Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:26 AM EST

PDB ID	:	3JB3
EMDB ID	:	EMD-6377
Title	:	Atomic model of cytoplasmic polyhedrosis virus with SAM, GTP and ATP
Authors	:	Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on	:	2015-07-06
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

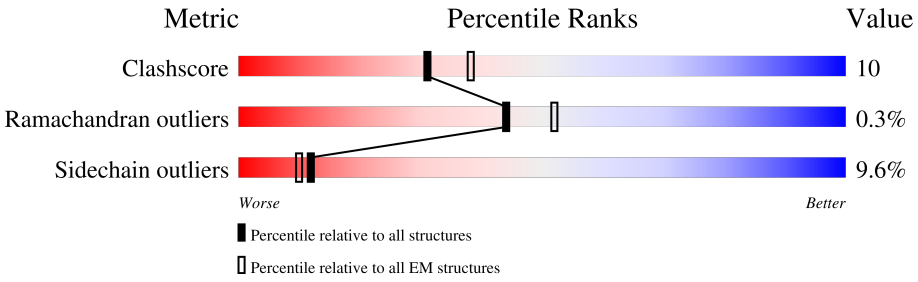
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	1058	11% 70% 26%
2	B	1333	63% 23% 11%
2	C	1333	66% 24% 6%
3	D	448	46% 17% 35%
3	E	448	49% 15% 35%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32368 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

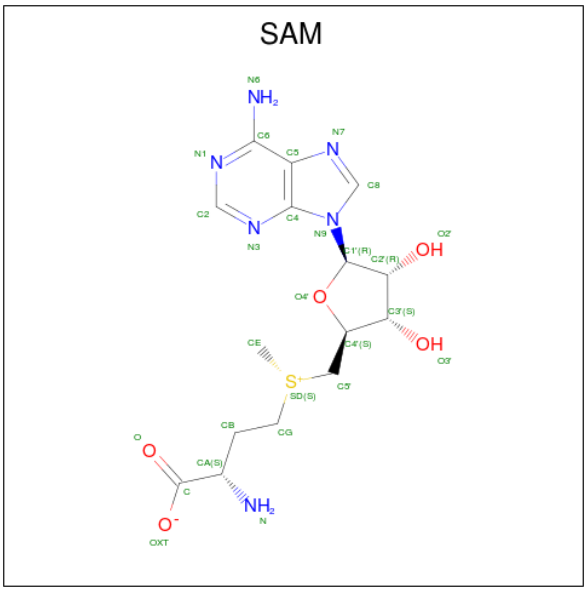
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1251	Total	C	N	O	S	0	0
			9857	6222	1713	1884	38		

- Molecule 3 is a protein called Viral structural protein 5.

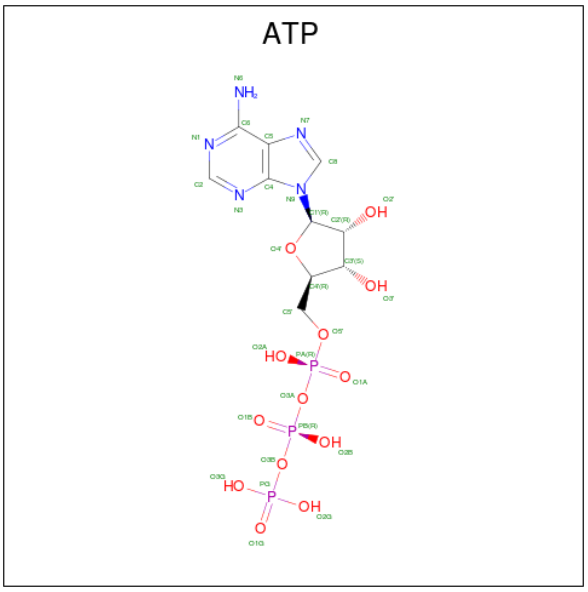
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



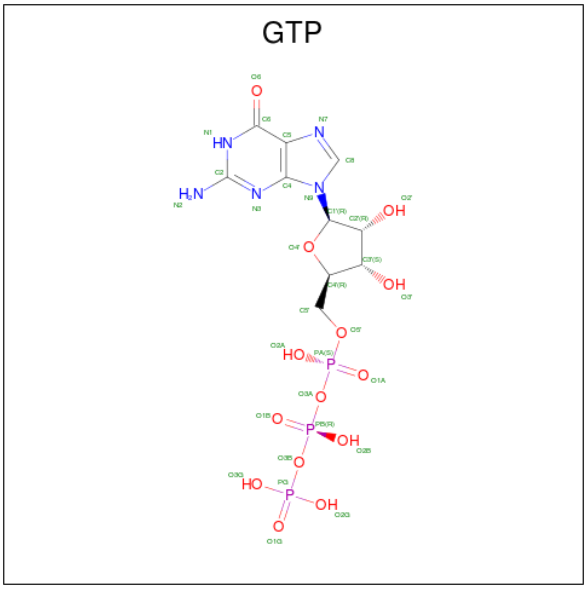
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			54	30	12	10	2	
4	A	1	Total	C	N	O	S	0
			54	30	12	10	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

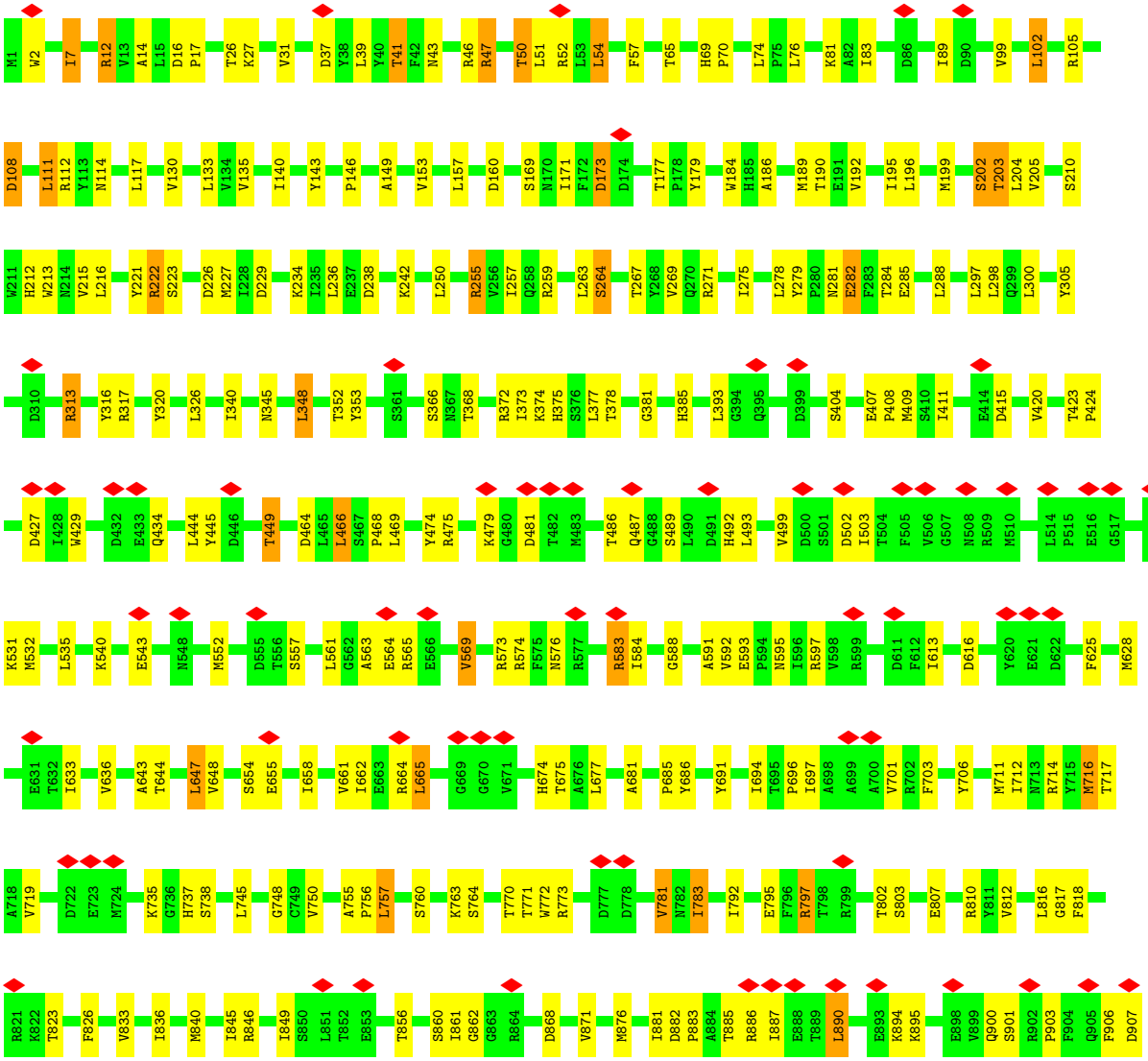
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	

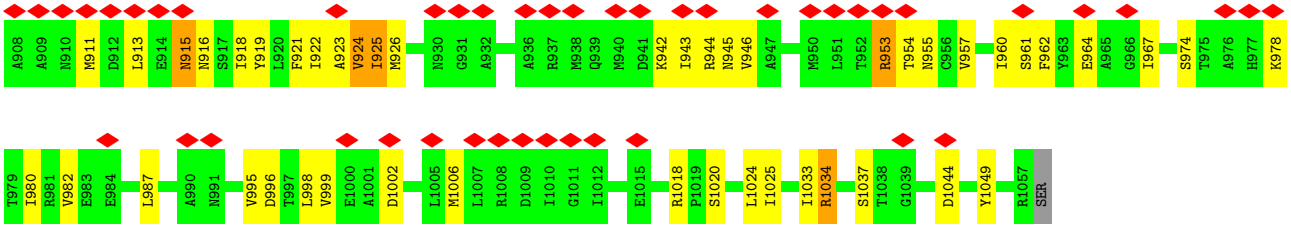
3 Residue-property plots (i)

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: Structural protein VP3

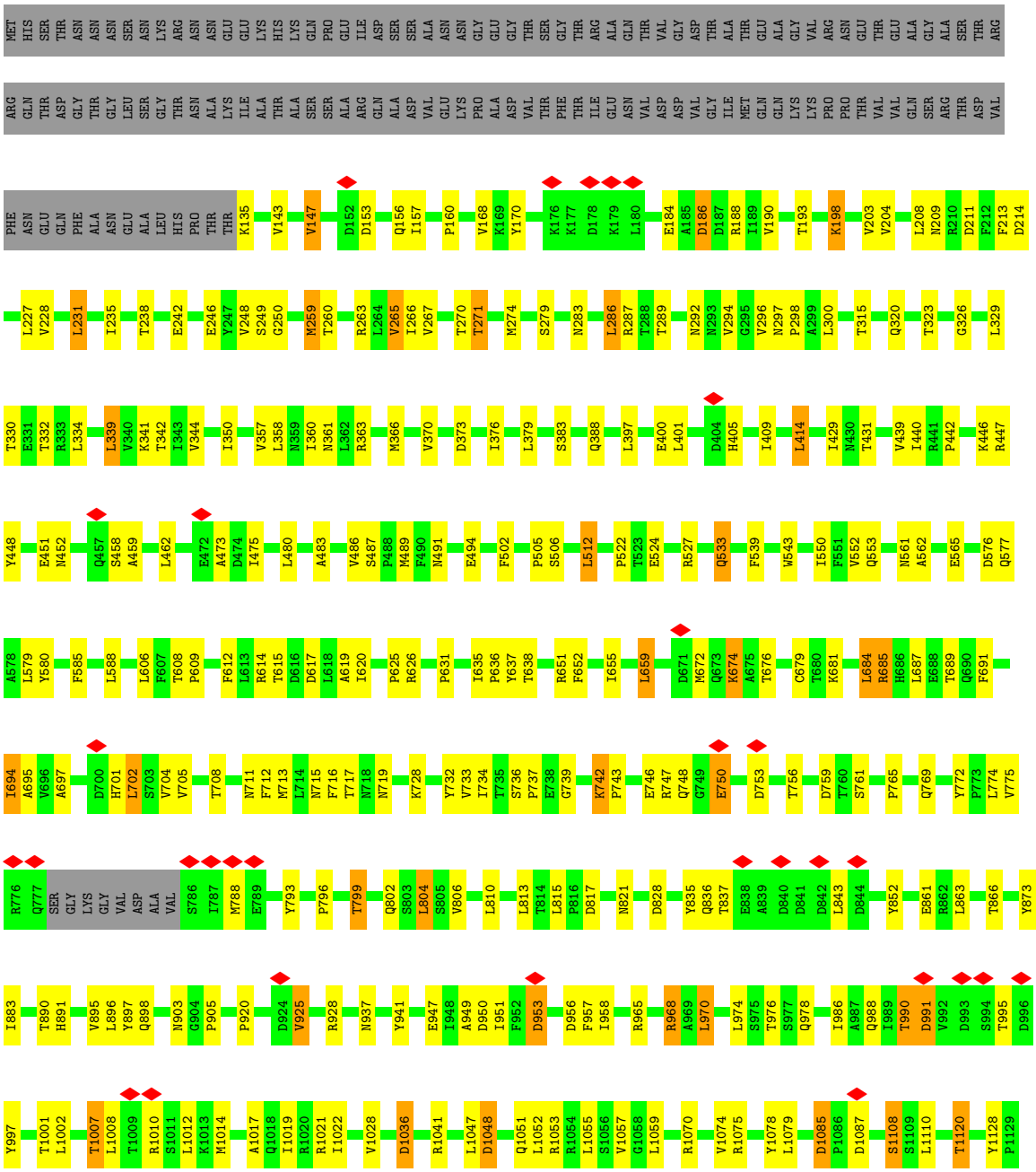
Chain A:

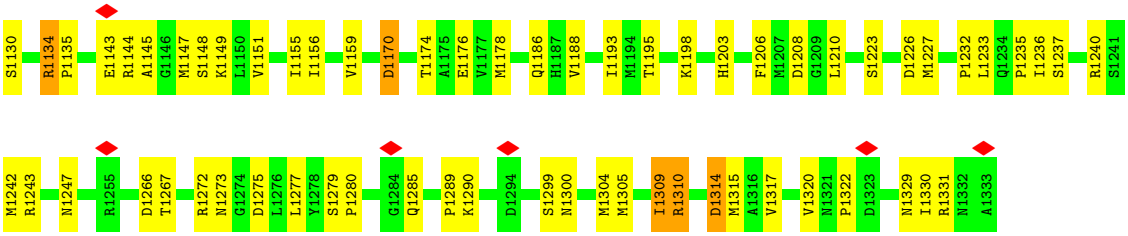




• Molecule 2: Capsid protein VP1

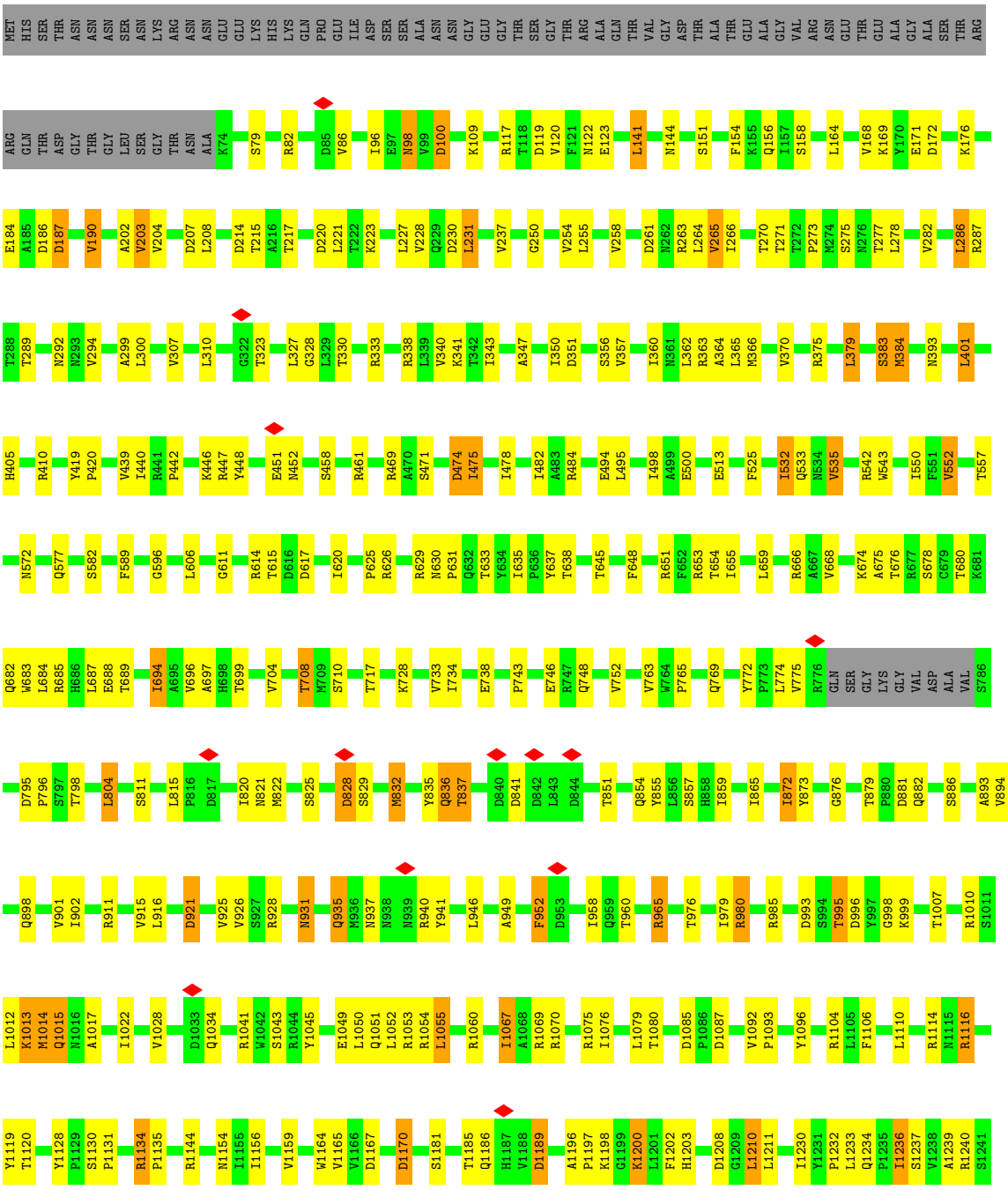
Chain B:

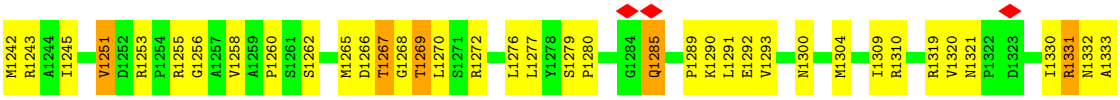




• Molecule 2: Capsid protein VP1

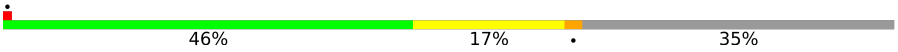
Chain C:

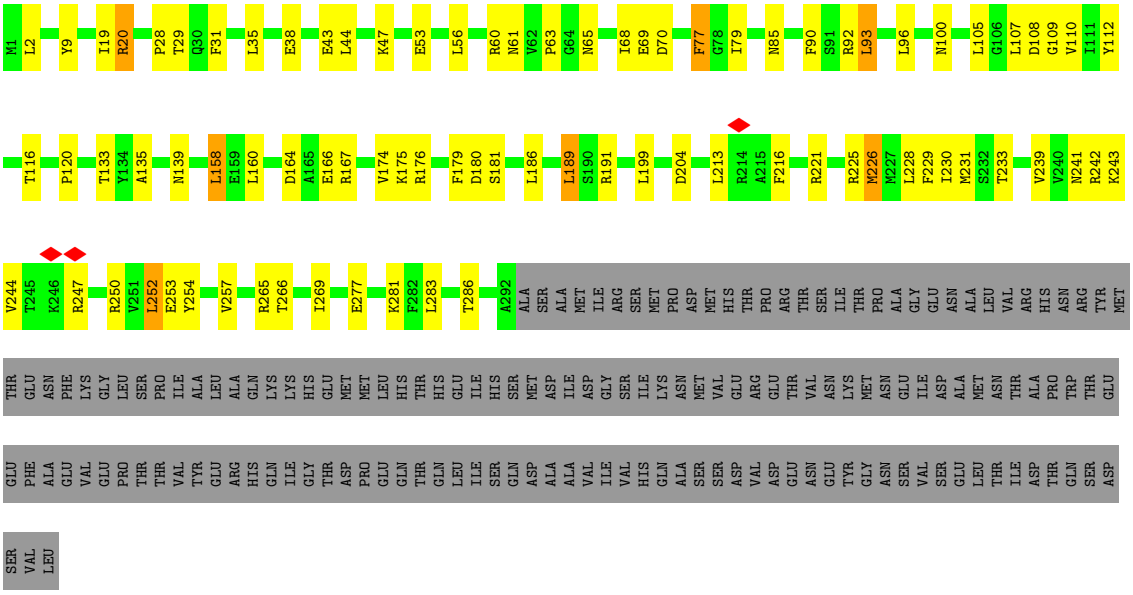




• Molecule 3: Viral structural protein 5

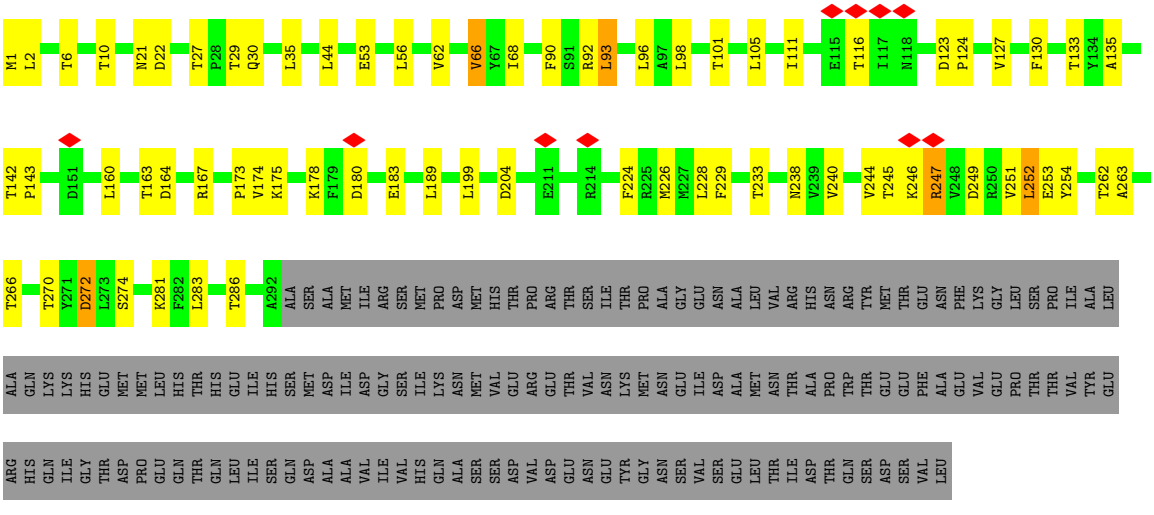
Chain D:





• Molecule 3: Viral structural protein 5

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	40898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	60535	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	25.770	Depositor
Minimum map value	-14.720	Depositor
Average map value	0.116	Depositor
Map value standard deviation	1.599	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	772.8, 772.8, 772.8	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, SAM, 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	0.28	0/8619	0.51	0/11737
2	B	0.34	0/9590	0.56	0/13056
2	C	0.34	0/10058	0.56	0/13695
3	D	0.32	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	0/44814

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	8434	0	8398	175	0
2	B	9397	0	9315	194	0
2	C	9857	0	9767	193	0
3	D	2281	0	2282	47	0
3	E	2281	0	2282	32	0
4	A	54	0	44	3	0
5	A	31	0	12	3	0
6	A	32	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
All	All	32368	0	32112	624	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 10.

