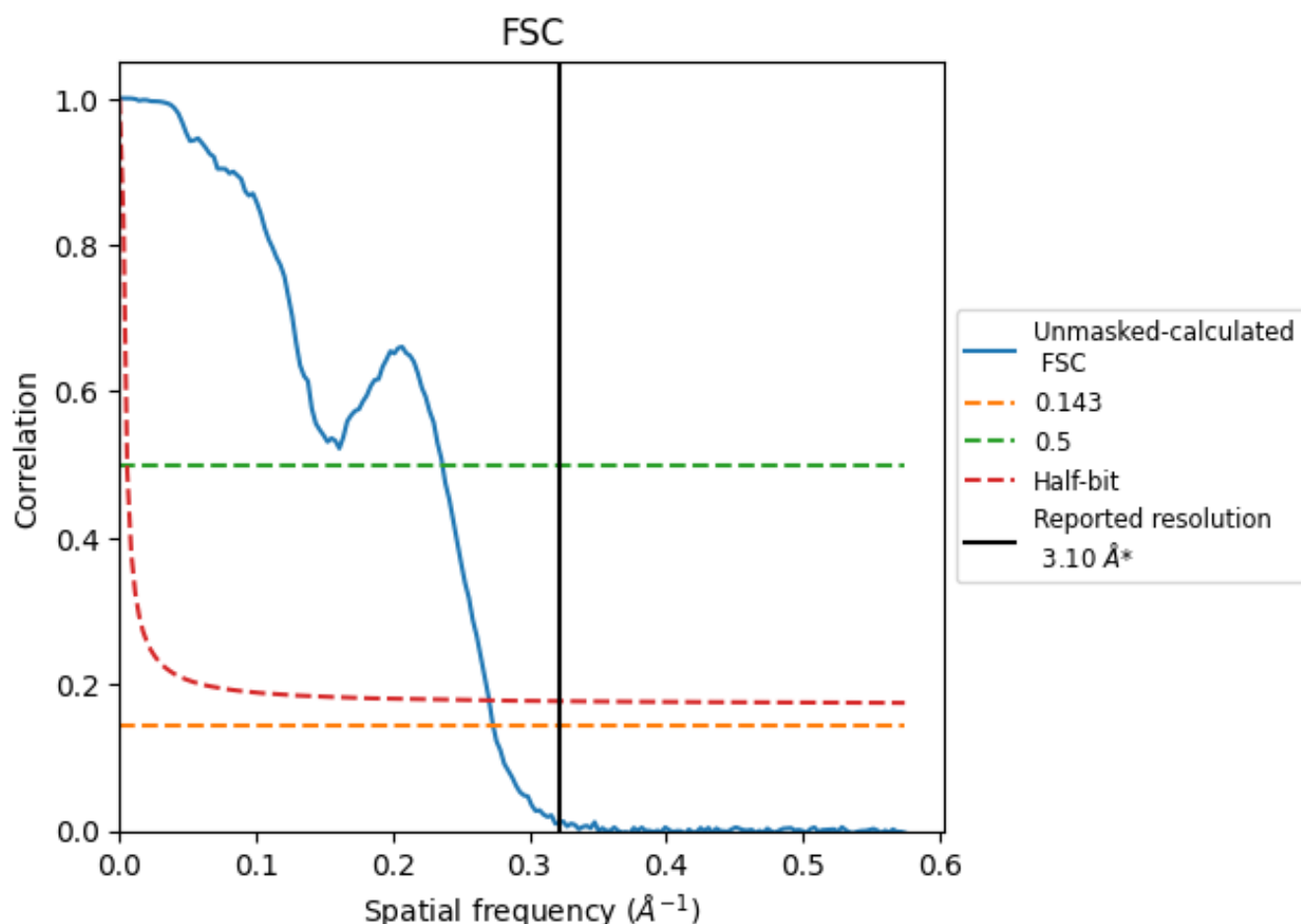


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

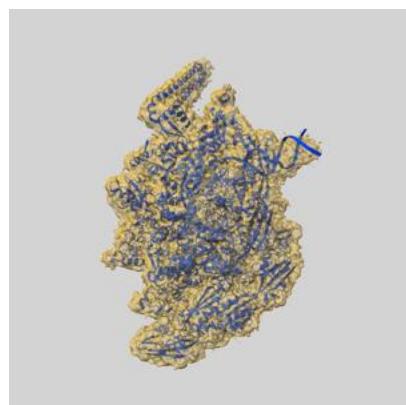
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.23	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.1 by more than 10 %

