Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:08 PM EST

PDB ID	:	3JAY
EMDB ID	:	EMD-6378
Title	:	Atomic model of transcribing cytoplasmic polyhedrosis virus
Authors	:	Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on	:	2015-07-06
Resolution	:	3.00 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:

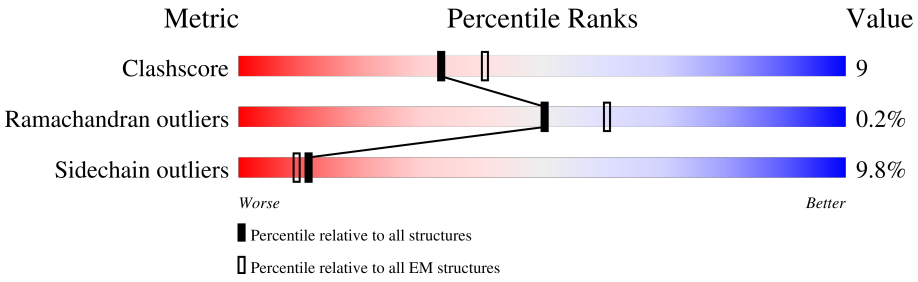
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 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	19% 70% 27%
2	B	1333	64% 22% 11%
2	C	1333	67% 24% 6%
3	D	448	49% 15% 35%
3	E	448	51% 12% 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		

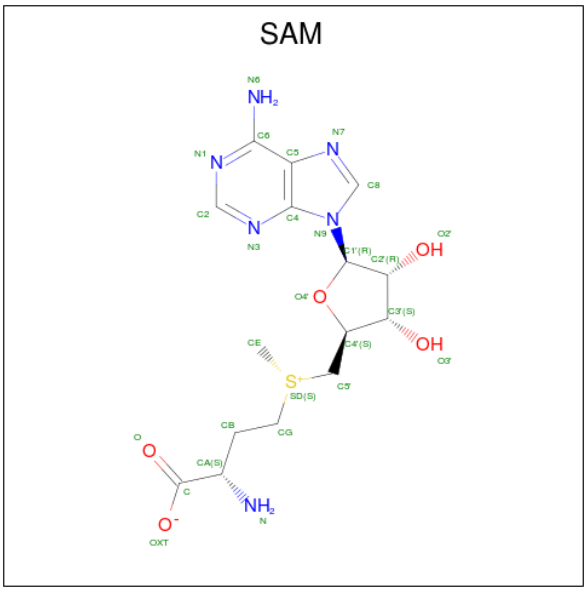
- Molecule 2 is a protein called Capsid protein VP1.

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.

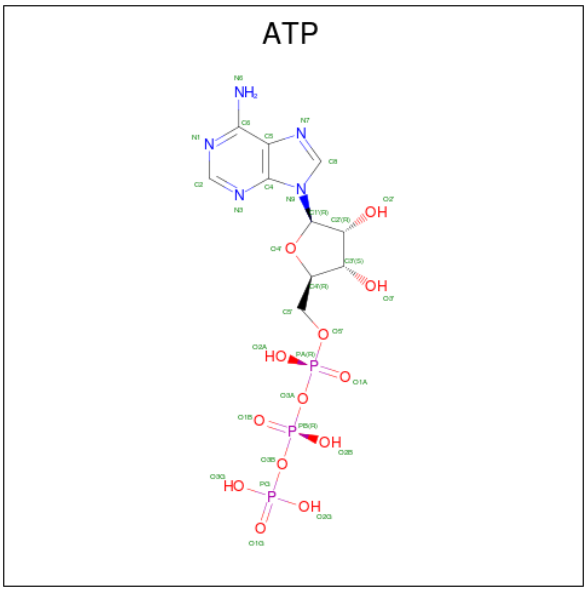
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

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



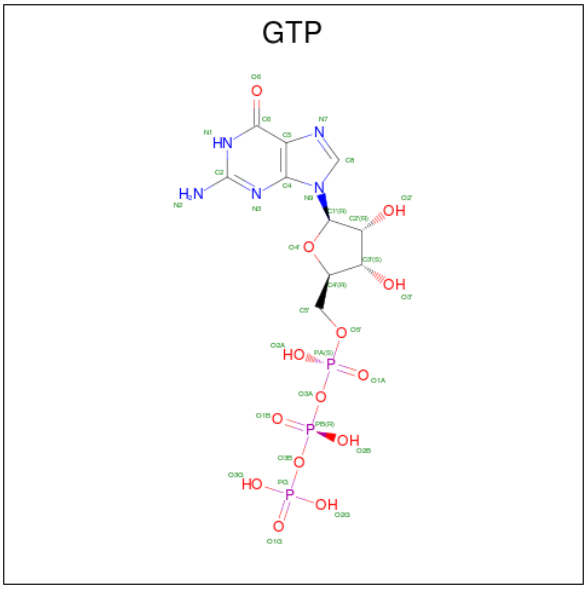
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			54	30	12	10	2	
4	A	1	Total	C	N	O	S	0
			54	30	12	10	2	

- 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	

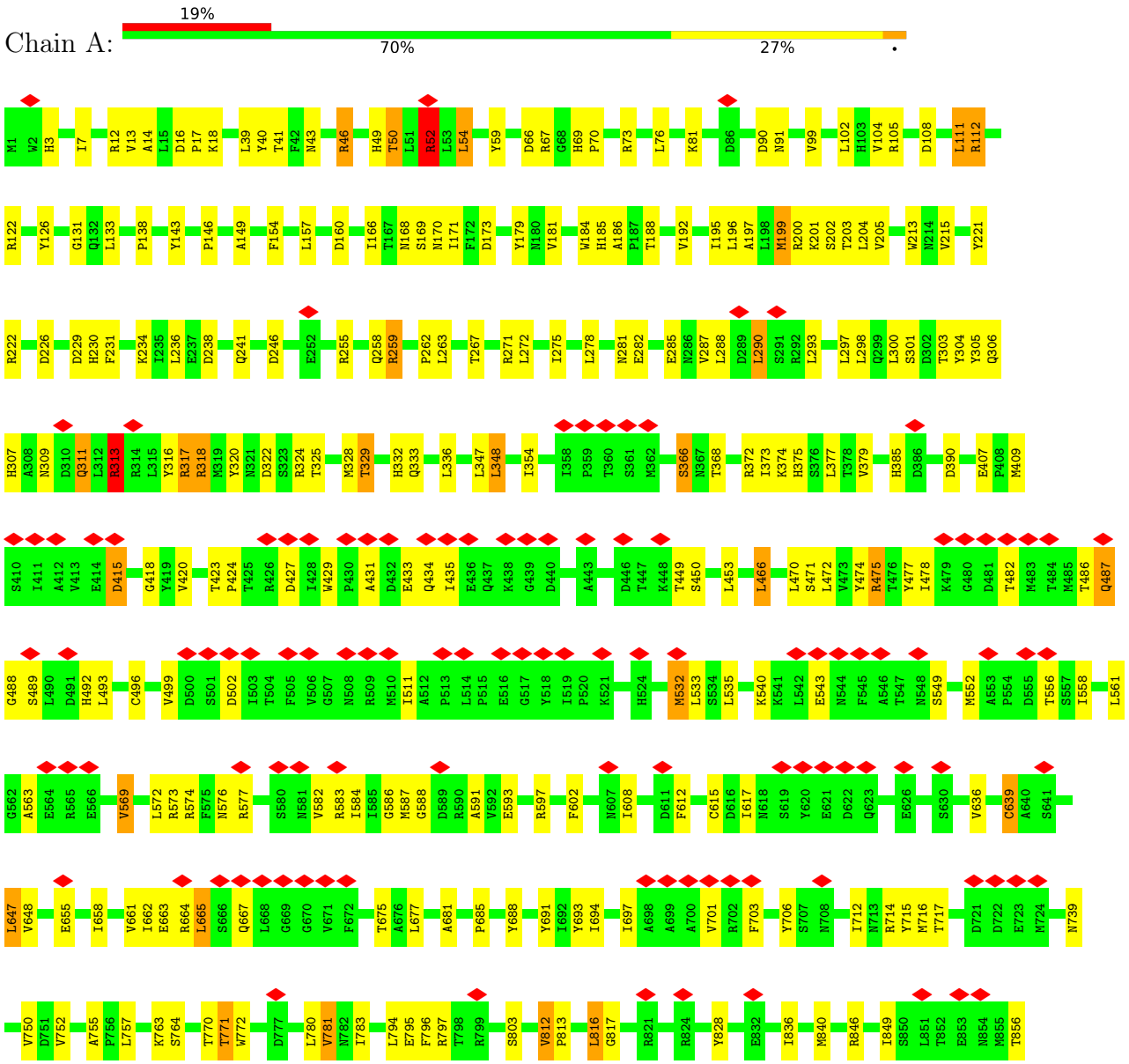
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

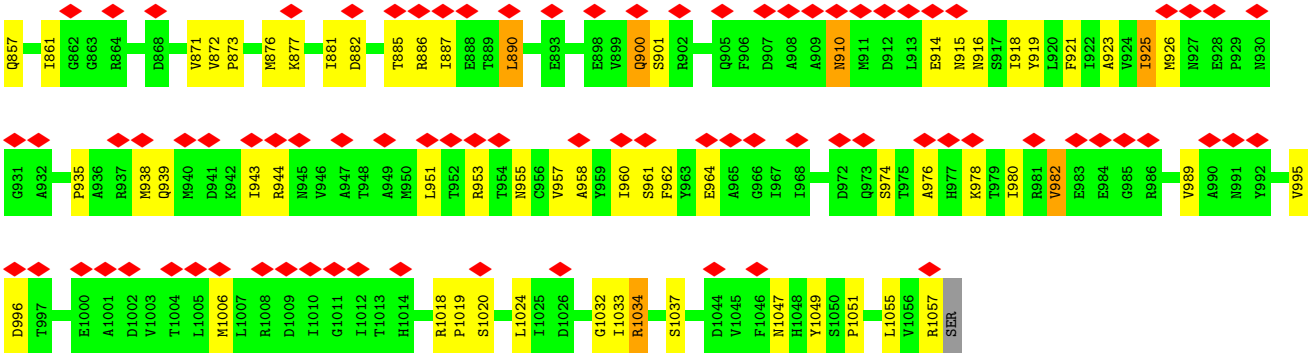
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	

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.