All (624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:HG22	1:A:271:ARG:HE	1.41	0.83
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.64	0.79
1:A:305:TYR:O	1:A:317:ARG:NH1	2.16	0.78
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.17	0.78
5:A:1103:ATP:H5'1	5:A:1103:ATP:H8	1.50	0.77
1:A:12:ARG:NH2	1:A:16:ASP:OD1	2.18	0.77
2:B:1289:PRO:HD2	3:D:20:ARG:HD3	1.71	0.73
2:C:1144:ARG:NH1	2:C:1170:ASP:OD1	2.21	0.73
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.22	0.72
2:B:626:ARG:NH2	2:B:712:PHE:O	2.23	0.72
1:A:926:MET:HB2	1:A:995:VAL:HG21	1.73	0.71
2:C:494:GLU:HG2	2:C:577:GLN:HG3	1.73	0.71
3:D:176:ARG:HG3	3:D:253:GLU:HB3	1.72	0.71
2:B:248:VAL:HG22	2:B:970:LEU:HB3	1.71	0.71
2:C:458:SER:HB3	2:C:675:ALA:HB1	1.72	0.70
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.21	0.70
1:A:487:GLN:O	1:A:492:HIS:ND1	2.24	0.70
2:C:996:ASP:HA	2:C:999:LYS:HD2	1.75	0.69
1:A:210:SER:O	1:A:255:ARG:NH1	2.25	0.69
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.74	0.69
2:C:1272:ARG:NH1	3:E:22:ASP:OD2	2.26	0.69
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.75	0.68
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.75	0.68
2:B:746:GLU:OE2	2:C:685:ARG:NH1	2.27	0.68
3:D:239:VAL:HG12	3:D:250:ARG:HD2	1.76	0.68
2:B:1273:ASN:ND2	2:B:1275:ASP:OD2	2.26	0.68
1:A:51:LEU:HD23	1:A:171:ILE:HD11	1.76	0.67
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.28	0.67
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.77	0.66
2:C:1240:ARG:HD2	2:C:1243:ARG:HB2	1.78	0.66
2:B:287:ARG:HE	2:B:330:THR:HG22	1.60	0.65
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:OD1	2:B:965:ARG:NH1	2.30	0.65
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.77	0.65
1:A:662:ILE:HD12	1:A:675:THR:HG21	1.77	0.65
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.78	0.65
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.78	0.65
2:B:1227:MET:HG3	2:C:123:GLU:HG2	1.77	0.65
2:C:829:SER:O	2:C:965:ARG:NH2	2.30	0.64
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.79	0.64
2:C:653:ARG:HG3	2:C:688:GLU:CD	2.18	0.64
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.31	0.64
1:A:173:ASP:N	1:A:173:ASP:OD1	2.31	0.64
1:A:267:THR:HG21	1:A:271:ARG:HH21	1.63	0.64
1:A:340:ILE:HD11	1:A:348:LEU:HD11	1.79	0.64
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.30	0.64
2:B:263:ARG:O	2:B:361:ASN:ND2	2.31	0.63
2:B:836:GLN:HE21	2:B:843:LEU:HA	1.63	0.63
2:C:795:ASP:OD1	2:C:1319:ARG:NH2	2.31	0.63
1:A:925:ILE:HG12	1:A:942:LYS:HD2	1.81	0.63
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.30	0.63
1:A:372:ARG:HD3	1:A:823:THR:HG21	1.80	0.63
1:A:27:LYS:NZ	1:A:37:ASP:OD1	2.27	0.63
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.32	0.63
2:B:388:GLN:HB2	2:B:1320:VAL:HB	1.81	0.63
1:A:686:TYR:HA	1:A:714:ARG:HH21	1.64	0.62
2:C:931:ASN:HD22	2:C:931:ASN:H	1.46	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.18	0.62
2:C:879:THR:HG22	2:C:881:ASP:H	1.65	0.62
2:C:1236:ILE:HG22	2:C:1237:SER:H	1.63	0.62
1:A:411:ILE:HD11	1:A:415:ASP:HB2	1.82	0.62
2:C:1289:PRO:HG2	2:C:1292:GLU:HB2	1.81	0.62
1:A:205:VAL:HG23	1:A:263:LEU:HB2	1.81	0.62
1:A:540:LYS:NZ	1:A:543:GLU:OE2	2.31	0.61
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.30	0.61
2:C:668:VAL:HG23	2:C:674:LYS:HD3	1.81	0.61
1:A:964:GLU:HB3	1:A:1049:TYR:HD1	1.66	0.61
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.34	0.61
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.82	0.61
1:A:677:LEU:HD23	1:A:711:MET:HB2	1.83	0.60
1:A:714:ARG:NH1	1:A:1044:ASP:OD2	2.34	0.60
2:B:235:ILE:HD12	2:C:774:LEU:HD22	1.83	0.60
3:D:283:LEU:HA	3:D:286:THR:HG22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:GLU:OE2	3:E:281:LYS:NZ	2.32	0.60
3:D:69:GLU:HG3	3:D:199:LEU:HG	1.83	0.60
3:E:272:ASP:OD1	3:E:274:SER:OG	2.18	0.60
3:D:93:LEU:HD12	3:D:96:LEU:HD12	1.83	0.60
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.36	0.59
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.83	0.59
2:B:1085:ASP:OD1	2:B:1085:ASP:N	2.36	0.59
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.36	0.59
1:A:189:MET:HE1	1:A:348:LEU:H	1.68	0.59
1:A:212:HIS:ND1	6:A:1104:GTP:O2A	2.33	0.59
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.85	0.59
3:D:108:ASP:OD2	3:D:112:TYR:OH	2.18	0.59
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.35	0.58
2:C:822:MET:O	2:C:825:SER:OG	2.22	0.58
2:C:1232:PRO:HB3	2:C:1236:ILE:HD11	1.84	0.58
1:A:14:ALA:HA	1:A:112:ARG:NH2	2.18	0.58
1:A:999:VAL:HG13	1:A:1002:ASP:HB2	1.86	0.58
2:C:615:THR:OG1	2:C:1333:ALA:O	2.19	0.58
1:A:227:MET:HG2	1:A:269:VAL:HG21	1.85	0.57
1:A:573:ARG:NH2	1:A:584:ILE:O	2.34	0.57
2:B:439:VAL:HG13	2:B:440:ILE:HG13	1.85	0.57
2:B:620:ILE:HD11	2:B:631:PRO:HG2	1.87	0.57
2:B:1108:SER:O	2:C:393:ASN:ND2	2.34	0.57
1:A:257:ILE:HG21	1:A:326:LEU:HD11	1.87	0.57
2:C:343:ILE:HD13	2:C:362:LEU:HD21	1.87	0.57
2:C:1269:THR:OG1	2:C:1270:LEU:N	2.25	0.57
2:C:851:THR:HG23	2:C:854:GLN:HB2	1.87	0.57
2:C:79:SER:OG	2:C:172:ASP:OD1	2.23	0.56
2:C:439:VAL:HG13	2:C:440:ILE:HG13	1.87	0.56
3:D:77:PHE:HB3	3:D:230:ILE:HG21	1.86	0.56
1:A:41:THR:HG23	1:A:50:THR:HG23	1.86	0.56
1:A:655:GLU:HG2	1:A:712:ILE:HG21	1.88	0.56
1:A:735:LYS:HB2	1:A:738:SER:HB2	1.87	0.56
2:B:524:GLU:HA	2:B:527:ARG:HD2	1.87	0.56
2:C:273:PRO:HB2	2:C:278:LEU:HD11	1.88	0.56
3:D:35:LEU:HD12	3:D:179:PHE:HB3	1.87	0.56
1:A:374:LYS:HG2	1:A:770:THR:HG22	1.88	0.56
2:B:576:ASP:OD2	2:B:747:ARG:NH1	2.36	0.56
2:C:615:THR:H	2:C:1333:ALA:HB1	1.71	0.56
1:A:267:THR:HG23	1:A:320:TYR:OH	2.06	0.56
1:A:697:ILE:HD11	1:A:701:VAL:HG22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.87	0.56
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.88	0.55
1:A:474:TYR:HD1	1:A:499:VAL:HG12	1.70	0.55
2:C:746:GLU:OE1	2:C:748:GLN:NE2	2.36	0.55
1:A:213:TRP:HB2	1:A:215:VAL:HG12	1.87	0.55
2:C:366:MET:HG3	3:E:266:THR:HG21	1.88	0.55
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.20	0.55
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.39	0.55
2:B:157:ILE:HG12	2:B:263:ARG:HD2	1.88	0.55
2:B:817:ASP:O	2:B:821:ASN:ND2	2.31	0.55
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.89	0.55
1:A:499:VAL:O	1:A:574:ARG:NH1	2.40	0.55
2:B:287:ARG:NH1	2:B:326:GLY:HA3	2.20	0.55
2:C:214:ASP:OD1	2:C:215:THR:N	2.39	0.55
2:C:865:ILE:HD11	2:C:1041:ARG:HB2	1.89	0.55
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.89	0.55
3:D:166:GLU:OE1	3:D:175:LYS:NZ	2.32	0.55
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	1.88	0.55
3:D:180:ASP:OD1	3:D:247:ARG:NH2	2.40	0.55
2:B:652:PHE:HA	2:B:655:ILE:HD12	1.88	0.54
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.89	0.54
2:C:795:ASP:O	2:C:798:THR:HG22	2.06	0.54
2:C:993:ASP:OD1	2:C:995:THR:OG1	2.22	0.54
2:C:1075:ARG:NH1	2:C:1167:ASP:OD1	2.40	0.54
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.88	0.54
2:B:626:ARG:NH1	2:B:715:ASN:O	2.40	0.54
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.89	0.54
2:B:1048:ASP:OD1	2:B:1048:ASP:N	2.40	0.54
1:A:203:THR:HG22	1:A:204:LEU:HG	1.90	0.54
1:A:836:ILE:HD11	1:A:1033:ILE:HG21	1.89	0.54
2:C:265:VAL:HB	2:C:1304:MET:HB3	1.90	0.54
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.88	0.54
2:B:168:VAL:HG22	2:B:204:VAL:HG22	1.88	0.54
2:B:339:LEU:HD11	3:D:63:PRO:HB2	1.90	0.54
1:A:427:ASP:HA	1:A:703:PHE:HA	1.90	0.54
2:B:287:ARG:HH11	2:B:326:GLY:HA3	1.73	0.54
2:C:100:ASP:HB2	2:C:338:ARG:HH22	1.73	0.54
2:C:186:ASP:OD1	2:C:282:VAL:HG21	2.08	0.54
1:A:288:LEU:HD21	1:A:300:LEU:HD22	1.90	0.53
1:A:685:PRO:O	1:A:714:ARG:NH2	2.40	0.53
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1008:LEU:HD11	2:B:1010:ARG:HB2	1.91	0.53
1:A:385:HIS:NE2	1:A:803:SER:OG	2.41	0.53
1:A:409:MET:HE1	1:A:1037:SER:HB3	1.88	0.53
2:C:347:ALA:HB1	2:C:1267:THR:HG21	1.91	0.53
2:C:926:VAL:HG21	2:C:937:ASN:HA	1.91	0.53
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.90	0.53
2:C:1069:ARG:HD2	2:C:1239:ALA:HB2	1.91	0.53
2:B:271:THR:HG22	2:B:292:ASN:OD1	2.06	0.53
2:C:254:VAL:O	2:C:258:VAL:HG12	2.09	0.53
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.89	0.53
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.91	0.53
2:B:502:PHE:CE2	2:B:539:PHE:HB2	2.44	0.53
3:D:229:PHE:O	3:D:233:THR:HG23	2.09	0.53
1:A:712:ILE:HG22	1:A:716:MET:HG3	1.91	0.52
2:B:370:VAL:HG22	2:B:400:GLU:O	2.09	0.52
2:C:1266:ASP:OD1	2:C:1279:SER:OG	2.25	0.52
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.90	0.52
2:B:990:THR:O	2:B:990:THR:OG1	2.24	0.52
1:A:764:SER:HA	1:A:795:GLU:HG2	1.91	0.52
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.24	0.52
2:C:190:VAL:HG23	2:C:300:LEU:HB3	1.91	0.52
2:B:619:ALA:HB2	2:B:711:ASN:HA	1.91	0.52
2:C:471:SER:O	2:C:765:PRO:HG3	2.09	0.52
2:B:705:VAL:HA	2:B:708:THR:HG22	1.90	0.52
2:B:1206:PHE:CE2	2:B:1232:PRO:HD3	2.45	0.52
2:C:614:ARG:HG3	2:C:1333:ALA:HA	1.91	0.52
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.27	0.52
2:C:100:ASP:OD1	2:C:338:ARG:NH2	2.42	0.52
2:C:384:MET:HA	2:C:708:THR:HG21	1.90	0.52
2:B:739:GLY:HA2	2:C:653:ARG:HD3	1.92	0.52
2:C:469:ARG:HH21	2:C:513:GLU:CD	2.13	0.52
3:E:245:THR:OG1	3:E:246:LYS:N	2.41	0.52
1:A:681:ALA:O	1:A:1037:SER:HB2	2.10	0.52
2:B:214:ASP:OD1	2:B:214:ASP:N	2.41	0.52
2:C:383:SER:HB3	2:C:796:PRO:HG3	1.92	0.52
1:A:74:LEU:HD13	1:A:83:ILE:HG21	1.91	0.51
2:B:505:PRO:HG2	2:B:672:MET:SD	2.50	0.51
2:C:498:ILE:HG22	2:C:500:GLU:H	1.74	0.51
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.92	0.51
3:E:238:ASN:HB3	3:E:253:GLU:HG3	1.92	0.51
1:A:411:ILE:HG23	1:A:469:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1014:MET:HA	2:B:1017:ALA:HB2	1.91	0.51
2:B:512:LEU:HD22	2:B:659:LEU:HD23	1.92	0.51
2:B:759:ASP:OD2	2:B:761:SER:OG	2.27	0.51
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.92	0.51
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.11	0.51
3:E:96:LEU:HA	3:E:101:THR:HG21	1.92	0.51
1:A:807:GLU:OE2	1:A:810:ARG:NH1	2.44	0.51
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.92	0.51
2:B:473:ALA:HB2	2:B:765:PRO:HB3	1.93	0.51
2:B:694:ILE:HG13	2:B:772:TYR:CE1	2.45	0.51
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.32	0.51
2:C:606:LEU:HA	2:C:651:ARG:HH21	1.76	0.51
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.92	0.51
1:A:797:ARG:NH2	1:A:876:MET:O	2.44	0.51
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.93	0.51
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.46	0.51
2:C:208:LEU:HD21	2:C:1067:ILE:HG13	1.93	0.51
2:B:287:ARG:NE	2:B:330:THR:HG22	2.25	0.51
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.92	0.51
1:A:887:ILE:HD11	1:A:901:SER:HB2	1.93	0.51
2:B:697:ALA:HB2	2:B:775:VAL:HG23	1.93	0.51
2:B:1128:TYR:CZ	2:B:1135:PRO:HD3	2.45	0.51
3:D:69:GLU:HB2	3:D:109:GLY:HA3	1.93	0.51
2:C:872:ILE:HD12	2:C:886:SER:HB2	1.92	0.50
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.46	0.50
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.94	0.50
1:A:479:LYS:NZ	1:A:481:ASP:OD2	2.31	0.50
1:A:856:THR:HG22	1:A:916:ASN:HB2	1.94	0.50
2:B:186:ASP:OD2	2:B:279:SER:OG	2.27	0.50
1:A:531:LYS:HD3	1:A:691:TYR:OH	2.12	0.50
2:B:1008:LEU:HG	2:B:1010:ARG:H	1.75	0.50
1:A:674:HIS:HA	1:A:701:VAL:HG21	1.93	0.50
1:A:860:SER:OG	1:A:868:ASP:OD2	2.23	0.50
2:B:267:VAL:HA	2:B:1304:MET:HE2	1.93	0.50
2:B:342:THR:HB	2:B:1309:ILE:HD11	1.94	0.50
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.26	0.50
2:B:873:TYR:HA	2:B:896:LEU:O	2.12	0.50
2:C:171:GLU:OE1	2:C:1181:SER:N	2.33	0.50
3:D:9:TYR:H	3:D:204:ASP:CG	2.14	0.50
1:A:552:MET:H	1:A:576:ASN:ND2	2.09	0.50
2:C:184:GLU:HA	2:C:187:ASP:OD2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ALA:HB2	1:A:781:VAL:HG11	1.93	0.50
2:C:828:ASP:OD1	2:C:960:THR:OG1	2.29	0.50
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.47	0.49
1:A:840:MET:HG2	1:A:1024:LEU:HA	1.93	0.49
2:B:742:LYS:HG3	2:B:1012:LEU:HD13	1.93	0.49
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.12	0.49
1:A:52:ARG:NH2	1:A:169:SER:OG	2.45	0.49
1:A:192:VAL:HG22	1:A:216:LEU:HD22	1.94	0.49
1:A:557:SER:HB3	1:A:583:ARG:HB3	1.94	0.49
2:B:357:VAL:HG23	2:B:1057:VAL:HG11	1.94	0.49
3:E:229:PHE:O	3:E:233:THR:HG23	2.12	0.49
1:A:881:ILE:HG23	1:A:900:GLN:HB3	1.94	0.49
3:D:213:LEU:O	3:D:216:PHE:HB3	2.12	0.49
1:A:12:ARG:O	1:A:12:ARG:NE	2.45	0.49
2:B:186:ASP:O	2:B:190:VAL:HB	2.12	0.49
2:B:360:ILE:HG12	2:B:363:ARG:NH2	2.27	0.49
1:A:665:LEU:HD21	1:A:694:ILE:HD12	1.94	0.49
2:B:1087:ASP:OD2	2:B:1240:ARG:NH2	2.45	0.49
2:C:1268:GLY:HA3	2:C:1277:LEU:O	2.12	0.49
1:A:535:LEU:HD22	1:A:647:LEU:HD11	1.95	0.49
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.93	0.49
2:B:439:VAL:HG23	2:B:701:HIS:CE1	2.47	0.49
3:E:124:PRO:HA	3:E:127:VAL:HG22	1.95	0.49
2:B:265:VAL:HG22	2:B:358:LEU:HD22	1.95	0.49
2:C:976:THR:HA	2:C:979:ILE:HD12	1.95	0.49
6:A:1104:GTP:O1B	6:A:1104:GTP:H5"	2.13	0.49
2:B:157:ILE:HD13	2:B:160:PRO:HB3	1.95	0.49
2:C:474:ASP:OD1	2:C:474:ASP:N	2.45	0.49
2:C:620:ILE:HD11	2:C:631:PRO:HG2	1.95	0.49
2:C:893:ALA:HB1	2:C:915:VAL:HA	1.95	0.49
2:B:153:ASP:OD1	2:B:153:ASP:N	2.42	0.49
2:B:170:TYR:CE1	2:B:198:LYS:HG2	2.47	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.94	0.49
2:C:1043:SER:O	2:C:1045:TYR:N	2.46	0.49
2:B:836:GLN:OE1	2:B:836:GLN:N	2.46	0.48
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.13	0.48
1:A:26:THR:HG22	1:A:57:PHE:HZ	1.78	0.48
2:C:617:ASP:OD1	2:C:617:ASP:N	2.46	0.48
1:A:943:ILE:HG12	1:A:960:ILE:HG21	1.95	0.48
2:B:332:THR:HG23	2:B:344:VAL:HG12	1.94	0.48
2:B:806:VAL:O	2:B:810:LEU:HG	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:997:TYR:O	2:B:1001:THR:HG23	2.13	0.48
2:C:611:GLY:HA3	2:C:635:ILE:O	2.13	0.48
2:C:697:ALA:HB2	2:C:775:VAL:HG23	1.95	0.48
1:A:102:LEU:HD23	1:A:135:VAL:HA	1.96	0.48
2:B:522:PRO:HD2	2:B:636:PRO:HB3	1.94	0.48
2:B:1036:ASP:N	2:B:1036:ASP:OD1	2.46	0.48
2:C:879:THR:HB	2:C:882:GLN:HB2	1.96	0.48
1:A:890:LEU:HD23	1:A:890:LEU:H	1.79	0.48
2:B:737:PRO:HA	2:B:861:GLU:HG2	1.94	0.48
2:C:552:VAL:HG13	2:C:572:ASN:HB2	1.94	0.48
1:A:962:PHE:HB2	1:A:998:LEU:HD23	1.95	0.48
2:B:458:SER:HB3	2:B:676:THR:HG22	1.96	0.48
2:C:704:VAL:O	2:C:708:THR:HG23	2.14	0.48
1:A:202:SER:O	1:A:264:SER:OG	2.17	0.47
2:B:446:LYS:HA	2:B:769:GLN:HB3	1.96	0.47
2:B:1007:THR:OG1	2:B:1008:LEU:N	2.45	0.47
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	1.96	0.47
2:C:168:VAL:HG13	2:C:204:VAL:HG22	1.95	0.47
2:C:821:ASN:OD1	2:C:1014:MET:N	2.46	0.47
2:C:1159:VAL:HA	2:C:1164:TRP:HB2	1.95	0.47
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.59	0.47
1:A:552:MET:H	1:A:576:ASN:HD21	1.62	0.47
1:A:919:TYR:HB3	1:A:921:PHE:HE1	1.79	0.47
2:B:184:GLU:O	2:B:188:ARG:HG3	2.12	0.47
2:C:363:ARG:HH12	3:E:183:GLU:CD	2.17	0.47
2:C:532:ILE:O	2:C:535:VAL:HG23	2.15	0.47
1:A:114:ASN:ND2	1:A:117:LEU:HD22	2.29	0.47
1:A:186:ALA:HB2	1:A:195:ILE:HD12	1.96	0.47
2:B:446:LYS:HB3	2:B:448:TYR:CE2	2.49	0.47
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.50	0.47