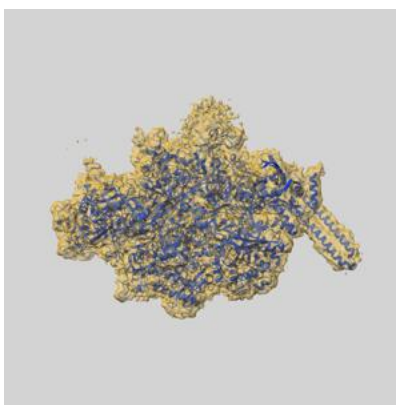
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28466 and PDB model 8EOS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

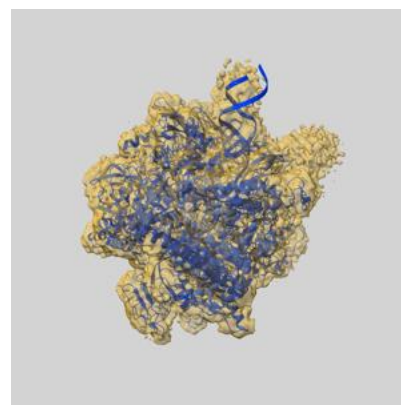
9.1 Map-model overlay [i](#)



X



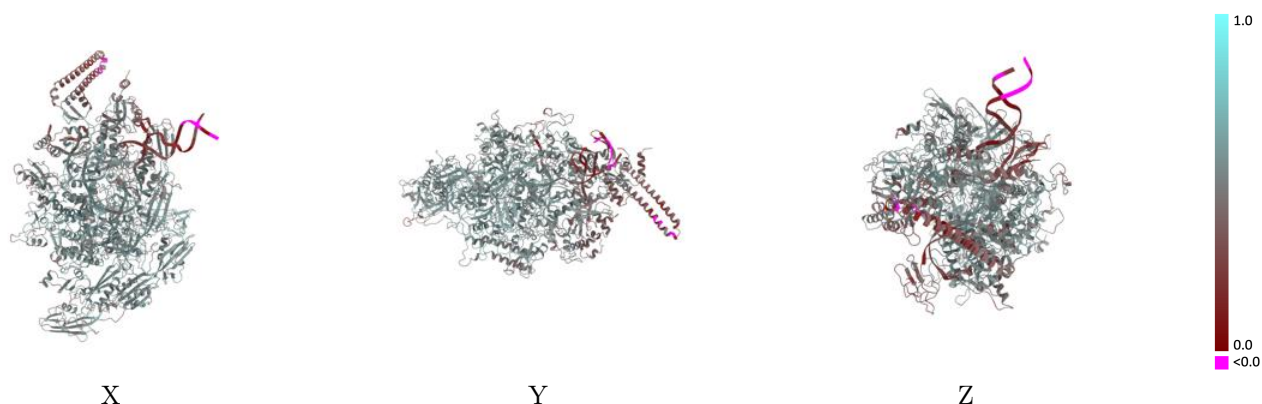
Y



Z

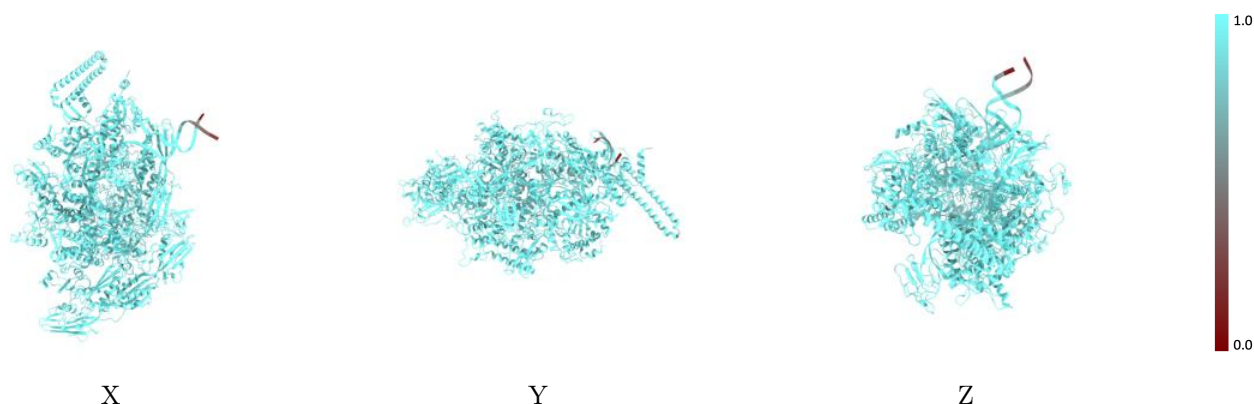
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