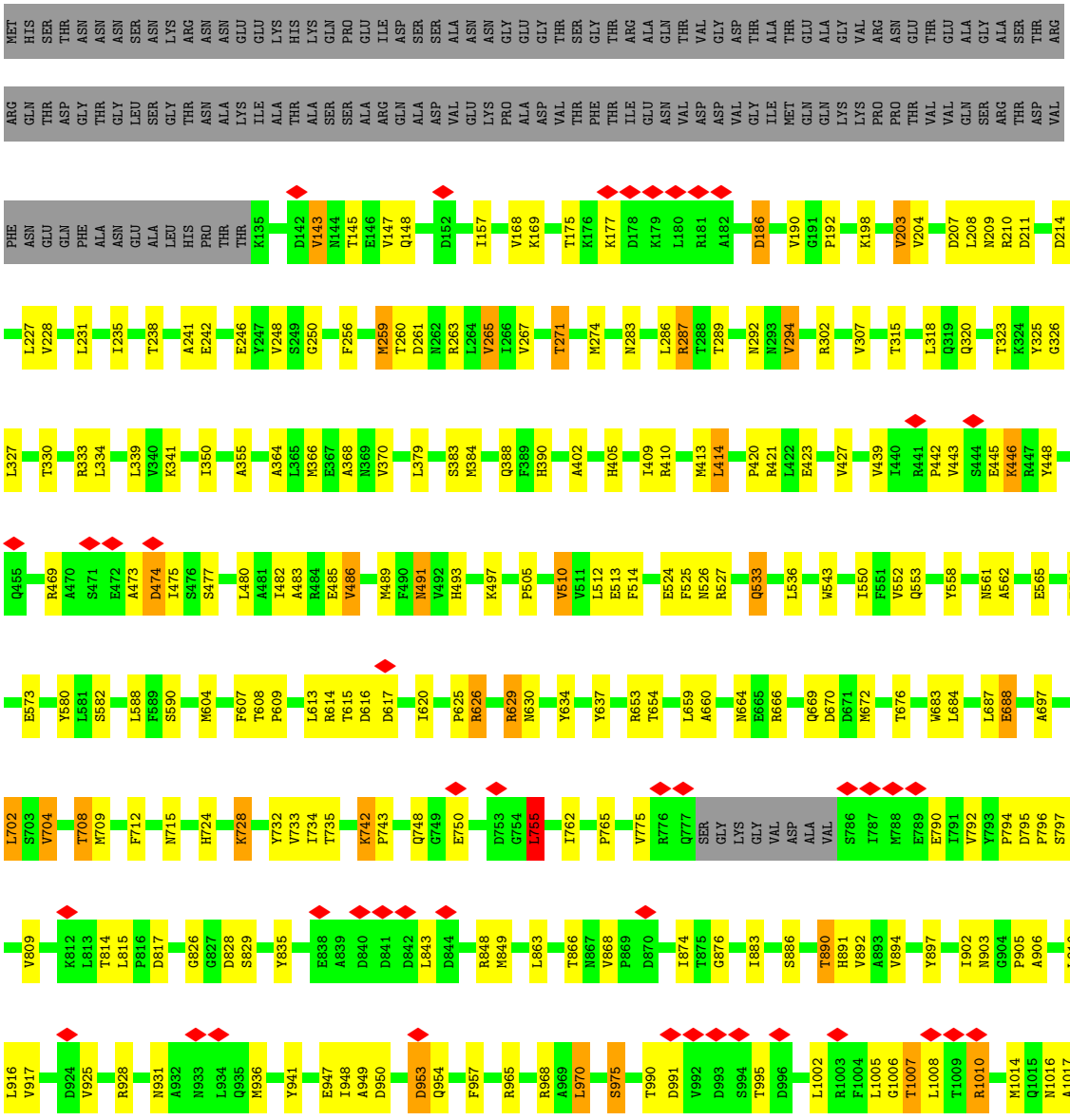
- Molecule 1: Structural protein VP3

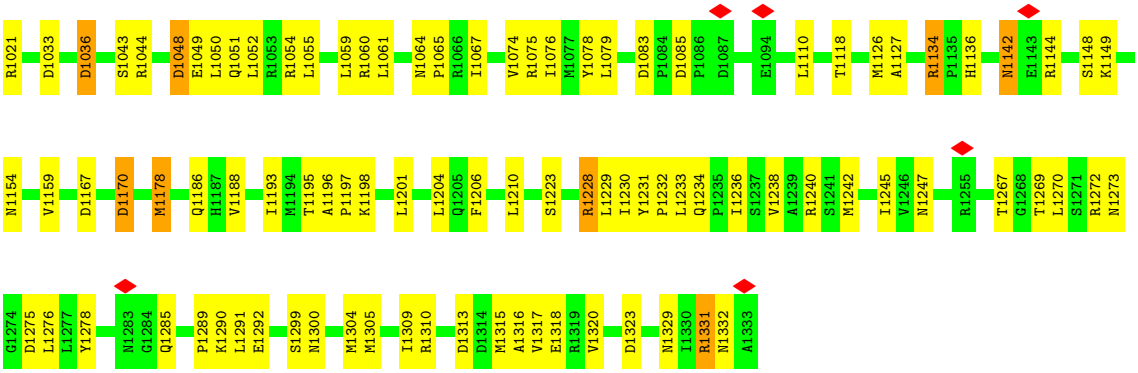




• Molecule 2: Capsid protein VP1

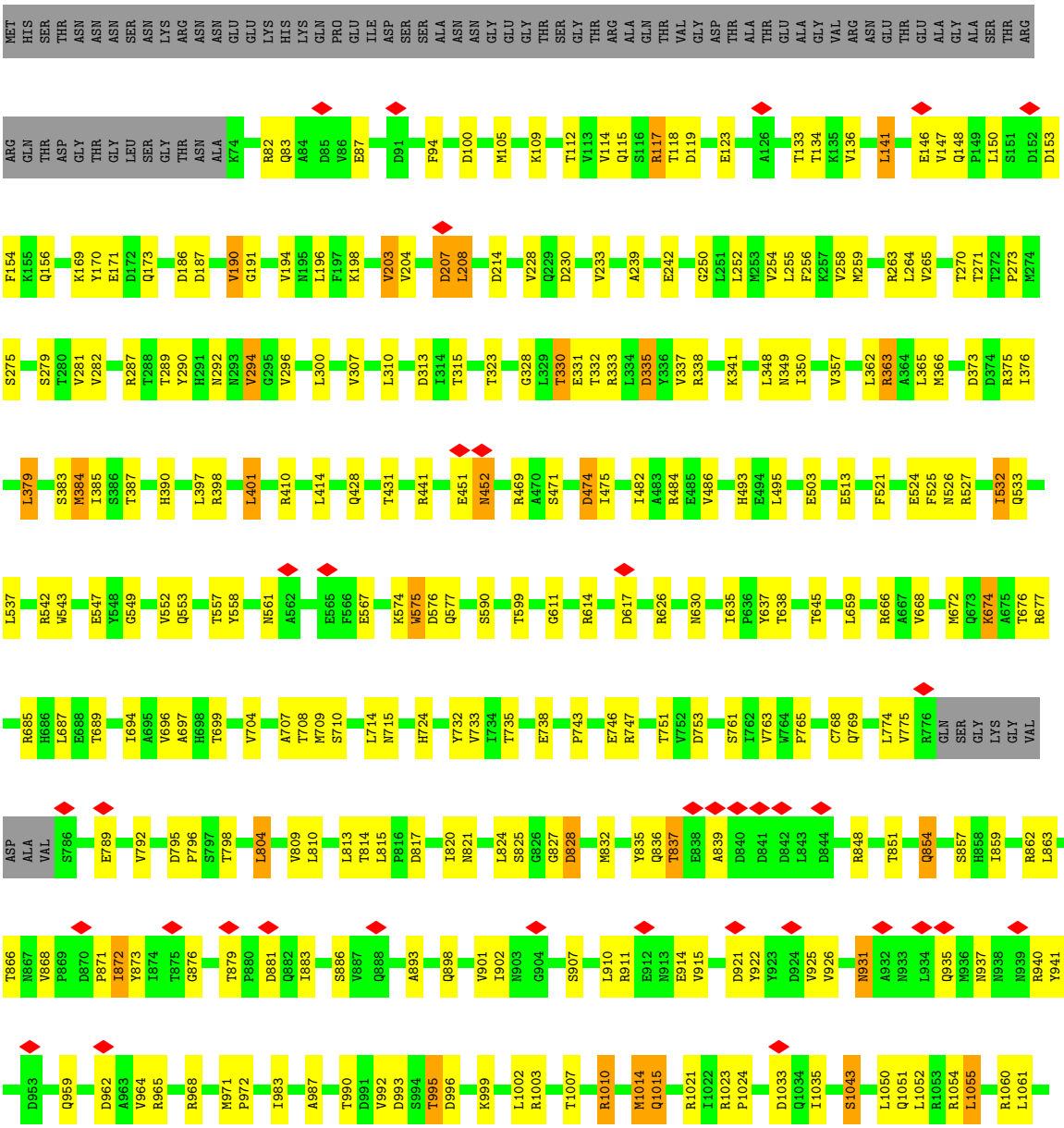
Chain B:

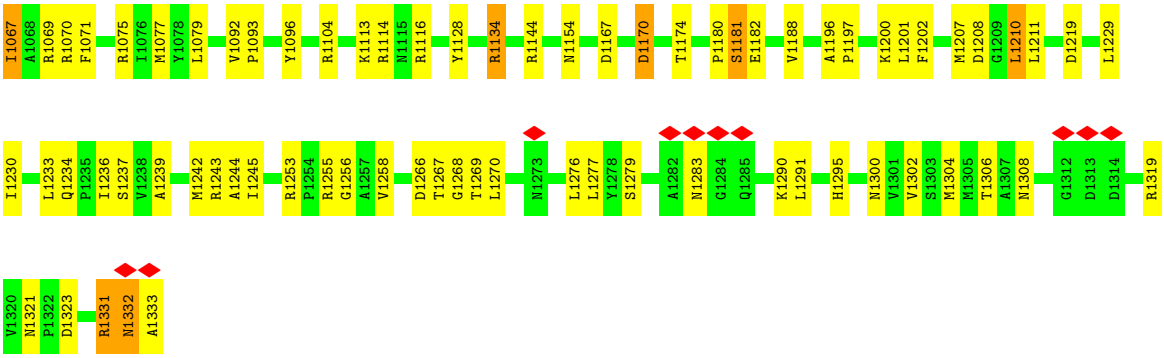




• Molecule 2: Capsid protein VP1

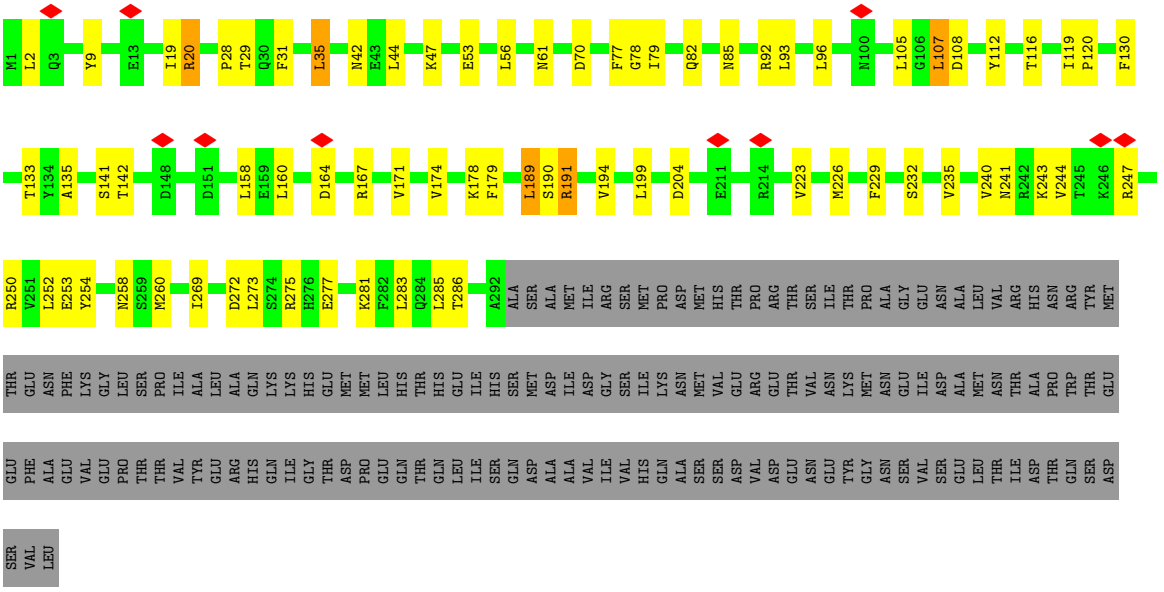
Chain C:





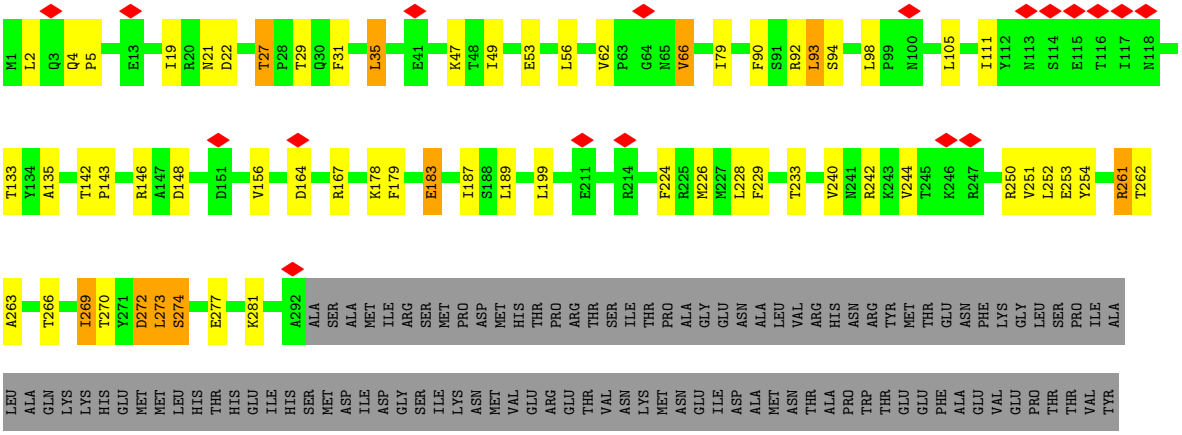
• Molecule 3: Viral structural protein 5

Chain D:



• Molecule 3: Viral structural protein 5

Chain E:



GLU ARG HIS GLN ILE GLY THR ASP PRO GLU GLN THR GLN LEU ILE SER GLN ASP ALA ALA VAL ILE VAL HIS GLN ALA SER SER ASP VAL ASP GLU ASN GLU TYR GLY ASN SER VAL SER GLU LEU THR ILE ASP THR GLN SER ASP SER VAL LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41624	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	29.318	Depositor
Minimum map value	-21.517	Depositor
Average map value	0.030	Depositor
Map value standard deviation	1.606	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: MG, SAM, ATP, GTP