2:C:633:THR:HG21	2:C:710:SER:HB2	1.96	0.47
2:B:612:PHE:CE2	2:B:614:ARG:HB2	2.49	0.47
2:C:738:GLU:OE2	2:C:857:SER:OG	2.21	0.47
2:B:505:PRO:HA	2:B:543:TRP:CZ2	2.50	0.47
2:B:891:HIS:HB3	3:D:242:ARG:HG2	1.96	0.47
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.14	0.47
3:E:44:LEU:HG	3:E:174:VAL:HG22	1.95	0.47
2:B:489:MET:HE1	2:B:580:TYR:HE2	1.78	0.47
2:C:405:HIS:CE1	2:C:625:PRO:HA	2.49	0.47
1:A:424:PRO:HG3	1:A:706:TYR:CZ	2.50	0.47
2:B:462:LEU:HA	2:B:506:SER:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1156:ILE:HD13	2:C:1156:ILE:HA	1.82	0.47
3:E:253:GLU:HA	3:E:254:TYR:HA	1.52	0.47
3:E:283:LEU:HA	3:E:286:THR:HG22	1.96	0.47
1:A:51:LEU:HB3	1:A:171:ILE:HG12	1.96	0.47
1:A:316:TYR:OH	5:A:1103:ATP:N1	2.31	0.47
2:B:227:LEU:HA	2:B:246:GLU:O	2.15	0.47
2:C:894:VAL:HG22	2:C:916:LEU:HB3	1.97	0.47
2:C:952:PHE:HB3	2:C:958:ILE:HD11	1.97	0.47
2:B:1143:GLU:HG2	2:B:1145:ALA:H	1.80	0.47
2:C:360:ILE:HD11	2:C:1054:ARG:HG2	1.95	0.47
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.96	0.47
3:D:253:GLU:HA	3:D:254:TYR:HA	1.49	0.47
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.79	0.46
1:A:564:GLU:OE1	4:A:1101:SAM:O3'	2.32	0.46
1:A:944:ARG:HB2	1:A:1006:MET:SD	2.55	0.46
2:B:561:ASN:HB3	2:B:565:GLU:HG2	1.97	0.46
2:B:585:PHE:CE1	2:B:728:LYS:HD3	2.51	0.46
2:B:1156:ILE:O	2:B:1159:VAL:HB	2.16	0.46
1:A:420:VAL:HG23	1:A:711:MET:HE1	1.96	0.46
1:A:911:MET:HE2	1:A:946:VAL:HA	1.97	0.46
2:B:719:ASN:OD1	2:B:719:ASN:N	2.38	0.46
2:B:903:ASN:ND2	2:B:905:PRO:HG2	2.31	0.46
2:C:231:LEU:HD12	2:C:985:ARG:HG2	1.97	0.46
2:C:837:THR:HG21	2:C:911:ARG:HG3	1.97	0.46
3:E:10:THR:N	3:E:204:ASP:OD2	2.47	0.46
1:A:420:VAL:HA	1:A:974:SER:HB2	1.96	0.46
1:A:563:ALA:HB3	1:A:588:GLY:H	1.80	0.46
1:A:907:ASP:O	1:A:911:MET:HG2	2.15	0.46
2:B:409:ILE:HD13	2:B:625:PRO:HB2	1.98	0.46
3:D:38:GLU:OE1	3:D:242:ARG:NH1	2.27	0.46
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.50	0.46
1:A:654:SER:O	1:A:658:ILE:HG12	2.16	0.46
2:B:429:ILE:HG23	2:B:799:THR:HG22	1.98	0.46
2:B:550:ILE:O	2:B:553:GLN:HG3	2.15	0.46
2:B:1134:ARG:H	2:B:1134:ARG:HG2	1.36	0.46
2:C:1050:LEU:HD23	2:C:1050:LEU:HA	1.72	0.46
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.39	0.46
2:B:684:LEU:HD12	2:B:684:LEU:HA	1.76	0.46
2:C:442:PRO:HD3	2:C:475:ILE:HG23	1.97	0.46
2:C:683:TRP:CH2	2:C:687:LEU:HD11	2.51	0.46
1:A:133:LEU:HD11	1:A:140:ILE:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HB3	1:A:313:ARG:HH21	1.81	0.46
1:A:849:ILE:HG12	1:A:918:ILE:HD13	1.98	0.46
1:A:862:GLY:HA3	1:A:924:VAL:HG11	1.98	0.46
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.15	0.46
3:E:178:LYS:HB3	3:E:251:VAL:HG22	1.97	0.46
1:A:915:ASN:HD21	1:A:954:THR:HG22	1.80	0.46
2:B:157:ILE:H	2:B:157:ILE:HG13	1.61	0.46
2:B:334:LEU:HA	2:B:341:LYS:HA	1.97	0.46
1:A:39:LEU:HG	1:A:54:LEU:HD21	1.98	0.45
1:A:281:ASN:O	1:A:285:GLU:HG2	2.16	0.45
1:A:771:THR:HG22	1:A:783:ILE:HB	1.97	0.45
1:A:919:TYR:HB3	1:A:921:PHE:CE1	2.52	0.45
2:C:1331:ARG:HG3	2:C:1332:ASN:H	1.80	0.45
1:A:271:ARG:O	1:A:275:ILE:HG13	2.15	0.45
2:C:543:TRP:CD2	2:C:666:ARG:HD3	2.50	0.45
1:A:282:GLU:H	1:A:282:GLU:HG2	1.48	0.45
1:A:474:TYR:CD1	1:A:499:VAL:HG12	2.51	0.45
1:A:845:ILE:HD12	1:A:922:ILE:HD11	1.98	0.45
2:C:774:LEU:HA	2:C:774:LEU:HD23	1.67	0.45
1:A:74:LEU:HB3	1:A:83:ILE:HD13	1.98	0.45
1:A:757:LEU:O	1:A:760:SER:OG	2.31	0.45
1:A:923:ALA:H	1:A:961:SER:HB3	1.81	0.45
2:B:897:TYR:CZ	2:B:928:ARG:HG2	2.51	0.45
2:C:495:LEU:HD22	2:C:532:ILE:HG22	1.98	0.45
2:C:979:ILE:HD13	2:C:1013:LYS:HB2	1.97	0.45
3:D:221:ARG:NH2	3:D:225:ARG:HD2	2.32	0.45
2:C:289:THR:O	2:C:328:GLY:HA3	2.16	0.45
2:C:401:LEU:HD12	2:C:401:LEU:HA	1.79	0.45
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.81	0.45
2:C:1116:ARG:HA	2:C:1116:ARG:HD2	1.83	0.45
1:A:552:MET:HB2	1:A:576:ASN:ND2	2.32	0.45
2:C:156:GLN:HB3	2:C:266:ILE:HD13	1.99	0.45
1:A:773:ARG:O	1:A:818:PHE:HA	2.17	0.45
2:B:1075:ARG:HB2	2:B:1233:LEU:HD21	1.99	0.45
2:B:1208:ASP:OD1	2:B:1243:ARG:NH1	2.49	0.45
2:C:1189:ASP:OD1	2:C:1189:ASP:N	2.50	0.45
1:A:658:ILE:O	1:A:662:ILE:HG12	2.17	0.45
2:B:802:GLN:O	2:B:806:VAL:HG23	2.16	0.45
2:B:863:LEU:HA	2:B:866:THR:HG22	1.98	0.45
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.98	0.45
1:A:255:ARG:NH2	6:A:1104:GTP:O1A	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:HG21	1:A:375:HIS:CE1	2.52	0.44
2:B:883:ILE:HG23	2:B:895:VAL:HG11	1.99	0.44
2:B:1002:LEU:HD23	2:B:1002:LEU:HA	1.73	0.44
2:C:1131:PRO:HG3	2:C:1154:ASN:ND2	2.32	0.44
2:C:164:LEU:HD21	2:C:1067:ILE:HD11	2.00	0.44
2:C:446:LYS:HB3	2:C:448:TYR:CE2	2.53	0.44
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.27	0.44
1:A:895:LYS:HA	1:A:895:LYS:HD3	1.84	0.44
2:B:397:LEU:HD23	2:B:397:LEU:HA	1.78	0.44
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.86	0.44
2:C:119:ASP:OD1	2:C:119:ASP:N	2.51	0.44
2:C:286:LEU:HD23	2:C:327:LEU:HD23	1.98	0.44
2:C:525:PHE:HZ	2:C:589:PHE:CE1	2.35	0.44
2:C:223:LYS:NZ	2:C:1203:HIS:HB2	2.33	0.44
2:C:835:TYR:CE2	2:C:941:TYR:HB3	2.53	0.44
2:C:1210:LEU:HD21	2:C:1255:ARG:O	2.17	0.44
1:A:12:ARG:HG3	1:A:213:TRP:CZ2	2.53	0.44
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.44
2:B:209:ASN:ND2	2:B:211:ASP:OD1	2.51	0.44
2:B:1240:ARG:HD2	2:B:1243:ARG:HB2	1.99	0.44
2:B:1267:THR:HG22	2:B:1299:SER:OG	2.18	0.44
1:A:918:ILE:HG23	1:A:957:VAL:HG13	1.99	0.44
2:B:1087:ASP:OD1	2:B:1237:SER:OG	2.36	0.44
2:B:1130:SER:O	2:B:1134:ARG:HD3	2.17	0.44
2:C:478:ILE:O	2:C:482:ILE:HG12	2.18	0.44
2:C:1243:ARG:HB3	2:C:1258:VAL:HG22	2.00	0.44
3:E:173:PRO:HG2	3:E:175:LYS:HE3	2.00	0.44
1:A:573:ARG:HA	1:A:584:ILE:HD12	1.99	0.44
2:C:96:ILE:H	2:C:96:ILE:HG12	1.60	0.44
2:C:156:GLN:OE1	2:C:1309:ILE:HG12	2.18	0.44
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.98	0.44
2:B:828:ASP:HA	2:C:645:THR:HG23	2.00	0.44
2:B:561:ASN:OD1	2:B:562:ALA:N	2.50	0.44
2:B:991:ASP:N	2:B:991:ASP:OD1	2.51	0.44
2:C:98:ASN:OD1	2:C:98:ASN:N	2.50	0.44
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.87	0.44
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.53	0.43
2:B:286:LEU:HD22	2:B:286:LEU:HA	1.85	0.43
2:B:1053:ARG:HD3	2:B:1053:ARG:HA	1.71	0.43
2:C:275:SER:HA	2:C:278:LEU:HD12	1.99	0.43
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:LEU:HD13	3:D:158:LEU:HA	1.83	0.43
2:B:489:MET:HE1	2:B:580:TYR:CE2	2.53	0.43
2:B:1120:THR:O	2:B:1120:THR:OG1	2.33	0.43
2:B:1233:LEU:HD23	2:B:1233:LEU:HA	1.72	0.43
2:B:1309:ILE:HD13	2:B:1309:ILE:HA	1.87	0.43
2:C:1114:ARG:HG3	2:C:1116:ARG:HD3	2.00	0.43
2:B:193:THR:HA	2:B:296:VAL:HG13	2.00	0.43
2:B:208:LEU:HD12	2:B:213:PHE:CE2	2.53	0.43
2:B:681:LYS:HG2	2:B:685:ARG:NH1	2.33	0.43
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	2.01	0.43
2:C:451:GLU:HA	2:C:452:ASN:HA	1.56	0.43
2:C:1211:LEU:HD12	2:C:1211:LEU:HA	1.85	0.43
2:C:1277:LEU:HD23	2:C:1289:PRO:HA	2.00	0.43
1:A:540:LYS:O	1:A:543:GLU:HG2	2.18	0.43
2:B:612:PHE:HE2	2:B:614:ARG:HB2	1.83	0.43
2:C:475:ILE:H	2:C:475:ILE:HG13	1.52	0.43
2:C:1096:TYR:CE2	2:C:1165:VAL:HG23	2.52	0.43
1:A:353:TYR:OH	3:D:43:GLU:OE1	2.30	0.43
1:A:373:ILE:HD13	1:A:817:GLY:HA2	2.00	0.43
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.86	0.43
1:A:906:PHE:O	1:A:945:ASN:HB3	2.19	0.43
5:A:1103:ATP:H5'1	5:A:1103:ATP:C8	2.42	0.43
2:B:793:TYR:CE1	2:B:1322:PRO:HG2	2.54	0.43
2:B:1188:VAL:HG11	2:B:1193:ILE:HD13	1.99	0.43
1:A:285:GLU:O	1:A:366:SER:HB3	2.18	0.43
2:B:414:LEU:HD11	2:B:1014:MET:SD	2.59	0.43
2:B:813:LEU:HD12	2:B:813:LEU:HA	1.86	0.43
2:C:356:SER:O	2:C:360:ILE:HG23	2.19	0.43
2:C:980:ARG:HA	2:C:1012:LEU:HD12	2.01	0.43
3:D:65:ASN:HB3	3:D:110:VAL:CG1	2.49	0.43
1:A:591:ALA:HB3	1:A:597:ARG:HA	2.00	0.43
2:C:351:ASP:OD1	2:C:351:ASP:N	2.51	0.43
2:C:832:MET:HE3	2:C:946:LEU:HB2	2.00	0.43
2:C:851:THR:CG2	2:C:854:GLN:HB2	2.48	0.43
1:A:381:GLY:H	1:A:802:THR:HB	1.84	0.43
2:B:620:ILE:HD13	2:B:620:ILE:HA	1.83	0.43
2:C:1049:GLU:O	2:C:1053:ARG:HG2	2.18	0.43
1:A:502:ASP:OD1	1:A:574:ARG:HD3	2.19	0.43
2:B:442:PRO:HG2	2:B:475:ILE:HB	2.00	0.43
2:C:836:GLN:HB2	2:C:940:ARG:HG2	2.01	0.43
2:C:1242:MET:SD	2:C:1260:PRO:HD3	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:ARG:HD2	2:B:635:ILE:HD11	1.99	0.43
2:B:1176:GLU:HB2	2:B:1203:HIS:CE1	2.54	0.43
2:C:176:LYS:HA	2:C:176:LYS:HD2	1.86	0.43
2:C:364:ALA:HB2	2:C:1050:LEU:HD21	2.01	0.43
3:D:2:LEU:HD23	3:D:2:LEU:HA	1.91	0.43
1:A:275:ILE:HG13	1:A:275:ILE:H	1.74	0.42
2:C:154:PHE:CE2	2:C:365:LEU:HB2	2.54	0.42
2:C:1015:GLN:H	2:C:1015:GLN:HG3	1.26	0.42
3:E:68:ILE:HG12	3:E:93:LEU:HG	1.99	0.42
3:E:233:THR:HG22	3:E:252:LEU:HD22	2.01	0.42
1:A:204:LEU:HD23	1:A:227:MET:HE2	2.01	0.42
1:A:408:PRO:HB2	1:A:468:PRO:HG2	2.01	0.42
1:A:913:LEU:O	1:A:953:ARG:NH2	2.50	0.42
1:A:913:LEU:O	1:A:953:ARG:HD2	2.18	0.42
2:B:1147:MET:HE3	2:B:1155:ILE:HD12	2.01	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.84	0.42
1:A:108:ASP:OD1	1:A:108:ASP:N	2.52	0.42
1:A:160:ASP:OD1	1:A:160:ASP:N	2.48	0.42
1:A:234:LYS:HB3	1:A:259:ARG:HA	2.01	0.42
2:B:326:GLY:H	2:B:1267:THR:HG21	1.84	0.42
2:C:341:LYS:HA	2:C:341:LYS:HD3	1.77	0.42
2:C:1210:LEU:HD22	2:C:1210:LEU:HA	1.88	0.42
1:A:14:ALA:HA	1:A:112:ARG:HH22	1.84	0.42
2:B:974:LEU:HD23	2:B:978:GLN:NE2	2.34	0.42
2:B:1314:ASP:OD1	2:B:1314:ASP:N	2.52	0.42
1:A:222:ARG:HD2	1:A:222:ARG:N	2.35	0.42
1:A:644:THR:O	1:A:696:PRO:HD2	2.19	0.42
2:B:459:ALA:HB2	2:B:679:CYS:SG	2.60	0.42
2:C:261:ASP:CG	2:C:263:ARG:HE	2.21	0.42
2:C:1200:LYS:NZ	2:C:1200:LYS:HB3	2.33	0.42
1:A:313:ARG:HD3	1:A:317:ARG:NH1	2.35	0.42
1:A:714:ARG:HD3	1:A:1044:ASP:OD1	2.19	0.42
1:A:916:ASN:N	1:A:955:ASN:O	2.51	0.42
2:B:614:ARG:NH1	2:B:617:ASP:OD1	2.52	0.42
2:B:925:VAL:O	2:B:928:ARG:HB2	2.19	0.42
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	2.01	0.42
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.20	0.42
3:D:38:GLU:HB2	3:D:176:ARG:HB3	2.01	0.42
2:B:1277:LEU:O	2:B:1290:LYS:HE3	2.19	0.42
2:C:1106:PHE:CE2	2:C:1119:TYR:HB2	2.54	0.42
1:A:890:LEU:O	1:A:894:LYS:HE3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:VAL:HG13	2:B:379:LEU:HD21	2.01	0.42
2:B:483:ALA:O	2:B:487:SER:OG	2.26	0.42
2:B:491:ASN:ND2	2:B:750:GLU:O	2.53	0.42
2:B:494:GLU:HG2	2:B:577:GLN:HG3	2.02	0.42
2:C:648:PHE:HB2	2:C:699:THR:HG21	2.02	0.42
2:C:694:ILE:HG13	2:C:772:TYR:CE1	2.55	0.42
2:C:931:ASN:HD22	2:C:931:ASN:N	2.16	0.42
3:E:123:ASP:HA	3:E:124:PRO:HD3	1.89	0.42
1:A:102:LEU:HA	1:A:102:LEU:HD12	1.80	0.42
1:A:613:ILE:HG13	1:A:643:ALA:HB2	2.00	0.42
1:A:772:TRP:HA	1:A:817:GLY:HA3	2.02	0.42
2:B:691:PHE:O	2:B:695:ALA:HB2	2.20	0.42
1:A:404:SER:HB3	1:A:826:PHE:CD1	2.55	0.42
1:A:882:ASP:HB3	1:A:885:THR:OG1	2.20	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.02	0.42
2:B:300:LEU:HD23	2:B:300:LEU:HA	1.85	0.42
2:B:451:GLU:O	2:B:452:ASN:HB2	2.20	0.42
2:C:550:ILE:HD13	2:C:596:GLY:HA3	2.02	0.42
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.72	0.42
1:A:238:ASP:OD2	1:A:279:TYR:OH	2.20	0.41
1:A:282:GLU:HG3	1:A:300:LEU:HD11	2.02	0.41
4:A:1102:SAM:HB2	4:A:1102:SAM:H5'2	1.77	0.41
2:B:297:ASN:HA	2:B:298:PRO:HD3	1.92	0.41
2:C:379:LEU:HD12	2:C:379:LEU:HA	1.88	0.41
2:C:876:GLY:HA2	2:C:902:ILE:HA	2.02	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.87	0.41
1:A:184:TRP:HB3	1:A:195:ILE:HD13	2.01	0.41
2:B:576:ASP:H	2:B:579:LEU:HD12	1.85	0.41
2:B:701:HIS:O	2:B:704:VAL:HG22	2.20	0.41
2:B:949:ALA:O	3:D:243:LYS:HE3	2.20	0.41
2:C:865:ILE:HD12	2:C:865:ILE:HA	1.91	0.41
1:A:7:ILE:HG22	1:A:250:LEU:HD11	2.03	0.41
1:A:616:ASP:OD2	4:A:1101:SAM:N	2.53	0.41
2:B:156:GLN:HB3	2:B:266:ILE:HD11	2.02	0.41
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.82	0.41
3:D:85:ASN:HD21	3:D:277:GLU:HG3	1.85	0.41
2:B:231:LEU:HB3	2:B:249:SER:HB2	2.03	0.41
2:B:439:VAL:HG21	2:B:702:LEU:HD13	2.02	0.41
2:B:1236:ILE:HG22	2:B:1237:SER:N	2.34	0.41
3:D:60:ARG:HE	3:D:60:ARG:HB2	1.74	0.41
1:A:143:TYR:CD1	1:A:146:PRO:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:OG	1:A:226:ASP:OD2	2.38	0.41
2:B:608:THR:HA	2:B:609:PRO:HD3	1.80	0.41
2:C:151:SER:O	2:C:1310:ARG:NH2	2.53	0.41
2:C:220:ASP:OD1	2:C:227:LEU:HB2	2.21	0.41
3:E:142:THR:HA	3:E:143:PRO:HD3	1.89	0.41
1:A:755:ALA:N	1:A:756:PRO:HD2	2.35	0.41
2:B:606:LEU:HA	2:B:651:ARG:HH21	1.86	0.41
2:C:804:LEU:HD13	2:C:804:LEU:HA	1.91	0.41
2:C:1067:ILE:HD12	2:C:1067:ILE:HA	1.87	0.41
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.03	0.41
3:D:186:LEU:HA	3:D:186:LEU:HD23	1.76	0.41
1:A:444:LEU:HD11	1:A:449:THR:HG23	2.02	0.41
2:B:774:LEU:HD23	2:B:774:LEU:HA	1.91	0.41
2:B:852:TYR:HB2	2:B:920:PRO:HA	2.03	0.41
2:B:329:LEU:HD11	2:B:344:VAL:HB	2.02	0.41
1:A:43:ASN:O	1:A:47:ARG:N	2.53	0.41
1:A:717:THR:CB	1:A:1020:SER:HB2	2.51	0.41
2:B:373:ASP:O	2:B:376:ILE:HG12	2.21	0.41
2:B:480:LEU:HD12	2:B:480:LEU:HA	1.82	0.41
2:B:772:TYR:CD1	2:B:772:TYR:N	2.89	0.41
2:B:1272:ARG:HH12	3:D:69:GLU:HB3	1.86	0.41
2:B:1280:PRO:HB3	2:B:1285:GLN:O	2.20	0.41
2:C:141:LEU:HD12	2:C:141:LEU:HA	1.73	0.41
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.94	0.41
2:C:442:PRO:CD	2:C:475:ILE:HG23	2.51	0.41
2:C:704:VAL:HA	2:C:1330:ILE:HG21	2.01	0.41
2:C:1076:ILE:HG22	2:C:1159:VAL:HG11	2.03	0.41
3:D:28:PRO:CB	3:D:226:MET:HG3	2.51	0.41
3:D:228:LEU:HA	3:D:231:MET:HE3	2.03	0.41
1:A:445:TYR:CD2	1:A:625:PHE:HB2	2.56	0.41
1:A:967:ILE:HG21	1:A:987:LEU:HD11	2.03	0.41
2:B:231:LEU:HD21	2:B:986:ILE:HG12	2.03	0.41
2:B:659:LEU:HD12	2:B:659:LEU:HA	1.73	0.41
2:C:582:SER:O	2:C:728:LYS:HE3	2.21	0.41
2:C:678:SER:O	2:C:682:GLN:HG3	2.20	0.41
2:C:835:TYR:HA	2:C:941:TYR:HA	2.02	0.41
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	2.01	0.41
3:E:27:THR:O	3:E:30:GLN:HG2	2.20	0.41
2:B:957:PHE:CG	2:B:958:ILE:HG13	2.56	0.40
2:C:169:LYS:HB2	2:C:203:VAL:HG23	2.02	0.40
2:C:680:THR:O	2:C:684:LEU:HG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1085:ASP:HB2	2:C:1087:ASP:OD1	2.21	0.40
3:E:263:ALA:O	3:E:270:THR:HG21	2.21	0.40
1:A:112:ARG:HB3	1:A:143:TYR:CZ	2.57	0.40
2:B:259:MET:HE1	2:B:1047:LEU:HD13	2.03	0.40
2:B:713:MET:HE1	2:B:804:LEU:HD13	2.03	0.40
2:C:287:ARG:O	2:C:289:THR:N	2.53	0.40
2:C:357:VAL:O	2:C:360:ILE:HG12	2.22	0.40
1:A:108:ASP:HB2	1:A:111:LEU:HD22	2.03	0.40
2:B:135:LYS:HD2	2:B:135:LYS:HA	1.82	0.40
2:B:674:LYS:HB2	2:B:674:LYS:HE2	1.91	0.40
2:B:716:PHE:CD1	2:B:717:THR:HG23	2.56	0.40
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	2.04	0.40
1:A:226:ASP:HA	1:A:229:ASP:OD2	2.22	0.40
1:A:278:LEU:HD11	1:A:316:TYR:HB2	2.03	0.40
1:A:883:PRO:HG3	1:A:903:PRO:HA	2.04	0.40
2:C:169:LYS:O	2:C:202:ALA:N	2.53	0.40
2:C:837:THR:O	2:C:935:GLN:HB3	2.21	0.40
3:E:224:PHE:O	3:E:228:LEU:HG	2.21	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	1055/1058 (100%)	1002 (95%)	53 (5%)	0	100	100
2	B	1187/1333 (89%)	1126 (95%)	58 (5%)	3 (0%)	41	73
2	C	1247/1333 (94%)	1191 (96%)	49 (4%)	7 (1%)	25	59
3	D	290/448 (65%)	282 (97%)	6 (2%)	2 (1%)	22	57
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	41	73
All	All	4069/4620 (88%)	3883 (95%)	173 (4%)	13 (0%)	44	73