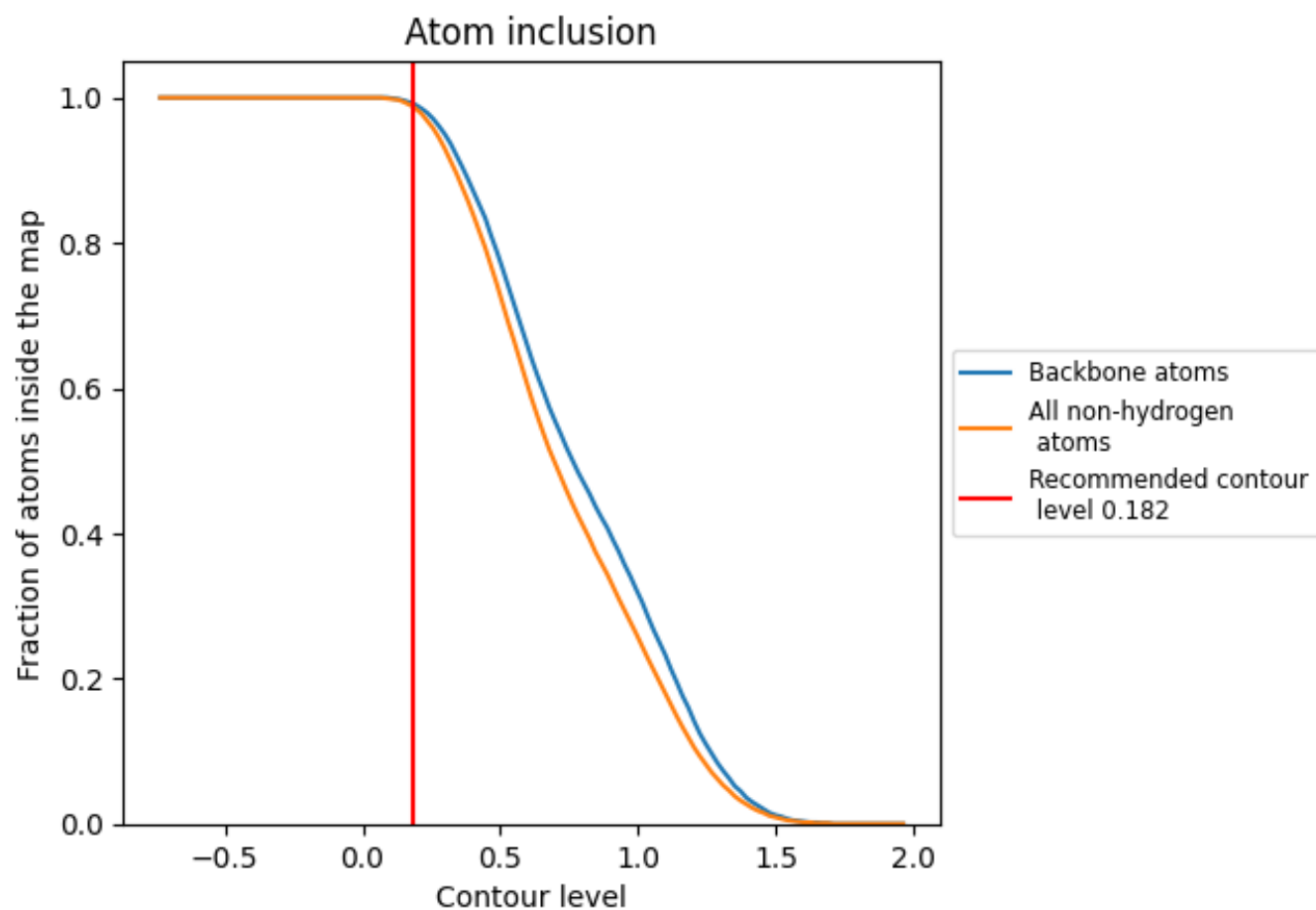
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9880	<div><div></div></div> 0.5020
A	<div><div></div></div> 0.9910	<div><div></div></div> 0.5350
B	<div><div></div></div> 0.9900	<div><div></div></div> 0.5150
C	<div><div></div></div> 0.9920	<div><div></div></div> 0.5270
D	<div><div></div></div> 0.9920	<div><div></div></div> 0.5050
E	<div><div></div></div> 0.9870	<div><div></div></div> 0.5220
G	<div><div></div></div> 0.9780	<div><div></div></div> 0.4060
N	<div><div></div></div> 0.9130	<div><div></div></div> 0.3060
R	<div><div></div></div> 1.0000	<div><div></div></div> 0.4830
T	<div><div></div></div> 0.9630	<div><div></div></div> 0.3740

1.0

0.0

<0.0