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	0.49	0/11737
2	B	0.33	0/9590	0.57	1/13056 (0.0%)
2	C	0.34	0/10058	0.55	0/13695
3	D	0.31	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	1/44814 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	755	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	46	ARG	Sidechain
1	A	52	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8399	170	0
2	B	9397	0	9315	190	0
2	C	9857	0	9767	180	0
3	D	2281	0	2282	43	0
3	E	2281	0	2282	31	0
4	A	54	0	44	1	0
5	A	31	0	12	0	0
6	A	32	0	12	1	0
7	A	1	0	0	0	0
All	All	32368	0	32113	589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (589) 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:52:ARG:NH2	1:A:52:ARG:HB2	1.72	1.02
1:A:43:ASN:OD1	1:A:46:ARG:HG2	1.72	0.89
1:A:41:THR:HG23	1:A:50:THR:HG23	1.56	0.88
2:C:383:SER:HB3	2:C:796:PRO:HG3	1.57	0.87
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.12	0.82
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.62	0.81
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.63	0.81
1:A:309:ASN:OD1	1:A:311:GLN:HG2	1.80	0.80
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.65	0.79
1:A:168:ASN:ND2	1:A:173:ASP:OD2	2.16	0.79
1:A:41:THR:CG2	1:A:50:THR:HG23	2.12	0.78
1:A:857:GLN:NE2	1:A:914:GLU:OE1	2.16	0.78
1:A:52:ARG:NH1	1:A:169:SER:OG	2.15	0.78
1:A:797:ARG:NH2	1:A:876:MET:O	2.18	0.77
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.16	0.77
1:A:52:ARG:HB2	1:A:52:ARG:HH21	1.48	0.75
1:A:52:ARG:HB2	1:A:52:ARG:CZ	2.16	0.74
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:O	1:A:317:ARG:NH1	2.21	0.74
2:C:1128:TYR:O	2:C:1134:ARG:NH1	2.20	0.74
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.21	0.73
2:C:709:MET:O	2:C:715:ASN:ND2	2.21	0.72
2:C:836:GLN:NE2	2:C:940:ARG:O	2.21	0.72
2:C:169:LYS:NZ	2:C:1182:GLU:OE2	2.23	0.72
1:A:12:ARG:NH2	1:A:16:ASP:OD1	2.23	0.71
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.23	0.70
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.74	0.69
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.26	0.69
1:A:685:PRO:O	1:A:714:ARG:NH2	2.26	0.69
2:C:493:HIS:O	2:C:577:GLN:NE2	2.26	0.69
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.26	0.69
1:A:958:ALA:HB3	1:A:1055:LEU:HB2	1.76	0.68
2:B:950:ASP:OD1	2:B:965:ARG:NH1	2.27	0.68
1:A:502:ASP:HA	1:A:574:ARG:HD3	1.76	0.67
2:B:817:ASP:OD2	2:B:1010:ARG:NH2	2.28	0.67
2:C:1170:ASP:OD1	2:C:1170:ASP:N	2.24	0.67
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.75	0.67
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.77	0.67
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.28	0.67
2:B:287:ARG:HE	2:B:330:THR:HG22	1.59	0.66
3:E:261:ARG:NH1	3:E:263:ALA:O	2.28	0.66
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.28	0.66
2:B:975:SER:HB2	2:C:696:VAL:HG21	1.77	0.66
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.20	0.66
1:A:202:SER:HB2	2:B:630:ASN:HB3	1.79	0.65
1:A:935:PRO:HG2	1:A:938:MET:HG3	1.77	0.65
1:A:662:ILE:HD12	1:A:675:THR:HG21	1.79	0.65
2:B:1273:ASN:ND2	2:B:1275:ASP:OD2	2.28	0.65
2:B:1060:ARG:NH1	2:B:1291:LEU:O	2.30	0.64
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.80	0.64
3:E:79:ILE:HG13	3:E:269:ILE:HG22	1.78	0.64
2:C:87:GLU:OE2	2:C:263:ARG:NH1	2.29	0.64
2:C:190:VAL:HG22	2:C:300:LEU:HB3	1.78	0.64
1:A:964:GLU:HB3	1:A:1049:TYR:HD1	1.62	0.64
2:B:209:ASN:ND2	2:B:211:ASP:OD1	2.32	0.63
2:B:267:VAL:HA	2:B:1304:MET:HE2	1.80	0.63
2:C:746:GLU:OE2	2:C:1010:ARG:NH2	2.25	0.63
3:E:53:GLU:OE2	3:E:281:LYS:NZ	2.31	0.63
2:C:287:ARG:HH11	2:C:330:THR:HB	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:MET:O	2:B:715:ASN:ND2	2.32	0.63
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.81	0.63
1:A:285:GLU:HB2	1:A:287:VAL:HG23	1.80	0.63
1:A:213:TRP:HB2	1:A:215:VAL:HG12	1.79	0.63
2:B:480:LEU:HD11	2:B:755:LEU:HD23	1.81	0.62
2:B:1170:ASP:N	2:B:1170:ASP:OD1	2.32	0.62
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.32	0.62
2:C:493:HIS:ND1	2:C:524:GLU:OE2	2.32	0.62
2:B:524:GLU:OE2	2:B:527:ARG:NH1	2.32	0.62
2:C:837:THR:HG21	2:C:911:ARG:HG3	1.82	0.62
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.81	0.62
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.33	0.62
2:C:1174:THR:HG23	2:C:1201:LEU:HD22	1.82	0.62
2:C:704:VAL:O	2:C:708:THR:HG23	2.00	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.17	0.62
2:B:626:ARG:NH2	2:B:712:PHE:O	2.33	0.61
2:C:146:GLU:O	2:C:148:GLN:NE2	2.31	0.61
2:C:94:PHE:HB3	2:C:105:MET:HG3	1.83	0.61
2:C:697:ALA:HB2	2:C:775:VAL:HG23	1.83	0.61
1:A:856:THR:HG23	1:A:857:GLN:HG2	1.83	0.61
2:C:153:ASP:HB3	2:C:401:LEU:HD22	1.83	0.61
2:C:357:VAL:HG13	2:C:1054:ARG:HD3	1.82	0.61
2:C:441:ARG:NH2	2:C:789:GLU:OE1	2.34	0.60
1:A:697:ILE:HD11	1:A:701:VAL:HG22	1.83	0.60
2:B:483:ALA:HA	2:B:709:MET:HE3	1.83	0.60
2:C:169:LYS:HB2	2:C:203:VAL:HG23	1.84	0.60
1:A:201:LYS:HD3	3:D:260:MET:HB3	1.82	0.60
2:C:156:GLN:OE1	2:C:1308:ASN:ND2	2.34	0.60
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.84	0.60
2:B:1048:ASP:OD1	2:B:1048:ASP:N	2.35	0.60
2:C:848:ARG:HE	2:C:914:GLU:HB3	1.66	0.60
2:B:666:ARG:NH1	2:B:670:ASP:OD2	2.35	0.59
1:A:558:ILE:HG13	1:A:612:PHE:HB2	1.82	0.59
2:B:248:VAL:HG22	2:B:970:LEU:HB3	1.84	0.59
2:B:1289:PRO:HD2	3:D:20:ARG:HD3	1.84	0.59
2:C:825:SER:HA	2:C:1015:GLN:HE21	1.66	0.59
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.02	0.59
1:A:772:TRP:HA	1:A:817:GLY:HA3	1.85	0.59
2:C:795:ASP:OD1	2:C:1319:ARG:NH2	2.35	0.59
1:A:192:VAL:HG21	1:A:347:LEU:HD13	1.85	0.59
2:C:866:THR:HG23	2:C:868:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:ASP:OD1	2:B:474:ASP:N	2.29	0.59
2:B:210:ARG:HH21	2:B:222:THR:HA	1.67	0.58
2:B:439:VAL:HG21	2:B:702:LEU:HD13	1.85	0.58
2:C:987:ALA:HB1	2:C:992:VAL:HG22	1.84	0.58
2:B:168:VAL:HG22	2:B:204:VAL:HG22	1.85	0.58
2:C:1069:ARG:HD2	2:C:1239:ALA:HB2	1.86	0.58
2:C:1236:ILE:HG22	2:C:1237:SER:H	1.68	0.58
2:C:384:MET:HA	2:C:708:THR:HG21	1.85	0.58
2:C:996:ASP:HA	2:C:999:LYS:HD2	1.85	0.58
2:C:1071:PHE:HD1	2:C:1234:GLN:HE21	1.51	0.58
3:E:178:LYS:HB3	3:E:251:VAL:HG22	1.85	0.58
1:A:104:VAL:HG23	1:A:138:PRO:HB2	1.86	0.58
1:A:304:TYR:HA	1:A:307:HIS:HB2	1.86	0.58
2:C:1266:ASP:OD1	2:C:1279:SER:OG	2.22	0.57
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.86	0.57
1:A:14:ALA:HA	1:A:112:ARG:HH22	1.70	0.57
2:B:469:ARG:NH1	2:B:513:GLU:OE2	2.35	0.57
2:B:704:VAL:O	2:B:708:THR:HG22	2.05	0.57
2:C:817:ASP:HA	2:C:983:ILE:HG12	1.87	0.56
2:C:879:THR:HG22	2:C:881:ASP:H	1.70	0.56
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.38	0.56
2:C:214:ASP:N	2:C:214:ASP:OD1	2.39	0.56
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.87	0.56
2:C:379:LEU:HD12	2:C:796:PRO:HB2	1.86	0.56
1:A:39:LEU:HG	1:A:54:LEU:HD21	1.88	0.56
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.33	0.56
2:B:613:LEU:HD13	2:B:634:TYR:HD1	1.70	0.56
2:B:326:GLY:H	2:B:1267:THR:HG21	1.70	0.56
3:D:35:LEU:HD12	3:D:179:PHE:HB3	1.86	0.56
3:D:78:GLY:O	3:D:275:ARG:NH2	2.39	0.56
1:A:373:ILE:HD13	1:A:817:GLY:N	2.20	0.55
1:A:43:ASN:OD1	1:A:46:ARG:CG	2.50	0.55
1:A:241:GLN:OE1	1:A:258:GLN:NE2	2.38	0.55
1:A:916:ASN:N	1:A:955:ASN:O	2.39	0.55
2:B:697:ALA:HB2	2:B:775:VAL:HG23	1.88	0.55
1:A:563:ALA:HB3	1:A:588:GLY:H	1.71	0.55
2:B:1188:VAL:HG21	2:B:1204:LEU:HD23	1.88	0.55
2:C:893:ALA:HB1	2:C:915:VAL:HA	1.89	0.55
2:C:452:ASN:N	2:C:452:ASN:OD1	2.39	0.55
2:B:573:GLU:OE2	2:C:674:LYS:NZ	2.39	0.55
2:C:259:MET:O	2:C:1054:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ASP:OD1	2:C:338:ARG:NH2	2.40	0.55
2:C:474:ASP:OD1	2:C:474:ASP:N	2.39	0.55
2:C:366:MET:HG2	3:E:266:THR:HG21	1.88	0.54
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.89	0.54
2:C:1077:MET:O	2:C:1229:LEU:HA	2.07	0.54
2:C:732:TYR:OH	2:C:1021:ARG:NH2	2.41	0.54
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.42	0.54
1:A:681:ALA:O	1:A:1037:SER:HB2	2.07	0.54
1:A:890:LEU:HD23	1:A:890:LEU:H	1.72	0.54
3:D:283:LEU:HA	3:D:286:THR:HG22	1.88	0.54
2:B:1126:MET:HE3	3:E:146:ARG:HB3	1.89	0.54
2:C:171:GLU:OE1	2:C:1181:SER:OG	2.20	0.54
1:A:278:LEU:HD11	1:A:316:TYR:HB2	1.90	0.54
2:B:614:ARG:NH1	2:B:617:ASP:OD1	2.39	0.54
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.90	0.54
2:C:543:TRP:CD2	2:C:666:ARG:HD3	2.43	0.54
3:E:156:VAL:HG13	3:E:228:LEU:HD22	1.88	0.54
1:A:615:CYS:HB3	1:A:648:VAL:HA	1.90	0.53
2:B:1007:THR:OG1	2:B:1008:LEU:N	2.39	0.53
1:A:887:ILE:HD11	1:A:901:SER:HB2	1.90	0.53
1:A:318:ARG:HG3	3:D:42:ASN:HA	1.90	0.53
2:C:428:GLN:HA	2:C:431:THR:HG22	1.89	0.53
1:A:108:ASP:HB2	1:A:111:LEU:HD22	1.91	0.53
1:A:221:TYR:OH	1:A:230:HIS:ND1	2.30	0.53
2:B:954:GLN:HE21	3:D:240:VAL:HG12	1.73	0.53
2:C:254:VAL:O	2:C:258:VAL:HG12	2.08	0.53
2:B:157:ILE:HG12	2:B:263:ARG:HD2	1.91	0.53
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.89	0.53
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.91	0.53
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.73	0.53
2:B:325:TYR:HA	2:B:1267:THR:HG23	1.90	0.53
2:C:289:THR:O	2:C:328:GLY:HA3	2.09	0.53
2:C:738:GLU:OE2	2:C:857:SER:OG	2.18	0.53
2:B:302:ARG:HD2	2:B:318:LEU:HD12	1.91	0.52
2:C:242:GLU:HB2	2:C:1200:LYS:HE2	1.90	0.52
1:A:41:THR:HG23	1:A:50:THR:CG2	2.35	0.52
1:A:466:LEU:HB3	1:A:470:LEU:HD23	1.91	0.52
2:C:196:LEU:HD23	2:C:296:VAL:HG11	1.91	0.52
1:A:267:THR:HG23	1:A:320:TYR:OH	2.09	0.52
2:B:169:LYS:HB2	2:B:203:VAL:HG23	1.92	0.52
2:B:558:TYR:HB3	2:B:568:PHE:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1331:ARG:HB2	2:B:1332:ASN:HA	1.90	0.52
3:D:253:GLU:HB3	3:D:254:TYR:CE1	2.44	0.52
1:A:573:ARG:NH2	1:A:584:ILE:O	2.39	0.52
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.45	0.52
2:C:883:ILE:HD13	2:C:910:LEU:HD21	1.91	0.52
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.39	0.52
1:A:836:ILE:HD11	1:A:1033:ILE:HG21	1.91	0.52
2:C:383:SER:HB2	2:C:387:THR:HG21	1.92	0.52
1:A:755:ALA:HB2	1:A:781:VAL:HG11	1.92	0.51
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.45	0.51
2:C:414:LEU:HD23	2:C:814:THR:HB	1.92	0.51
1:A:496:CYS:O	1:A:574:ARG:NH1	2.43	0.51
2:B:1005:LEU:HB2	2:B:1006:GLY:HA2	1.91	0.51
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.91	0.51
2:B:491:ASN:OD1	2:B:491:ASN:N	2.41	0.51
2:B:792:VAL:HG12	2:B:794:PRO:HD3	1.91	0.51
1:A:420:VAL:HA	1:A:974:SER:HB2	1.92	0.51
2:C:611:GLY:HA3	2:C:635:ILE:O	2.10	0.51
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.92	0.51
1:A:487:GLN:O	1:A:492:HIS:ND1	2.31	0.51
1:A:205:VAL:HG23	1:A:263:LEU:HB2	1.93	0.51
2:B:903:ASN:HD22	2:B:905:PRO:HG2	1.75	0.51
1:A:372:ARG:HD2	1:A:772:TRP:CE3	2.45	0.51
1:A:918:ILE:HG23	1:A:957:VAL:HG13	1.93	0.51
2:B:1305:MET:HE2	2:B:1309:ILE:HG21	1.93	0.51
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.93	0.51
2:C:851:THR:HG23	2:C:854:GLN:HB2	1.93	0.50
2:C:743:PRO:HB2	2:C:746:GLU:HG2	1.93	0.50
2:B:931:ASN:ND2	2:B:936:MET:O	2.44	0.50
2:C:576:ASP:OD1	2:C:747:ARG:NH2	2.44	0.50
1:A:166:ILE:HG21	1:A:179:TYR:CE1	2.47	0.50
1:A:424:PRO:HG3	1:A:706:TYR:CZ	2.46	0.50
1:A:910:ASN:OD1	1:A:910:ASN:N	2.45	0.50
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.12	0.50
2:C:233:VAL:HG23	2:C:239:ALA:HB2	1.92	0.50
2:B:370:VAL:HG11	2:B:402:ALA:HB2	1.93	0.50
2:C:668:VAL:HG23	2:C:674:LYS:HD3	1.94	0.50
1:A:290:LEU:HD12	1:A:293:LEU:HD13	1.91	0.50
1:A:472:LEU:HD23	1:A:475:ARG:HH21	1.76	0.50
1:A:943:ILE:HG12	1:A:960:ILE:HG21	1.94	0.50
2:B:287:ARG:NE	2:B:330:THR:HG22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:HG22	1:A:204:LEU:HG	1.93	0.49
2:B:1289:PRO:HG3	3:D:191:ARG:NH2	2.27	0.49
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.47	0.49
1:A:336:LEU:HG	1:A:348:LEU:HD22	1.94	0.49
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.45	0.49
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.95	0.49
2:C:114:VAL:HG22	2:C:136:VAL:HG23	1.93	0.49
2:C:672:MET:O	2:C:676:THR:HG23	2.12	0.49
3:D:273:LEU:O	3:D:277:GLU:HG3	2.11	0.49
2:B:558:TYR:CE1	2:B:590:SER:HB3	2.47	0.49
1:A:540:LYS:NZ	1:A:543:GLU:OE2	2.29	0.49
2:B:866:THR:HG23	2:B:868:VAL:HG13	1.94	0.49
2:C:561:ASN:ND2	2:C:567:GLU:OE2	2.44	0.49
1:A:170:ASN:ND2	1:A:173:ASP:OD1	2.45	0.49
2:B:505:PRO:HG2	2:B:672:MET:SD	2.53	0.49
1:A:272:LEU:HA	1:A:275:ILE:HD11	1.95	0.49
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.95	0.49
1:A:374:LYS:HG2	1:A:770:THR:HG22	1.94	0.49
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.95	0.49
1:A:474:TYR:HD1	1:A:499:VAL:HG12	1.77	0.49
1:A:186:ALA:HB2	1:A:195:ILE:HD12	1.94	0.48
1:A:301:SER:HB2	1:A:316:TYR:OH	2.12	0.48
1:A:288:LEU:HD21	1:A:300:LEU:HD22	1.94	0.48
1:A:764:SER:HA	1:A:795:GLU:HG2	1.93	0.48
2:B:514:PHE:HB3	2:B:607:PHE:HE2	1.78	0.48
2:B:876:GLY:HA2	2:B:902:ILE:HA	1.94	0.48
1:A:923:ALA:H	1:A:961:SER:HB3	1.77	0.48
2:C:150:LEU:HD21	2:C:398:ARG:HB3	1.94	0.48
2:C:549:GLY:O	2:C:553:GLN:HB2	2.13	0.48
1:A:427:ASP:HA	1:A:703:PHE:HA	1.96	0.48
1:A:688:TYR:HB2	1:A:715:TYR:HB2	1.95	0.48
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.48	0.48
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.94	0.48
1:A:385:HIS:NE2	1:A:803:SER:OG	2.44	0.48
1:A:658:ILE:O	1:A:662:ILE:HG12	2.14	0.48
2:C:638:THR:O	2:C:699:THR:HB	2.14	0.48
2:C:810:LEU:HA	2:C:813:LEU:HB3	1.96	0.48
1:A:849:ILE:HG12	1:A:918:ILE:HD13	1.95	0.48
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.28	0.48
2:C:294:VAL:O	2:C:349:ASN:ND2	2.46	0.48
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:272:ASP:OD1	3:E:274:SER:OG	2.15	0.48
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.96	0.48
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.95	0.48
1:A:588:GLY:H	1:A:591:ALA:HB2	1.79	0.48
2:B:795:ASP:OD1	2:B:795:ASP:N	2.47	0.48
2:B:1044:ARG:NH1	2:B:1049:GLU:OE2	2.41	0.48
1:A:739:ASN:HB2	1:A:796:PHE:CE1	2.49	0.48
2:B:890:THR:O	2:B:890:THR:OG1	2.29	0.48
2:C:810:LEU:O	2:C:814:THR:HG23	2.14	0.48
3:E:224:PHE:O	3:E:228:LEU:HG	2.14	0.48
2:C:207:ASP:OD1	2:C:207:ASP:N	2.47	0.47
2:C:824:LEU:O	2:C:1015:GLN:NE2	2.47	0.47
2:C:1211:LEU:HD11	2:C:1244:ALA:HA	1.95	0.47
1:A:552:MET:H	1:A:576:ASN:ND2	2.11	0.47
2:C:1236:ILE:HG22	2:C:1237:SER:N	2.29	0.47
1:A:752:VAL:HG23	1:A:816:LEU:HD21	1.95	0.47
1:A:980:ILE:HG23	1:A:989:VAL:HG12	1.95	0.47
2:B:526:ASN:HB2	2:B:724:HIS:CE1	2.49	0.47
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.72	0.47
2:B:261:ASP:CG	2:B:263:ARG:HE	2.17	0.47
2:B:405:HIS:CE1	2:B:625:PRO:HA	2.50	0.47