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	769	GLN
2	C	1251	VAL
3	D	61	ASN
2	B	1310	ARG
2	C	340	VAL
2	C	1014	MET
3	E	116	THR
2	C	901	VAL
2	C	1331	ARG
2	C	1236	ILE
3	D	244	VAL
2	B	1235	PRO
2	B	1309	ILE

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	942/943 (100%)	850 (90%)	92 (10%)	8 29
2	B	1038/1153 (90%)	946 (91%)	92 (9%)	9 34
2	C	1090/1153 (94%)	974 (89%)	116 (11%)	6 26
3	D	240/379 (63%)	221 (92%)	19 (8%)	12 40
3	E	240/379 (63%)	218 (91%)	22 (9%)	9 33
All	All	3550/4007 (89%)	3209 (90%)	341 (10%)	12 31

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	7	ILE
1	A	12	ARG
1	A	31	VAL
1	A	41	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	46	ARG
1	A	47	ARG
1	A	50	THR
1	A	54	LEU
1	A	65	THR
1	A	76	LEU
1	A	81	LYS
1	A	89	ILE
1	A	99	VAL
1	A	102	LEU
1	A	105	ARG
1	A	108	ASP
1	A	111	LEU
1	A	130	VAL
1	A	153	VAL
1	A	157	LEU
1	A	173	ASP
1	A	177	THR
1	A	190	THR
1	A	196	LEU
1	A	199	MET
1	A	202	SER
1	A	203	THR
1	A	222	ARG
1	A	236	LEU
1	A	242	LYS
1	A	255	ARG
1	A	264	SER
1	A	282	GLU
1	A	284	THR
1	A	297	LEU
1	A	298	LEU
1	A	313	ARG
1	A	345	ASN
1	A	348	LEU
1	A	352	THR
1	A	368	THR
1	A	377	LEU
1	A	378	THR
1	A	423	THR
1	A	449	THR
1	A	464	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	LEU
1	A	475	ARG
1	A	493	LEU
1	A	503	ILE
1	A	532	MET
1	A	561	LEU
1	A	565	ARG
1	A	569	VAL
1	A	583	ARG
1	A	592	VAL
1	A	593	GLU
1	A	595	ASN
1	A	628	MET
1	A	633	ILE
1	A	647	LEU
1	A	664	ARG
1	A	665	LEU
1	A	716	MET
1	A	719	VAL
1	A	737	HIS
1	A	745	LEU
1	A	750	VAL
1	A	757	LEU
1	A	763	LYS
1	A	781	VAL
1	A	783	ILE
1	A	792	ILE
1	A	797	ARG
1	A	812	VAL
1	A	816	LEU
1	A	833	VAL
1	A	861	ILE
1	A	886	ARG
1	A	890	LEU
1	A	915	ASN
1	A	924	VAL
1	A	925	ILE
1	A	953	ARG
1	A	978	LYS
1	A	980	ILE
1	A	982	VAL
1	A	996	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1018	ARG
1	A	1025	ILE
1	A	1034	ARG
2	B	143	VAL
2	B	147	VAL
2	B	186	ASP
2	B	198	LYS
2	B	203	VAL
2	B	231	LEU
2	B	238	THR
2	B	242	GLU
2	B	259	MET
2	B	260	THR
2	B	265	VAL
2	B	270	THR
2	B	271	THR
2	B	274	MET
2	B	283	ASN
2	B	286	LEU
2	B	289	THR
2	B	294	VAL
2	B	315	THR
2	B	320	GLN
2	B	323	THR
2	B	339	LEU
2	B	366	MET
2	B	414	LEU
2	B	431	THR
2	B	447	ARG
2	B	486	VAL
2	B	512	LEU
2	B	533	GLN
2	B	552	VAL
2	B	615	THR
2	B	637	TYR
2	B	638	THR
2	B	659	LEU
2	B	674	LYS
2	B	684	LEU
2	B	685	ARG
2	B	687	LEU
2	B	689	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	694	ILE
2	B	702	LEU
2	B	736	SER
2	B	742	LYS
2	B	748	GLN
2	B	750	GLU
2	B	753	ASP
2	B	756	THR
2	B	788	MET
2	B	799	THR
2	B	804	LEU
2	B	815	LEU
2	B	837	THR
2	B	890	THR
2	B	925	VAL
2	B	937	ASN
2	B	951	ILE
2	B	953	ASP
2	B	968	ARG
2	B	970	LEU
2	B	976	THR
2	B	988	GLN
2	B	990	THR
2	B	991	ASP
2	B	995	THR
2	B	1007	THR
2	B	1036	ASP
2	B	1041	ARG
2	B	1048	ASP
2	B	1052	LEU
2	B	1070	ARG
2	B	1074	VAL
2	B	1079	LEU
2	B	1085	ASP
2	B	1108	SER
2	B	1110	LEU
2	B	1120	THR
2	B	1134	ARG
2	B	1170	ASP
2	B	1174	THR
2	B	1178	MET
2	B	1186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1198	LYS
2	B	1210	LEU
2	B	1223	SER
2	B	1247	ASN
2	B	1305	MET
2	B	1310	ARG
2	B	1314	ASP
2	B	1315	MET
2	B	1317	VAL
2	B	1329	ASN
2	B	1331	ARG
2	C	82	ARG
2	C	86	VAL
2	C	98	ASN
2	C	100	ASP
2	C	109	LYS
2	C	117	ARG
2	C	120	VAL
2	C	141	LEU
2	C	144	ASN
2	C	158	SER
2	C	187	ASP
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	217	THR
2	C	221	LEU
2	C	230	ASP
2	C	231	LEU
2	C	237	VAL
2	C	255	LEU
2	C	264	LEU
2	C	265	VAL
2	C	270	THR
2	C	277	THR
2	C	286	LEU
2	C	294	VAL
2	C	310	LEU
2	C	323	THR
2	C	330	THR
2	C	370	VAL
2	C	375	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	379	LEU
2	C	383	SER
2	C	384	MET
2	C	401	LEU
2	C	447	ARG
2	C	474	ASP
2	C	475	ILE
2	C	484	ARG
2	C	532	ILE
2	C	533	GLN
2	C	535	VAL
2	C	542	ARG
2	C	552	VAL
2	C	557	THR
2	C	626	ARG
2	C	629	ARG
2	C	630	ASN
2	C	637	TYR
2	C	638	THR
2	C	654	THR
2	C	659	LEU
2	C	689	THR
2	C	694	ILE
2	C	696	VAL
2	C	708	THR
2	C	717	THR
2	C	752	VAL
2	C	763	VAL
2	C	804	LEU
2	C	811	SER
2	C	815	LEU
2	C	828	ASP
2	C	832	MET
2	C	836	GLN
2	C	837	THR
2	C	841	ASP
2	C	855	TYR
2	C	859	ILE
2	C	872	ILE
2	C	921	ASP
2	C	925	VAL
2	C	931	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	935	GLN
2	C	952	PHE
2	C	965	ARG
2	C	980	ARG
2	C	995	THR
2	C	1007	THR
2	C	1010	ARG
2	C	1013	LYS
2	C	1015	GLN
2	C	1022	ILE
2	C	1028	VAL
2	C	1034	GLN
2	C	1052	LEU
2	C	1055	LEU
2	C	1067	ILE
2	C	1070	ARG
2	C	1079	LEU
2	C	1080	THR
2	C	1104	ARG
2	C	1110	LEU
2	C	1116	ARG
2	C	1120	THR
2	C	1134	ARG
2	C	1170	ASP
2	C	1185	THR
2	C	1186	GLN
2	C	1189	ASP
2	C	1198	LYS
2	C	1200	LYS
2	C	1202	PHE
2	C	1210	LEU
2	C	1230	ILE
2	C	1233	LEU
2	C	1234	GLN
2	C	1251	VAL
2	C	1253	ARG
2	C	1262	SER
2	C	1267	THR
2	C	1269	THR
2	C	1285	GLN
2	C	1293	VAL
2	C	1320	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1321	ASN
3	D	20	ARG
3	D	29	THR
3	D	47	LYS
3	D	77	PHE
3	D	92	ARG
3	D	93	LEU
3	D	100	ASN
3	D	116	THR
3	D	133	THR
3	D	139	ASN
3	D	158	LEU
3	D	160	LEU
3	D	181	SER
3	D	189	LEU
3	D	191	ARG
3	D	226	MET
3	D	252	LEU
3	D	257	VAL
3	D	265	ARG
3	E	1	MET
3	E	2	LEU
3	E	6	THR
3	E	21	ASN
3	E	29	THR
3	E	35	LEU
3	E	66	VAL
3	E	93	LEU
3	E	98	LEU
3	E	130	PHE
3	E	133	THR
3	E	160	LEU
3	E	163	THR
3	E	189	LEU
3	E	226	MET
3	E	240	VAL
3	E	244	VAL
3	E	247	ARG
3	E	249	ASP
3	E	252	LEU
3	E	262	THR
3	E	272	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	576	ASN
1	A	837	HIS
2	B	430	ASN
2	B	1138	HIS
2	C	931	ASN
3	D	85	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	GTP	A	1104	7	26,34,34	1.10	1 (3%)	32,54,54	1.45	5 (15%)
4	SAM	A	1102	-	24,29,29	1.21	3 (12%)	23,42,42	1.60	4 (17%)
5	ATP	A	1103	-	26,33,33	0.90	1 (3%)	31,52,52	1.51	5 (16%)
4	SAM	A	1101	-	24,29,29	1.20	3 (12%)	23,42,42	1.56	4 (17%)