2:C:931:ASN:O	2:C:931:ASN:ND2	2.44	0.47
2:C:1268:GLY:HA3	2:C:1277:LEU:O	2.14	0.47
1:A:59:TYR:HB3	6:A:1104:GTP:C6	2.50	0.47
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.97	0.47
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.96	0.47
1:A:40:TYR:OH	1:A:49:HIS:ND1	2.40	0.47
1:A:840:MET:HG2	1:A:1024:LEU:HA	1.96	0.47
2:B:604:MET:HE1	2:B:607:PHE:CE1	2.50	0.47
2:B:712:PHE:HB2	2:B:715:ASN:ND2	2.30	0.47
2:C:186:ASP:OD2	2:C:279:SER:OG	2.18	0.47
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.28	0.47
2:C:1075:ARG:NH1	2:C:1167:ASP:OD1	2.47	0.47
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.76	0.47
1:A:499:VAL:O	1:A:574:ARG:NH1	2.48	0.47
2:B:241:ALA:HB2	2:B:1197:PRO:HB2	1.97	0.47
2:B:443:VAL:HG22	2:B:445:GLU:H	1.79	0.47
3:E:35:LEU:HD12	3:E:179:PHE:HB3	1.96	0.47
1:A:126:TYR:HA	1:A:131:GLY:HA3	1.96	0.47
2:B:829:SER:HB3	2:B:947:GLU:HA	1.96	0.47
2:C:525:PHE:HD2	2:C:724:HIS:CE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1210:LEU:HD21	2:C:1255:ARG:O	2.15	0.46
2:C:827:GLY:HA3	2:C:964:VAL:HG11	1.97	0.46
2:B:364:ALA:HB2	2:B:1050:LEU:HD21	1.97	0.46
2:C:817:ASP:O	2:C:821:ASN:ND2	2.39	0.46
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.98	0.46
1:A:552:MET:HB2	1:A:576:ASN:ND2	2.31	0.46
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.97	0.46
3:E:178:LYS:HA	3:E:250:ARG:O	2.16	0.46
1:A:281:ASN:O	1:A:285:GLU:HG2	2.15	0.46
2:B:207:ASP:OD1	2:B:207:ASP:N	2.47	0.46
2:B:660:ALA:O	2:B:664:ASN:HB2	2.16	0.46
1:A:925:ILE:HD11	1:A:939:GLN:HB3	1.98	0.46
2:B:616:ASP:O	2:B:620:ILE:HG12	2.15	0.46
2:B:863:LEU:HA	2:B:866:THR:HG22	1.98	0.46
2:C:1033:ASP:OD1	2:C:1033:ASP:N	2.46	0.46
2:B:829:SER:O	2:C:645:THR:HG21	2.16	0.46
2:B:1050:LEU:HD23	2:B:1050:LEU:HA	1.74	0.46
2:C:141:LEU:HD12	2:C:141:LEU:HA	1.81	0.46
2:C:804:LEU:HD13	2:C:804:LEU:HA	1.85	0.46
2:C:1128:TYR:HB3	2:C:1134:ARG:HD3	1.98	0.46
2:C:1200:LYS:HE3	2:C:1200:LYS:HB2	1.74	0.46
2:B:368:ALA:HA	3:D:82:GLN:HG3	1.98	0.46
2:C:154:PHE:HE2	2:C:365:LEU:HD13	1.81	0.46
2:C:191:GLY:HA2	2:C:194:VAL:HG22	1.96	0.46
1:A:677:LEU:HD13	1:A:706:TYR:CZ	2.51	0.46
2:B:259:MET:HB2	2:B:1055:LEU:HD23	1.98	0.46
2:B:1118:THR:CG2	2:B:1127:ALA:HB1	2.46	0.46
2:B:1206:PHE:HE2	2:B:1232:PRO:HD3	1.81	0.46
2:C:835:TYR:HA	2:C:941:TYR:HA	1.98	0.46
1:A:409:MET:HB3	1:A:409:MET:HE3	1.65	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:683:TRP:CH2	2:B:687:LEU:HD11	2.51	0.45
1:A:647:LEU:HD13	1:A:691:TYR:HB3	1.99	0.45
2:B:897:TYR:CZ	2:B:928:ARG:HG2	2.51	0.45
2:B:925:VAL:HA	2:B:928:ARG:HD2	1.99	0.45
2:B:1228:ARG:HG2	2:B:1231:TYR:CE1	2.51	0.45
2:C:674:LYS:HG3	2:C:677:ARG:NH2	2.32	0.45
3:E:142:THR:HA	3:E:143:PRO:HD3	1.84	0.45
1:A:328:MET:HE1	1:A:336:LEU:HD22	1.97	0.45
1:A:449:THR:HG22	1:A:450:SER:H	1.80	0.45
2:C:614:ARG:HG3	2:C:1333:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:876:GLY:HA2	2:C:902:ILE:HA	1.97	0.45
3:E:273:LEU:O	3:E:277:GLU:HG3	2.16	0.45
1:A:226:ASP:HA	1:A:229:ASP:OD2	2.17	0.45
1:A:431:ALA:O	1:A:435:ILE:HG13	2.16	0.45
2:C:828:ASP:OD2	2:C:862:ARG:NH2	2.50	0.45
3:E:148:ASP:OD1	3:E:148:ASP:N	2.50	0.45
1:A:231:PHE:HE2	1:A:262:PRO:HD3	1.82	0.45
1:A:617:ILE:HD12	4:A:1101:SAM:C4	2.46	0.45
2:C:337:VAL:HG22	3:E:187:ILE:HG13	1.99	0.45
2:C:872:ILE:HD12	2:C:886:SER:HB2	1.99	0.45
3:E:49:ILE:H	3:E:49:ILE:HG13	1.54	0.45
3:E:253:GLU:HA	3:E:254:TYR:HA	1.58	0.45
2:B:1206:PHE:CE2	2:B:1232:PRO:HD3	2.51	0.45
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.98	0.45
2:B:214:ASP:OD1	2:B:214:ASP:N	2.41	0.45
2:B:493:HIS:ND1	2:B:524:GLU:OE1	2.48	0.45
2:B:1076:ILE:HG22	2:B:1159:VAL:HG21	1.99	0.45
1:A:712:ILE:HG22	1:A:716:MET:HG3	1.99	0.45
2:B:1085:ASP:OD1	2:B:1085:ASP:N	2.50	0.45
2:C:537:LEU:HD23	2:C:537:LEU:HA	1.76	0.45
3:D:253:GLU:HA	3:D:254:TYR:HA	1.70	0.45
2:B:505:PRO:HA	2:B:543:TRP:CZ2	2.53	0.44
3:D:108:ASP:OD2	3:D:112:TYR:OH	2.18	0.44
1:A:828:TYR:HA	1:A:1032:GLY:O	2.17	0.44
2:B:883:ILE:HD13	2:B:910:LEU:HD21	1.98	0.44
2:B:1075:ARG:NH2	2:B:1167:ASP:OD2	2.31	0.44
2:C:945:VAL:HG21	2:C:962:ASP:OD1	2.17	0.44
1:A:573:ARG:HA	1:A:584:ILE:HD12	1.99	0.44
2:B:334:LEU:HA	2:B:341:LYS:HA	2.00	0.44
2:B:421:ARG:HG2	2:B:750:GLU:CD	2.38	0.44
2:B:653:ARG:HA	2:B:688:GLU:CD	2.37	0.44
2:C:482:ILE:HD13	2:C:521:PHE:HE1	1.82	0.44
2:C:575:TRP:HZ3	2:C:577:GLN:OE1	1.99	0.44
2:B:267:VAL:HG22	2:B:1304:MET:HG3	1.99	0.44
2:B:482:ILE:HD13	2:B:702:LEU:HD11	1.99	0.44
2:C:1114:ARG:HG3	2:C:1116:ARG:HD3	1.99	0.44
2:B:271:THR:HG22	2:B:292:ASN:OD1	2.16	0.44
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.51	0.44
2:B:1270:LEU:HD12	2:B:1270:LEU:HA	1.75	0.44
2:C:265:VAL:HB	2:C:1304:MET:HG2	2.00	0.44
2:C:348:LEU:HD12	2:C:1302:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:GLU:HA	2:C:452:ASN:HA	1.58	0.44
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.99	0.44
1:A:14:ALA:HA	1:A:112:ARG:NH2	2.33	0.44
1:A:375:HIS:CD2	1:A:771:THR:HG23	2.52	0.44
1:A:477:TYR:HA	1:A:482:THR:HG22	1.99	0.44
2:B:953:ASP:OD1	3:D:243:LYS:HE2	2.18	0.44
2:C:617:ASP:OD1	2:C:617:ASP:N	2.51	0.44
1:A:184:TRP:HB3	1:A:195:ILE:HD13	1.99	0.44
3:D:253:GLU:HB3	3:D:254:TYR:CD1	2.53	0.44
3:E:4:GLN:HA	3:E:5:PRO:HD3	1.82	0.44
1:A:511:ILE:H	1:A:511:ILE:HG13	1.64	0.44
2:B:410:ARG:HD3	2:B:1043:SER:HA	1.99	0.44
2:B:894:VAL:HG22	2:B:916:LEU:HB3	1.99	0.44
2:B:1142:ASN:OD1	2:B:1142:ASN:N	2.51	0.44
2:C:170:TYR:CE1	2:C:198:LYS:HG2	2.52	0.44
1:A:285:GLU:O	1:A:366:SER:HB3	2.17	0.44
2:B:379:LEU:O	2:B:383:SER:OG	2.28	0.44
2:C:373:ASP:HA	2:C:376:ILE:HG12	2.00	0.44
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.98	0.44
1:A:90:ASP:OD1	1:A:91:ASN:N	2.51	0.43
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.99	0.43
1:A:322:ASP:OD2	1:A:325:THR:OG1	2.30	0.43
1:A:675:THR:HA	1:A:693:TYR:O	2.18	0.43
2:B:1148:SER:HB2	2:C:390:HIS:CD2	2.53	0.43
2:B:1267:THR:HG22	2:B:1299:SER:HB3	1.99	0.43
2:B:414:LEU:HD13	2:B:814:THR:HG21	2.00	0.43
2:B:489:MET:HE3	2:B:580:TYR:HE2	1.83	0.43
3:D:28:PRO:HG3	3:D:223:VAL:HG22	1.99	0.43
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.43
1:A:615:CYS:HB2	1:A:639:CYS:SG	2.58	0.43
2:B:903:ASN:ND2	2:B:905:PRO:HG2	2.32	0.43
2:B:1060:ARG:HE	2:B:1060:ARG:HA	1.83	0.43
2:B:1148:SER:HB2	2:C:390:HIS:CG	2.53	0.43
2:B:1292:GLU:OE2	3:D:20:ARG:NH1	2.46	0.43
2:C:252:LEU:HD23	2:C:252:LEU:HA	1.83	0.43
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.75	0.43
2:B:469:ARG:NE	2:B:513:GLU:OE1	2.51	0.43
2:B:1313:ASP:OD1	2:B:1313:ASP:N	2.51	0.43
2:C:341:LYS:HA	2:C:341:LYS:HD3	1.86	0.43
2:C:1093:PRO:HB2	2:C:1096:TYR:CE1	2.54	0.43
1:A:602:PHE:CG	1:A:608:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:HE2	2:B:1178:MET:HE2	2.00	0.43
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.54	0.43
2:B:1230:ILE:HG13	2:C:119:ASP:HA	2.00	0.43
2:C:256:PHE:HE2	2:C:990:THR:HG21	1.84	0.43
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	2.01	0.43
2:C:495:LEU:HD13	2:C:532:ILE:HG22	2.01	0.43
3:E:27:THR:HB	3:E:29:THR:HG22	1.99	0.43
1:A:271:ARG:O	1:A:275:ILE:HG13	2.19	0.43
2:B:1076:ILE:HG23	2:B:1229:LEU:HG	2.01	0.43
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.51	0.43
2:C:117:ARG:HD2	2:C:117:ARG:HA	1.71	0.43
2:C:674:LYS:HG3	2:C:677:ARG:HH21	1.83	0.43
2:C:968:ARG:HA	2:C:971:MET:HE3	2.01	0.43
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.01	0.43
2:B:608:THR:HA	2:B:609:PRO:HD3	1.88	0.43
3:D:53:GLU:CD	3:D:53:GLU:H	2.22	0.43
1:A:238:ASP:OD2	1:A:259:ARG:NE	2.52	0.43
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.77	0.43
2:C:1050:LEU:HD23	2:C:1050:LEU:HA	1.65	0.43
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.88	0.43
1:A:143:TYR:CD2	1:A:146:PRO:HA	2.54	0.43
1:A:470:LEU:HD13	1:A:470:LEU:HA	1.90	0.43
1:A:532:MET:HA	1:A:535:LEU:HD12	1.99	0.43
2:B:186:ASP:O	2:B:190:VAL:HB	2.19	0.43
2:C:526:ASN:HB2	2:C:724:HIS:CE1	2.53	0.43
1:A:962:PHE:CE1	1:A:1051:PRO:HB2	2.53	0.42
2:B:186:ASP:OD1	2:B:186:ASP:N	2.51	0.42
2:B:355:ALA:HB3	2:B:1276:LEU:HD11	2.01	0.42
2:B:561:ASN:OD1	2:B:562:ALA:N	2.51	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.81	0.42
3:D:272:ASP:OD1	3:D:273:LEU:N	2.48	0.42
1:A:313:ARG:HD2	1:A:317:ARG:NH1	2.34	0.42
2:B:388:GLN:HB2	2:B:1320:VAL:HB	1.99	0.42
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.53	0.42
2:B:1118:THR:HG21	2:B:1127:ALA:HB1	2.00	0.42
2:C:848:ARG:HH21	2:C:914:GLU:HG2	1.84	0.42
3:E:229:PHE:O	3:E:233:THR:HG23	2.19	0.42
2:B:886:SER:O	2:B:890:THR:HG23	2.20	0.42
2:C:993:ASP:OD1	2:C:995:THR:OG1	2.29	0.42
2:C:1331:ARG:HG3	2:C:1332:ASN:H	1.83	0.42
1:A:925:ILE:O	1:A:925:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:ALA:O	2:B:910:LEU:HG	2.19	0.42
2:C:558:TYR:CE1	2:C:590:SER:HB3	2.54	0.42
2:C:1144:ARG:N	2:C:1170:ASP:OD2	2.47	0.42
3:D:9:TYR:H	3:D:204:ASP:CG	2.21	0.42
3:D:35:LEU:HD21	3:D:229:PHE:CE1	2.55	0.42
3:D:178:LYS:HA	3:D:250:ARG:O	2.20	0.42
2:C:839:ALA:HB2	2:C:935:GLN:NE2	2.35	0.42
2:C:1181:SER:H	2:C:1181:SER:HG	1.50	0.42
1:A:418:GLY:C	1:A:976:ALA:HB2	2.40	0.42
1:A:586:GLY:O	1:A:587:MET:HG3	2.20	0.42
2:B:473:ALA:HB2	2:B:765:PRO:HB3	2.01	0.42
2:B:1002:LEU:HD23	2:B:1002:LEU:HA	1.71	0.42
1:A:561:LEU:HD11	1:A:602:PHE:HZ	1.85	0.42
3:E:263:ALA:O	3:E:270:THR:HG21	2.19	0.42
1:A:66:ASP:CG	1:A:122:ARG:HH22	2.23	0.42
1:A:488:GLY:HA3	1:A:549:SER:HA	2.01	0.42
2:C:714:LEU:HA	2:C:714:LEU:HD23	1.80	0.42
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.54	0.42
1:A:415:ASP:OD1	1:A:415:ASP:N	2.52	0.42
2:B:477:SER:OG	2:B:762:ILE:HD11	2.20	0.42
2:C:273:PRO:HD3	2:C:290:TYR:HE1	1.84	0.42
2:C:524:GLU:HA	2:C:527:ARG:HD2	2.02	0.42
3:D:77:PHE:HA	3:D:269:ILE:HD13	2.02	0.42
1:A:143:TYR:CE2	1:A:146:PRO:HA	2.55	0.42
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.55	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.00	0.42
2:B:420:PRO:HG2	2:B:750:GLU:OE1	2.20	0.42
2:C:383:SER:CB	2:C:387:THR:HG21	2.50	0.42
2:C:751:THR:OG1	2:C:753:ASP:OD1	2.33	0.42
1:A:329:THR:HG22	1:A:332:HIS:ND1	2.34	0.41
1:A:717:THR:HB	1:A:1020:SER:HB2	2.01	0.41
2:B:442:PRO:HG2	2:B:475:ILE:HB	2.01	0.41
2:B:446:LYS:HB3	2:B:448:TYR:CD2	2.55	0.41
2:B:474:ASP:O	2:B:477:SER:OG	2.23	0.41
2:B:957:PHE:HE1	2:B:1016:ASN:HB3	1.85	0.41
2:B:1014:MET:HA	2:B:1017:ALA:HB2	2.02	0.41
2:C:208:LEU:HD21	2:C:1067:ILE:HG13	2.02	0.41
2:C:574:LYS:NZ	2:C:574:LYS:HB3	2.35	0.41
2:C:707:ALA:O	2:C:710:SER:OG	2.38	0.41
2:C:751:THR:HG22	2:C:1002:LEU:HD23	2.01	0.41
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.55	0.41
3:D:130:PHE:CZ	3:D:199:LEU:HD22	2.55	0.41
2:B:143:VAL:HG11	2:B:1316:ALA:HB1	2.02	0.41
2:B:525:PHE:HD2	2:B:724:HIS:CE1	2.38	0.41
2:B:536:LEU:HD23	2:B:536:LEU:HA	1.91	0.41
2:B:874:ILE:HD11	2:B:917:VAL:HG13	2.01	0.41
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.53	0.41
3:D:281:LYS:O	3:D:285:LEU:HG	2.20	0.41
1:A:812:VAL:HA	1:A:813:PRO:HA	1.80	0.41
2:B:510:VAL:O	2:B:513:GLU:HB3	2.21	0.41
2:C:547:GLU:OE2	2:C:599:THR:OG1	2.36	0.41
2:C:971:MET:HA	2:C:972:PRO:HD3	1.96	0.41
2:C:1180:PRO:HD3	2:C:1208:ASP:O	2.20	0.41
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.54	0.41
2:B:804:LEU:HA	2:B:804:LEU:HD12	1.80	0.41
2:B:1036:ASP:OD1	2:B:1036:ASP:N	2.53	0.41
2:B:1076:ILE:CG2	2:B:1159:VAL:HG21	2.51	0.41
2:C:332:THR:O	2:C:335:ASP:HB2	2.20	0.41
1:A:944:ARG:HB2	1:A:1006:MET:SD	2.60	0.41
2:B:1064:ASN:HA	2:B:1065:PRO:HD3	1.86	0.41
2:B:1278:TYR:CZ	2:B:1290:LYS:HG2	2.55	0.41
2:C:922:TYR:O	2:C:925:VAL:HG23	2.21	0.41
2:C:1197:PRO:HG2	2:C:1200:LYS:HB3	2.02	0.41
1:A:569:VAL:HG22	1:A:584:ILE:HG22	2.03	0.41
1:A:663:GLU:OE2	1:A:667:GLN:NE2	2.53	0.41
2:B:742:LYS:HB3	2:B:742:LYS:HE2	1.89	0.41
1:A:333:GLN:HG3	1:A:354:ILE:HD12	2.02	0.41
1:A:872:VAL:HA	1:A:873:PRO:HD3	1.96	0.41
2:B:550:ILE:O	2:B:553:GLN:HG3	2.20	0.41
2:B:735:THR:O	2:B:1017:ALA:HA	2.20	0.41
2:B:795:ASP:HA	2:B:796:PRO:HD3	1.96	0.41
2:B:1050:LEU:O	2:B:1054:ARG:HG3	2.21	0.41
1:A:665:LEU:HD21	1:A:694:ILE:HD12	2.03	0.41
2:B:235:ILE:HG13	2:C:774:LEU:HD22	2.02	0.41
2:B:497:LYS:HA	2:B:497:LYS:HD3	1.86	0.41
2:C:926:VAL:HG21	2:C:937:ASN:HA	2.03	0.41
3:D:85:ASN:HB3	3:D:141:SER:HB3	2.02	0.41
1:A:591:ALA:HB3	1:A:597:ARG:HA	2.02	0.41
1:A:655:GLU:HG2	1:A:712:ILE:HG21	2.02	0.41
2:B:192:PRO:HG3	2:B:294:VAL:HG23	2.03	0.41
2:B:307:VAL:HG21	2:B:1245:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:HIS:HB2	2:B:1318:GLU:HB3	2.02	0.41
2:B:524:GLU:HA	2:B:527:ARG:HD2	2.03	0.41
2:B:948:ILE:HD13	2:B:948:ILE:HA	1.86	0.41
2:B:1232:PRO:HB3	2:B:1236:ILE:HD11	2.02	0.41
2:C:385:ILE:HG12	2:C:708:THR:HG22	2.02	0.41
1:A:474:TYR:CD1	1:A:499:VAL:HG12	2.55	0.41
1:A:915:ASN:OD1	1:A:953:ARG:HG3	2.20	0.41
1:A:926:MET:HB2	1:A:995:VAL:HG21	2.03	0.41
2:B:227:LEU:HA	2:B:246:GLU:O	2.21	0.41
2:B:409:ILE:O	2:B:413:MET:HG2	2.21	0.41
2:B:582:SER:O	2:B:728:LYS:HE3	2.21	0.41
2:B:849:MET:HA	2:B:917:VAL:O	2.20	0.41
2:C:1323:ASP:OD1	2:C:1323:ASP:N	2.53	0.41
3:D:190:SER:O	3:D:194:VAL:HG23	2.21	0.41
1:A:41:THR:HG22	1:A:50:THR:HG23	1.99	0.40
1:A:67:ARG:NH1	1:A:171:ILE:O	2.47	0.40
1:A:552:MET:H	1:A:576:ASN:HD21	1.69	0.40
1:A:882:ASP:HB3	1:A:885:THR:OG1	2.22	0.40
2:B:145:THR:OG1	2:B:1317:VAL:HG23	2.21	0.40
2:C:471:SER:O	2:C:765:PRO:HG3	2.21	0.40
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.82	0.40
1:A:197:ALA:O	1:A:200:ARG:HG2	2.21	0.40
1:A:379:VAL:HG11	1:A:794:LEU:HG	2.03	0.40
1:A:1019:PRO:HG2	1:A:1047:ASN:OD1	2.21	0.40
2:C:204:VAL:HB	2:C:1242:MET:HB2	2.04	0.40
1:A:615:CYS:SG	1:A:617:ILE:HG12	2.61	0.40
1:A:881:ILE:HG23	1:A:900:GLN:HB3	2.04	0.40
1:A:919:TYR:HB3	1:A:921:PHE:HE1	1.86	0.40
2:B:809:VAL:HG11	2:B:1002:LEU:HG	2.04	0.40
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.22	0.40
2:B:1289:PRO:HG2	2:B:1292:GLU:HB2	2.03	0.40
3:D:235:VAL:HB	3:D:258:ASN:OD1	2.22	0.40
1:A:154:PHE:CG	1:A:185:HIS:HB2	2.56	0.40
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	2.02	0.40
2:B:863:LEU:O	2:B:866:THR:HG22	2.22	0.40
2:C:863:LEU:HD13	2:C:871:PRO:HD3	2.03	0.40
2:C:1071:PHE:HD1	2:C:1234:GLN:NE2	2.18	0.40
2:C:1269:THR:OG1	2:C:1270:LEU:N	2.54	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%)	1009 (96%)	45 (4%)	1 (0%)	51 85
2	B	1187/1333 (89%)	1129 (95%)	55 (5%)	3 (0%)	41 76
2	C	1247/1333 (94%)	1188 (95%)	55 (4%)	4 (0%)	41 76
3	D	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	41 76
3	E	290/448 (65%)	283 (98%)	7 (2%)	0	100 100
All	All	4069/4620 (88%)	3888 (96%)	172 (4%)	9 (0%)	50 82