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
6	GTP	A	1104	7	-	3/18/38/38	0/3/3/3
4	SAM	A	1102	-	-	4/12/33/33	0/3/3/3
5	ATP	A	1103	-	-	5/18/38/38	0/3/3/3
4	SAM	A	1101	-	-	6/12/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N3	4.01	1.38	1.32
4	A	1102	SAM	C2-N3	3.88	1.38	1.32
6	A	1104	GTP	C5-C6	-3.87	1.39	1.47
4	A	1102	SAM	C2-N1	2.51	1.38	1.33
4	A	1101	SAM	C2-N1	2.48	1.38	1.33
5	A	1103	ATP	C5-C4	2.40	1.47	1.40
4	A	1102	SAM	OXT-C	-2.08	1.23	1.30
4	A	1101	SAM	OXT-C	-2.08	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	SAM	N3-C2-N1	-5.54	120.02	128.68
4	A	1102	SAM	N3-C2-N1	-5.41	120.23	128.68
6	A	1104	GTP	C8-N7-C5	3.65	109.94	102.99
5	A	1103	ATP	C3'-C2'-C1'	3.40	106.10	100.98
6	A	1104	GTP	C5-C6-N1	3.25	119.69	113.95
5	A	1103	ATP	PB-O3B-PG	-3.22	121.79	132.83
6	A	1104	GTP	PB-O3B-PG	-3.00	122.52	132.83
5	A	1103	ATP	N3-C2-N1	-2.95	124.07	128.68
6	A	1104	GTP	C2-N1-C6	-2.88	119.79	125.10
4	A	1102	SAM	C3'-C2'-C1'	2.87	105.29	100.98
5	A	1103	ATP	PA-O3A-PB	-2.85	123.03	132.83
4	A	1101	SAM	OXT-C-O	-2.76	117.82	124.09
4	A	1102	SAM	OXT-C-O	-2.64	118.10	124.09
4	A	1101	SAM	C3'-C2'-C1'	2.32	104.47	100.98
4	A	1102	SAM	OXT-C-CA	2.20	120.89	113.38
4	A	1101	SAM	OXT-C-CA	2.18	120.81	113.38
5	A	1103	ATP	C4-C5-N7	-2.18	107.13	109.40
6	A	1104	GTP	O6-C6-C5	-2.13	120.21	124.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	O-C-CA-N
4	A	1101	SAM	C-CA-CB-CG
4	A	1102	SAM	N-CA-CB-CG
4	A	1102	SAM	C-CA-CB-CG
4	A	1102	SAM	CB-CG-SD-C5'
5	A	1103	ATP	C5'-O5'-PA-O2A
5	A	1103	ATP	C5'-O5'-PA-O3A
6	A	1104	GTP	PB-O3B-PG-O3G
5	A	1103	ATP	O4'-C4'-C5'-O5'
4	A	1101	SAM	OXT-C-CA-N
5	A	1103	ATP	PB-O3A-PA-O5'
4	A	1101	SAM	N-CA-CB-CG
5	A	1103	ATP	C5'-O5'-PA-O1A
4	A	1102	SAM	C3'-C4'-C5'-SD
4	A	1101	SAM	O-C-CA-CB
4	A	1101	SAM	OXT-C-CA-CB
6	A	1104	GTP	PB-O3B-PG-O1G
6	A	1104	GTP	O4'-C4'-C5'-O5'

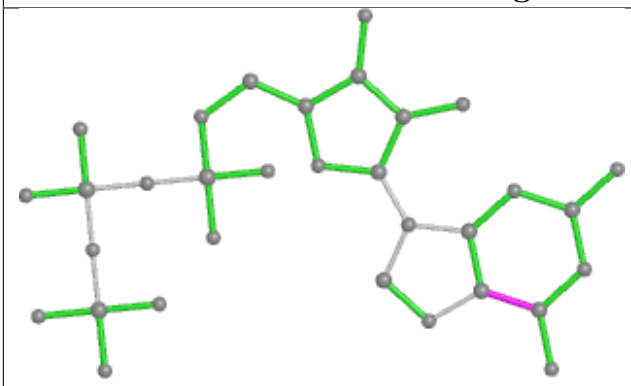
There are no ring outliers.

4 monomers are involved in 9 short contacts:

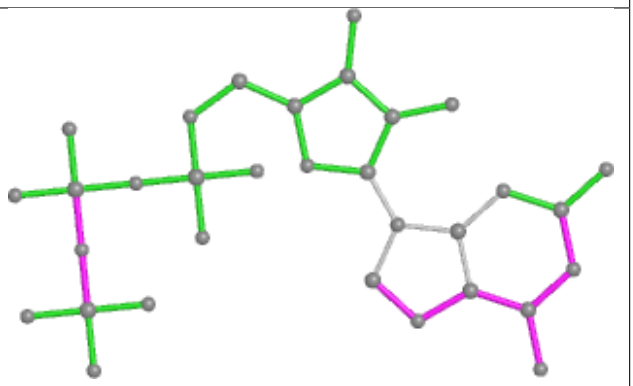
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1104	GTP	3	0
4	A	1102	SAM	1	0
5	A	1103	ATP	3	0
4	A	1101	SAM	2	0

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 then 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.