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1136	HIS
2	C	769	GLN
2	B	790	GLU
2	B	1310	ARG
2	C	1014	MET
2	C	1331	ARG
3	D	61	ASN
1	A	982	VAL
2	C	901	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	942/943 (100%)	853 (91%)	89 (9%)	8 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1038/1153 (90%)	933 (90%)	105 (10%)	7 29
2	C	1090/1153 (94%)	978 (90%)	112 (10%)	7 28
3	D	240/379 (63%)	220 (92%)	20 (8%)	11 39
3	E	240/379 (63%)	217 (90%)	23 (10%)	8 32
All	All	3550/4007 (89%)	3201 (90%)	349 (10%)	11 30

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	7	ILE
1	A	18	LYS
1	A	50	THR
1	A	52	ARG
1	A	54	LEU
1	A	73	ARG
1	A	76	LEU
1	A	81	LYS
1	A	99	VAL
1	A	102	LEU
1	A	105	ARG
1	A	111	LEU
1	A	112	ARG
1	A	133	LEU
1	A	157	LEU
1	A	160	ASP
1	A	181	VAL
1	A	188	THR
1	A	196	LEU
1	A	199	MET
1	A	222	ARG
1	A	236	LEU
1	A	246	ASP
1	A	255	ARG
1	A	259	ARG
1	A	282	GLU
1	A	290	LEU
1	A	297	LEU
1	A	298	LEU
1	A	303	THR
1	A	306	GLN

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	313	ARG
1	A	317	ARG
1	A	318	ARG
1	A	324	ARG
1	A	329	THR
1	A	348	LEU
1	A	366	SER
1	A	368	THR
1	A	377	LEU
1	A	390	ASP
1	A	415	ASP
1	A	423	THR
1	A	433	GLU
1	A	453	LEU
1	A	466	LEU
1	A	471	SER
1	A	475	ARG
1	A	478	ILE
1	A	487	GLN
1	A	493	LEU
1	A	532	MET
1	A	533	LEU
1	A	556	THR
1	A	569	VAL
1	A	572	LEU
1	A	577	ARG
1	A	582	VAL
1	A	583	ARG
1	A	593	GLU
1	A	639	CYS
1	A	647	LEU
1	A	664	ARG
1	A	665	LEU
1	A	750	VAL
1	A	757	LEU
1	A	763	LYS
1	A	771	THR
1	A	780	LEU
1	A	781	VAL
1	A	783	ILE
1	A	812	VAL

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Mol	Chain	Res	Type
1	A	816	LEU
1	A	861	ILE
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	900	GLN
1	A	910	ASN
1	A	925	ILE
1	A	951	LEU
1	A	978	LYS
1	A	982	VAL
1	A	996	ASP
1	A	1018	ARG
1	A	1034	ARG
1	A	1057	ARG
2	B	143	VAL
2	B	147	VAL
2	B	148	GLN
2	B	175	THR
2	B	177	LYS
2	B	186	ASP
2	B	198	LYS
2	B	203	VAL
2	B	208	LEU
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	271	THR
2	B	274	MET
2	B	283	ASN
2	B	286	LEU
2	B	287	ARG
2	B	289	THR
2	B	294	VAL
2	B	315	THR
2	B	320	GLN
2	B	323	THR
2	B	327	LEU
2	B	333	ARG

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Mol	Chain	Res	Type
2	B	339	LEU
2	B	366	MET
2	B	384	MET
2	B	414	LEU
2	B	446	LYS
2	B	474	ASP
2	B	485	GLU
2	B	486	VAL
2	B	491	ASN
2	B	510	VAL
2	B	512	LEU
2	B	533	GLN
2	B	552	VAL
2	B	565	GLU
2	B	615	THR
2	B	626	ARG
2	B	629	ARG
2	B	637	TYR
2	B	654	THR
2	B	659	LEU
2	B	669	GLN
2	B	676	THR
2	B	684	LEU
2	B	688	GLU
2	B	702	LEU
2	B	704	VAL
2	B	708	THR
2	B	728	LYS
2	B	742	LYS
2	B	748	GLN
2	B	755	LEU
2	B	797	SER
2	B	804	LEU
2	B	815	LEU
2	B	828	ASP
2	B	843	LEU
2	B	848	ARG
2	B	890	THR
2	B	892	VAL
2	B	953	ASP
2	B	970	LEU
2	B	975	SER

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Mol	Chain	Res	Type
2	B	991	ASP
2	B	995	THR
2	B	1007	THR
2	B	1010	ARG
2	B	1033	ASP
2	B	1036	ASP
2	B	1048	ASP
2	B	1052	LEU
2	B	1061	LEU
2	B	1067	ILE
2	B	1074	VAL
2	B	1079	LEU
2	B	1083	ASP
2	B	1110	LEU
2	B	1134	ARG
2	B	1142	ASN
2	B	1170	ASP
2	B	1178	MET
2	B	1186	GLN
2	B	1193	ILE
2	B	1198	LYS
2	B	1201	LEU
2	B	1210	LEU
2	B	1223	SER
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1238	VAL
2	B	1240	ARG
2	B	1247	ASN
2	B	1269	THR
2	B	1285	GLN
2	B	1315	MET
2	B	1323	ASP
2	B	1329	ASN
2	B	1331	ARG
2	C	82	ARG
2	C	83	GLN
2	C	109	LYS
2	C	112	THR
2	C	115	GLN
2	C	117	ARG

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Mol	Chain	Res	Type
2	C	118	THR
2	C	133	THR
2	C	134	THR
2	C	141	LEU
2	C	147	VAL
2	C	173	GLN
2	C	187	ASP
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	208	LEU
2	C	230	ASP
2	C	255	LEU
2	C	264	LEU
2	C	270	THR
2	C	275	SER
2	C	281	VAL
2	C	282	VAL
2	C	294	VAL
2	C	310	LEU
2	C	315	THR
2	C	323	THR
2	C	330	THR
2	C	331	GLU
2	C	335	ASP
2	C	362	LEU
2	C	363	ARG
2	C	375	ARG
2	C	379	LEU
2	C	384	MET
2	C	397	LEU
2	C	401	LEU
2	C	452	ASN
2	C	474	ASP
2	C	475	ILE
2	C	484	ARG
2	C	486	VAL
2	C	503	GLU
2	C	532	ILE
2	C	533	GLN
2	C	542	ARG
2	C	552	VAL