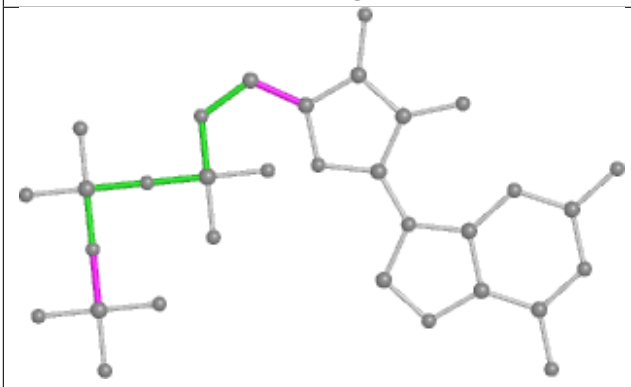
Ligand GTP A 1104



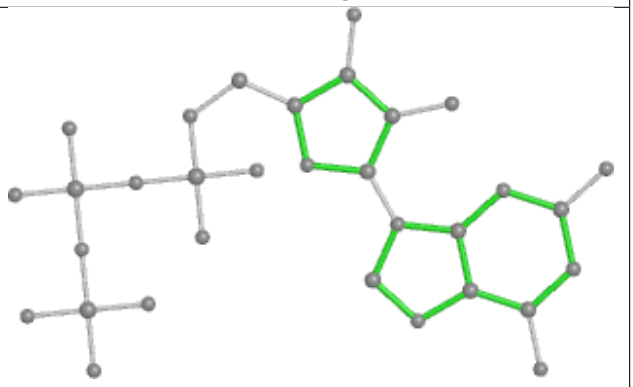
Bond lengths



Bond angles

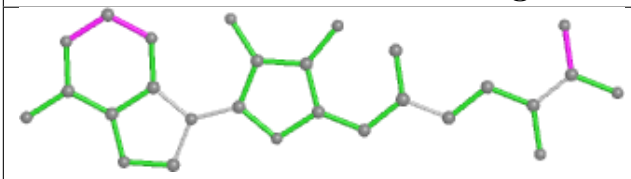


Torsions

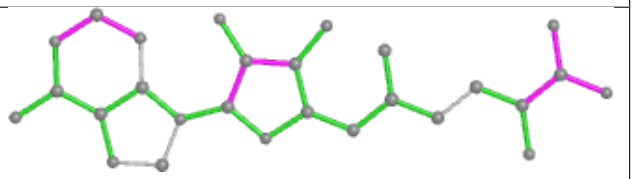


Rings

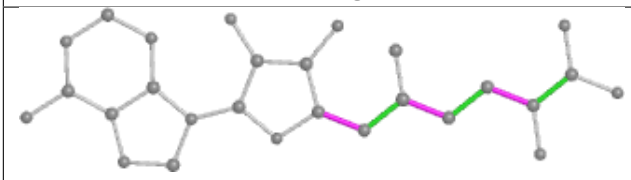
Ligand SAM A 1102



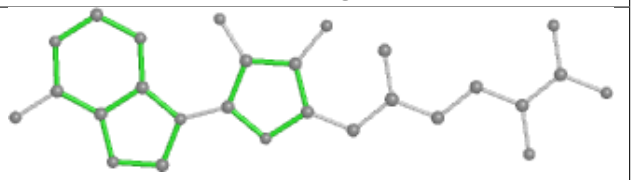
Bond lengths



Bond angles

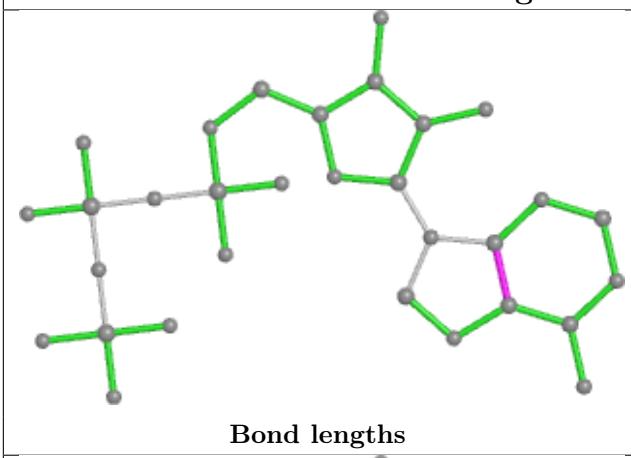


Torsions

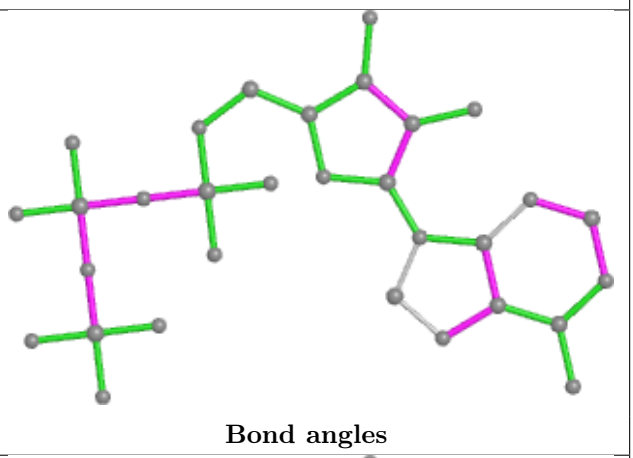


Rings

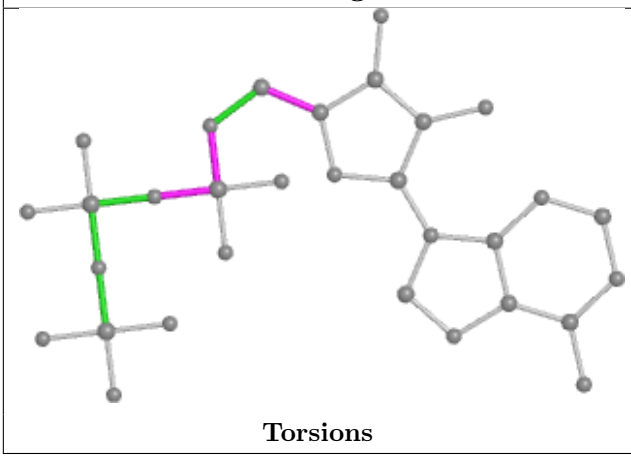
Ligand ATP A 1103



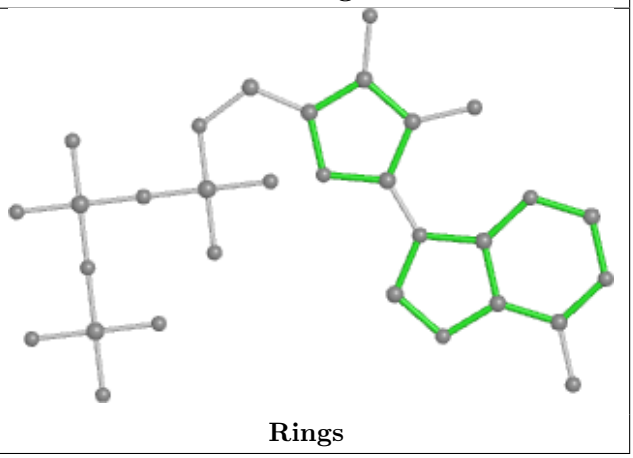
Bond lengths



Bond angles

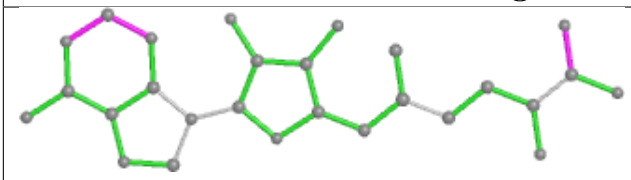


Torsions

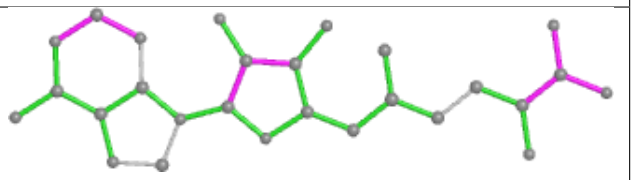


Rings

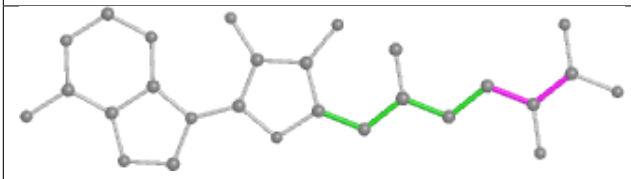
Ligand SAM A 1101



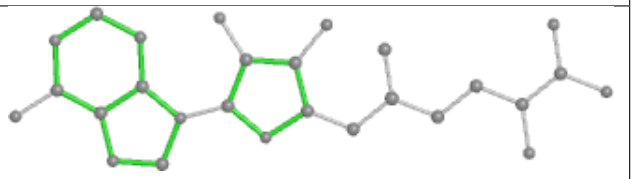
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

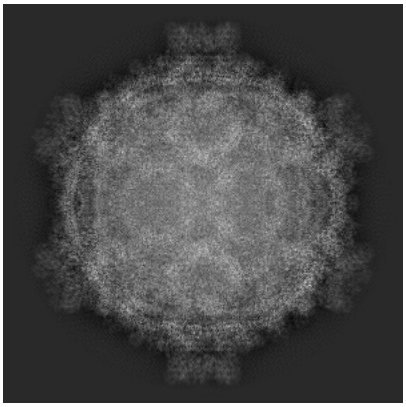
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6377. These allow visual inspection of the internal detail of the map and identification of artifacts.

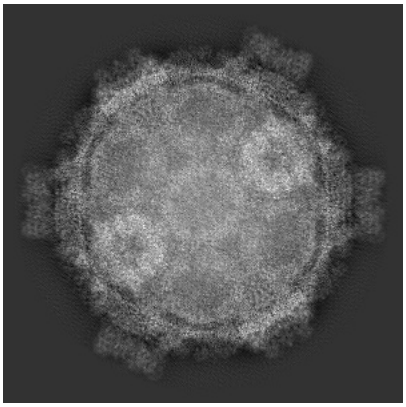
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

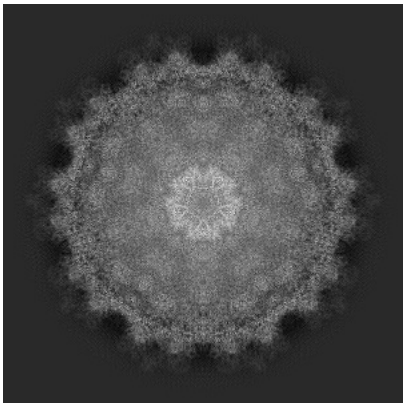
6.1.1 Primary map



X



Y

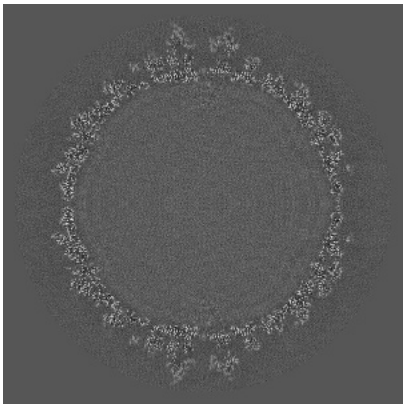


Z

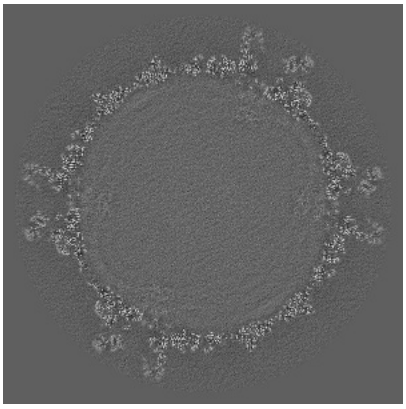
The images above show the map projected in three orthogonal directions.

6.2 Central slices

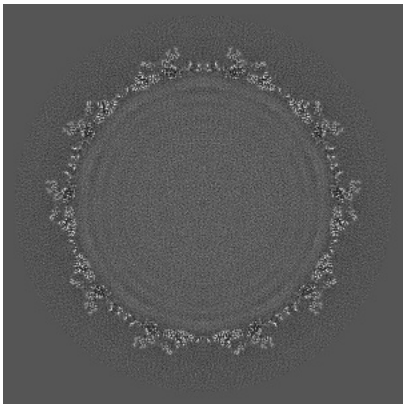
6.2.1 Primary map



X Index: 350



Y Index: 350

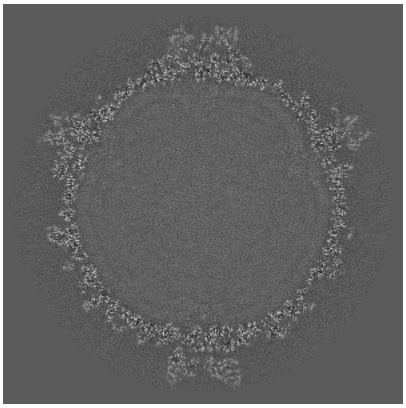


Z Index: 350

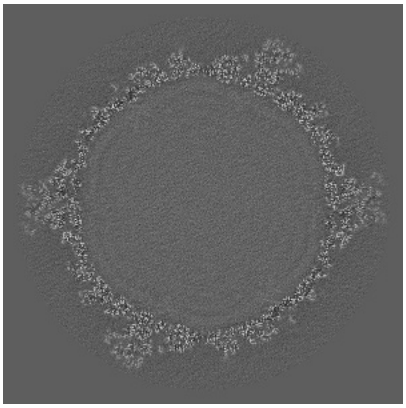
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

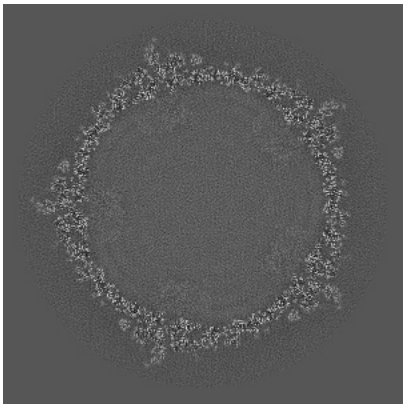
6.3.1 Primary map



X Index: 373



Y Index: 397

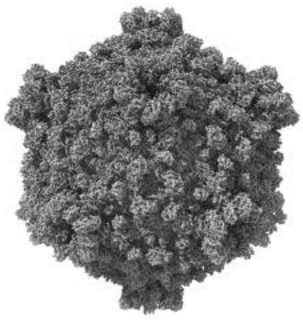


Z Index: 279

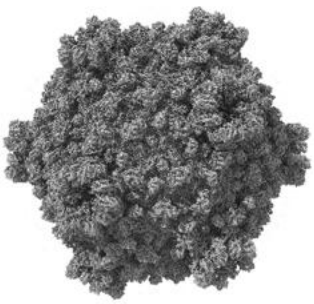
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

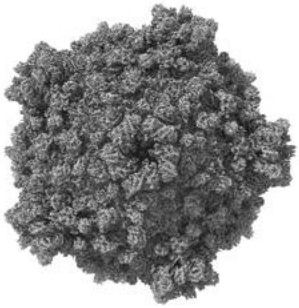
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

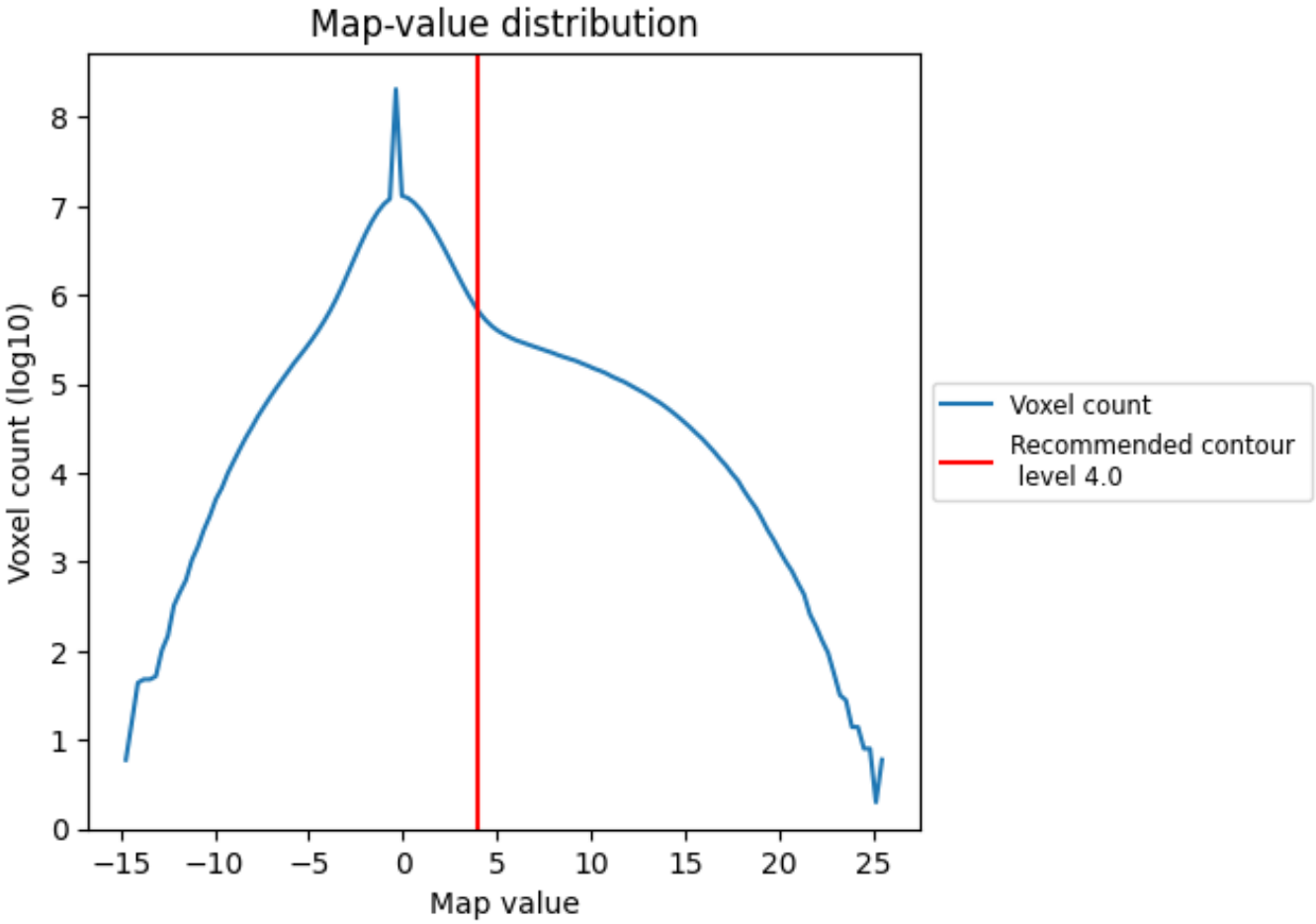
6.5 Mask visualisation (i)

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

7 Map analysis

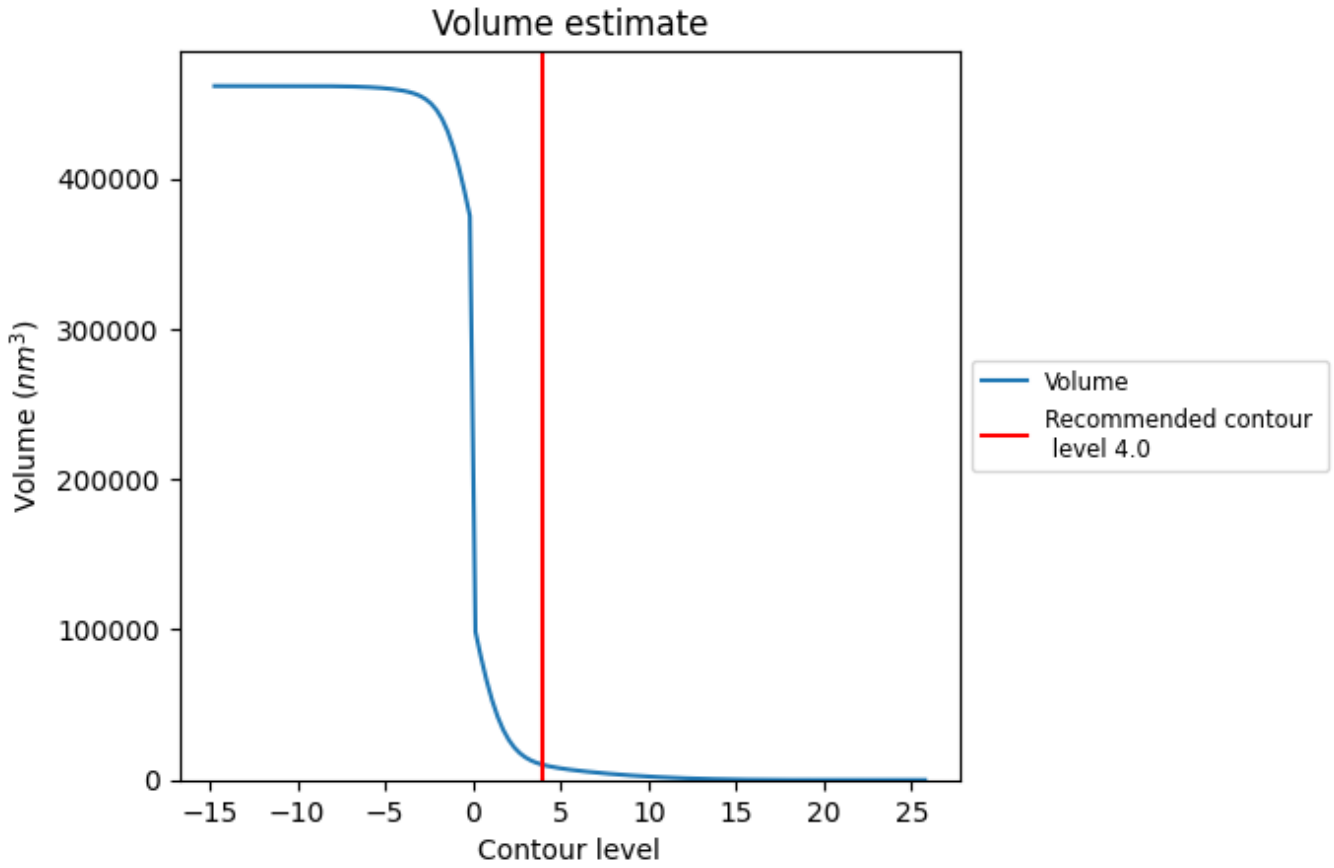
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

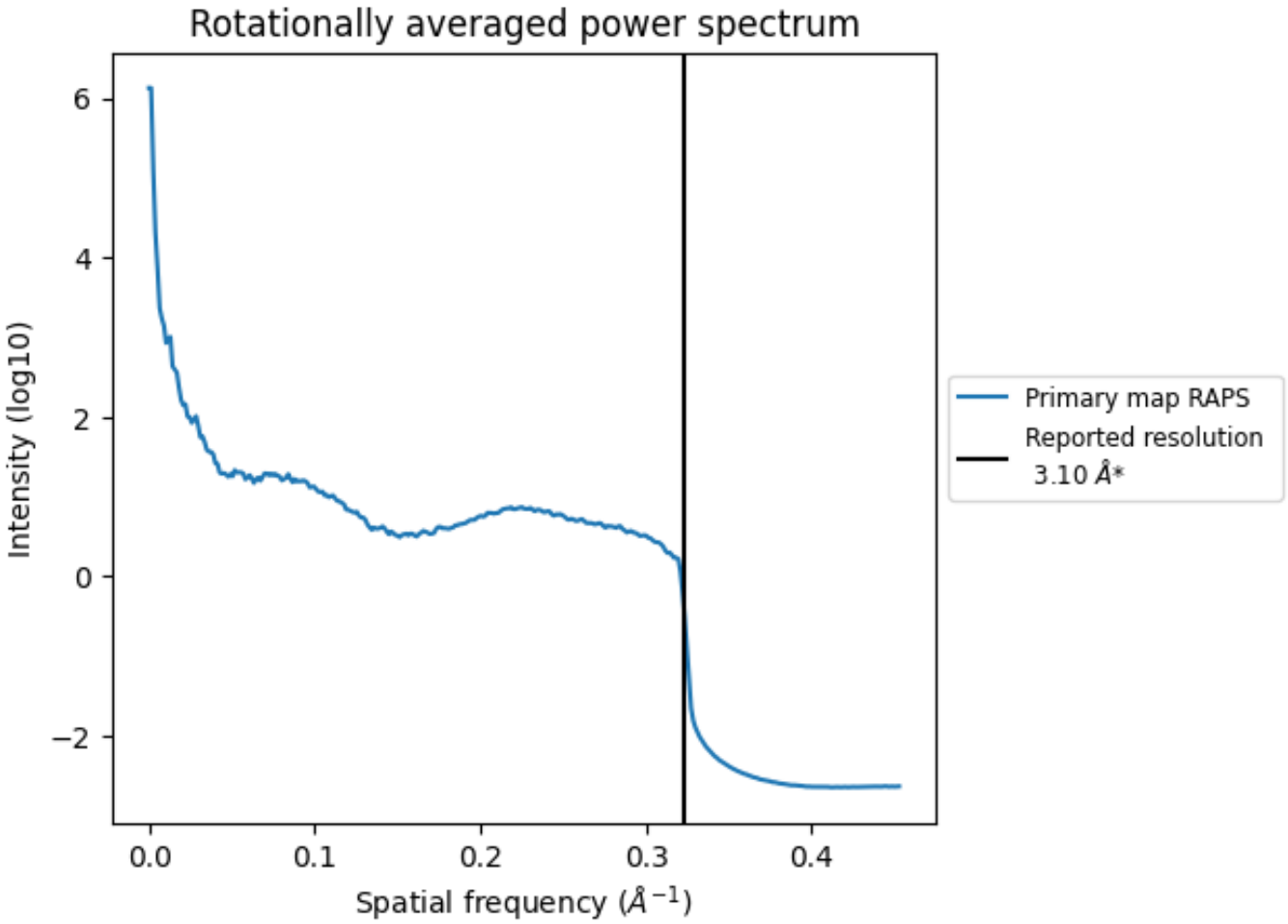
7.2 Volume estimate



The volume at the recommended contour level is 10082 nm^3; this corresponds to an approximate mass of 9107 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)



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation (i)

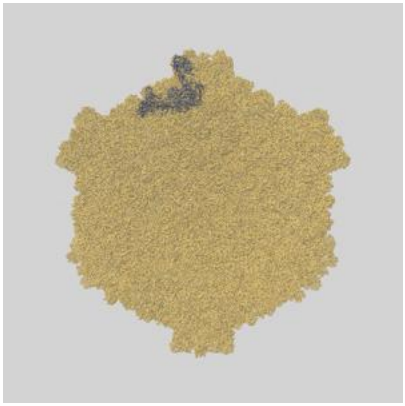
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

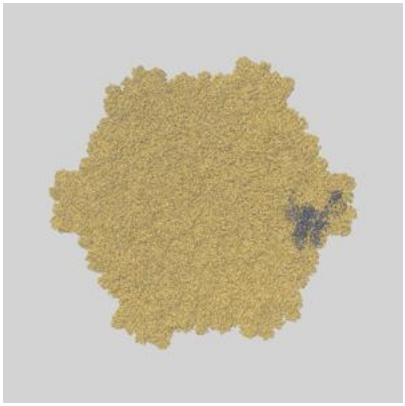
This section contains information regarding the fit between EMDB map EMD-6377 and PDB model 3JB3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

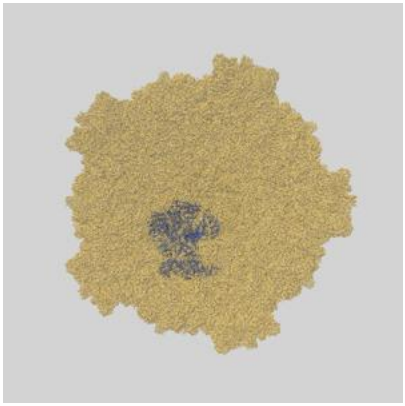
9.1.1 Map-model overlay



X

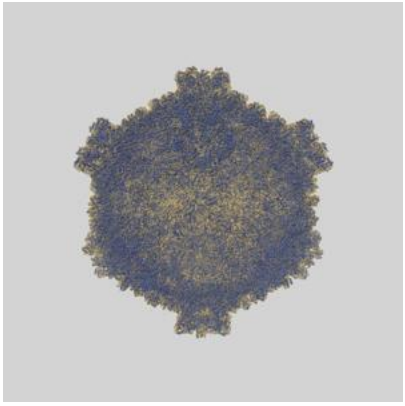


Y

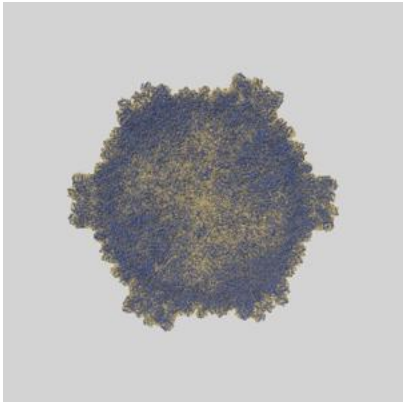


Z

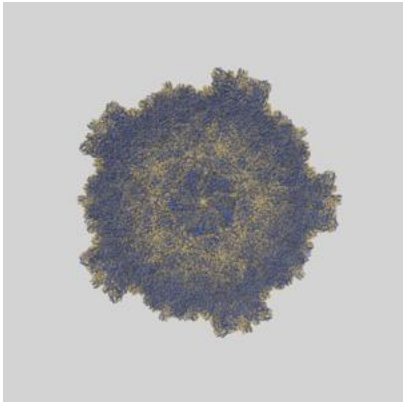
9.1.2 Map-model assembly overlay



X



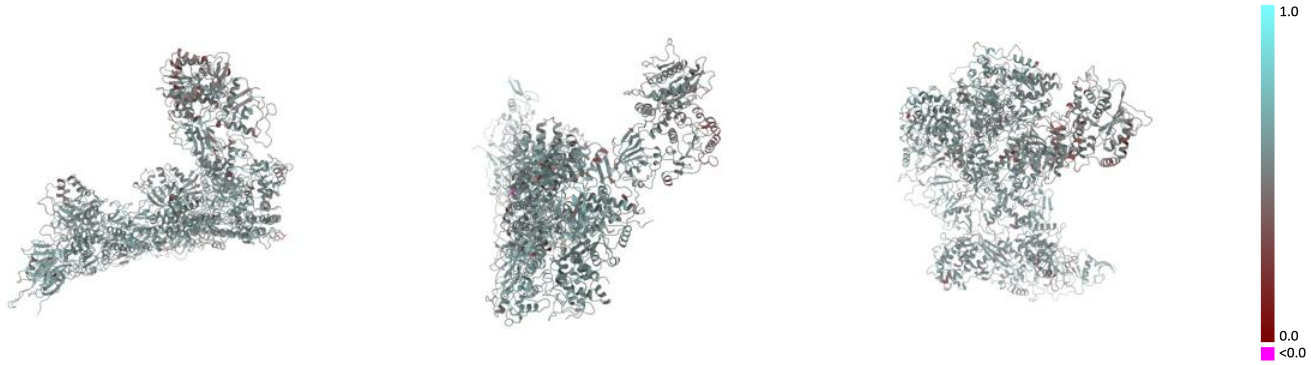
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

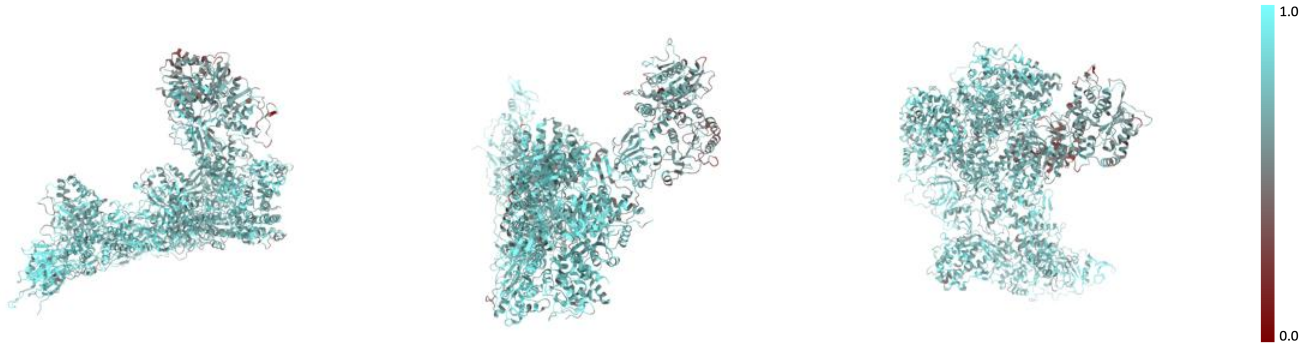
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

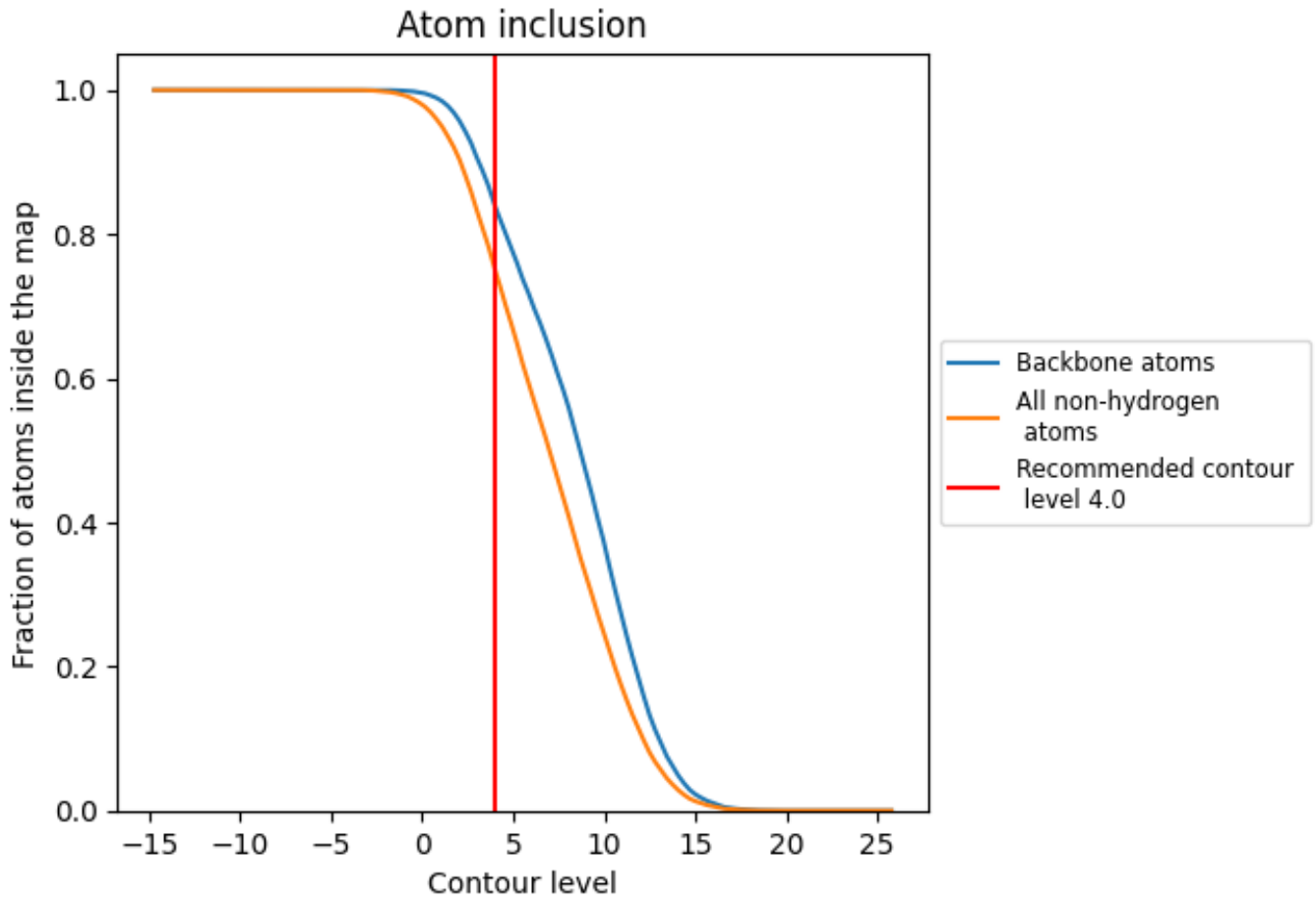
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7502	0.5310
A	0.6710	0.5050
B	0.7701	0.5390
C	0.7853	0.5410
D	0.7876	0.5460
E	0.7759	0.5350