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Mol	Chain	Res	Type
2	C	557	THR
2	C	575	TRP
2	C	626	ARG
2	C	630	ASN
2	C	637	TYR
2	C	659	LEU
2	C	674	LYS
2	C	685	ARG
2	C	687	LEU
2	C	689	THR
2	C	694	ILE
2	C	735	THR
2	C	761	SER
2	C	763	VAL
2	C	768	CYS
2	C	792	VAL
2	C	798	THR
2	C	804	LEU
2	C	809	VAL
2	C	815	LEU
2	C	828	ASP
2	C	832	MET
2	C	837	THR
2	C	854	GLN
2	C	859	ILE
2	C	872	ILE
2	C	907	SER
2	C	921	ASP
2	C	931	ASN
2	C	945	VAL
2	C	959	GLN
2	C	965	ARG
2	C	995	THR
2	C	1003	ARG
2	C	1007	THR
2	C	1010	ARG
2	C	1014	MET
2	C	1015	GLN
2	C	1035	ILE
2	C	1043	SER
2	C	1052	LEU
2	C	1055	LEU

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Mol	Chain	Res	Type
2	C	1061	LEU
2	C	1067	ILE
2	C	1070	ARG
2	C	1079	LEU
2	C	1104	ARG
2	C	1113	LYS
2	C	1134	ARG
2	C	1170	ASP
2	C	1181	SER
2	C	1188	VAL
2	C	1202	PHE
2	C	1210	LEU
2	C	1219	ASP
2	C	1230	ILE
2	C	1233	LEU
2	C	1258	VAL
2	C	1267	THR
2	C	1283	ASN
2	C	1295	HIS
2	C	1306	THR
2	C	1321	ASN
2	C	1332	ASN
3	D	2	LEU
3	D	20	ARG
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	92	ARG
3	D	93	LEU
3	D	96	LEU
3	D	107	LEU
3	D	116	THR
3	D	133	THR
3	D	142	THR
3	D	158	LEU
3	D	160	LEU
3	D	171	VAL
3	D	189	LEU
3	D	191	ARG
3	D	226	MET
3	D	232	SER
3	D	252	LEU

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Mol	Chain	Res	Type
3	E	2	LEU
3	E	21	ASN
3	E	27	THR
3	E	35	LEU
3	E	47	LYS
3	E	66	VAL
3	E	93	LEU
3	E	94	SER
3	E	98	LEU
3	E	133	THR
3	E	183	GLU
3	E	189	LEU
3	E	226	MET
3	E	240	VAL
3	E	242	ARG
3	E	244	VAL
3	E	252	LEU
3	E	261	ARG
3	E	262	THR
3	E	269	ILE
3	E	272	ASP
3	E	273	LEU
3	E	274	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	241	GLN
1	A	258	GLN
1	A	375	HIS
1	A	576	ASN
2	B	724	HIS
2	B	1138	HIS
2	C	724	HIS
2	C	1015	GLN
2	C	1234	GLN
2	C	1308	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 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	$\#\|Z\| > 2$
4	SAM	A	1101	-	24,29,29	1.18	3 (12%)	23,42,42	1.61	4 (17%)
4	SAM	A	1102	-	24,29,29	1.20	3 (12%)	23,42,42	1.62	4 (17%)
5	ATP	A	1103	-	26,33,33	0.89	1 (3%)	31,52,52	1.46	6 (19%)
6	GTP	A	1104	7	26,34,34	1.11	1 (3%)	32,54,54	1.47	6 (18%)

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
4	SAM	A	1101	-	-	4/12/33/33	0/3/3/3
4	SAM	A	1102	-	-	2/12/33/33	0/3/3/3
5	ATP	A	1103	-	-	0/18/38/38	0/3/3/3
6	GTP	A	1104	7	-	5/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1104	GTP	C5-C6	-3.96	1.39	1.47
4	A	1102	SAM	C2-N3	3.84	1.38	1.32
4	A	1101	SAM	C2-N3	3.81	1.38	1.32
4	A	1102	SAM	C2-N1	2.46	1.38	1.33
5	A	1103	ATP	C5-C4	2.38	1.47	1.40
4	A	1101	SAM	C2-N1	2.36	1.38	1.33
4	A	1102	SAM	OXT-C	-2.13	1.23	1.30
4	A	1101	SAM	OXT-C	-2.12	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	SAM	N3-C2-N1	-5.58	119.96	128.68
4	A	1102	SAM	N3-C2-N1	-5.51	120.07	128.68
5	A	1103	ATP	C3'-C2'-C1'	3.49	106.23	100.98
5	A	1103	ATP	N3-C2-N1	-3.36	123.43	128.68
6	A	1104	GTP	C5-C6-N1	3.23	119.66	113.95
5	A	1103	ATP	PB-O3B-PG	-3.13	122.08	132.83
6	A	1104	GTP	C8-N7-C5	3.12	108.93	102.99
4	A	1102	SAM	C3'-C2'-C1'	2.90	105.34	100.98
6	A	1104	GTP	PB-O3B-PG	-2.90	122.88	132.83
6	A	1104	GTP	C2-N1-C6	-2.87	119.81	125.10
4	A	1102	SAM	OXT-C-O	-2.80	117.72	124.09
4	A	1101	SAM	OXT-C-O	-2.79	117.75	124.09
4	A	1101	SAM	C3'-C2'-C1'	2.71	105.06	100.98
6	A	1104	GTP	C3'-C2'-C1'	2.51	104.75	100.98
5	A	1103	ATP	C4-C5-N7	-2.32	106.98	109.40
4	A	1102	SAM	OXT-C-CA	2.28	121.14	113.38
6	A	1104	GTP	O6-C6-C5	-2.25	119.98	124.37
4	A	1101	SAM	OXT-C-CA	2.18	120.82	113.38
5	A	1103	ATP	O3G-PG-O2G	2.08	115.58	107.64
5	A	1103	ATP	C2-N1-C6	2.06	122.27	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	SAM	CB-CG-SD-CE
6	A	1104	GTP	PB-O3B-PG-O3G
6	A	1104	GTP	C5'-O5'-PA-O1A
4	A	1101	SAM	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	C-CA-CB-CG
4	A	1101	SAM	O-C-CA-N
6	A	1104	GTP	C5'-O5'-PA-O3A
6	A	1104	GTP	PB-O3A-PA-O2A
6	A	1104	GTP	PB-O3B-PG-O1G
4	A	1101	SAM	N-CA-CB-CG
4	A	1102	SAM	CB-CG-SD-C5'

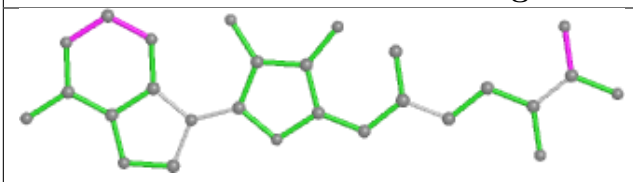
There are no ring outliers.

2 monomers are involved in 2 short contacts:

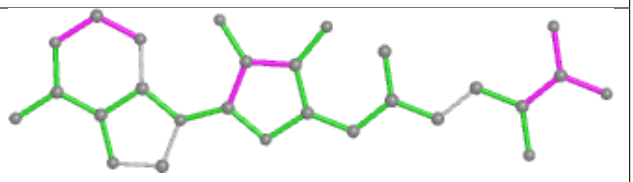
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	1	0
6	A	1104	GTP	1	0

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.

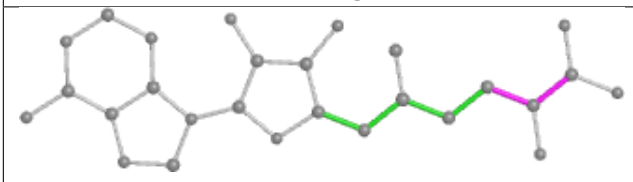
Ligand SAM A 1101



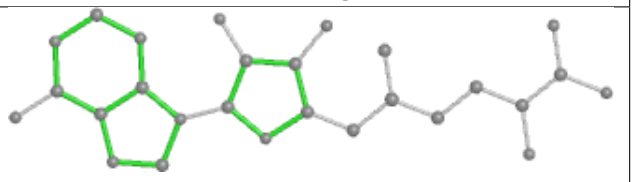
Bond lengths



Bond angles

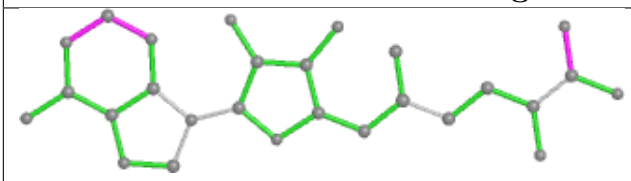


Torsions

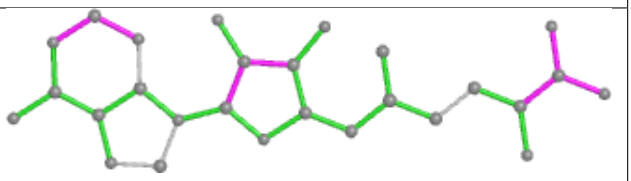


Rings

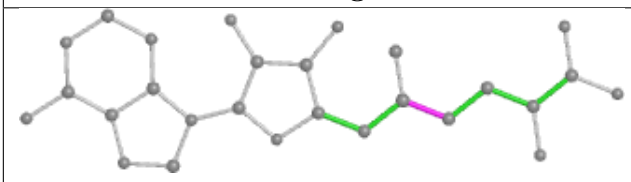
Ligand SAM A 1102



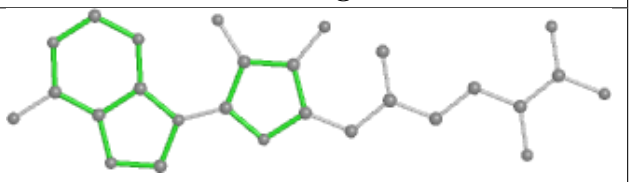
Bond lengths



Bond angles

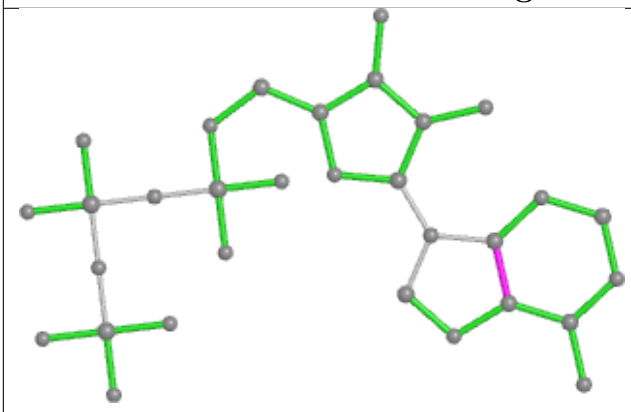


Torsions

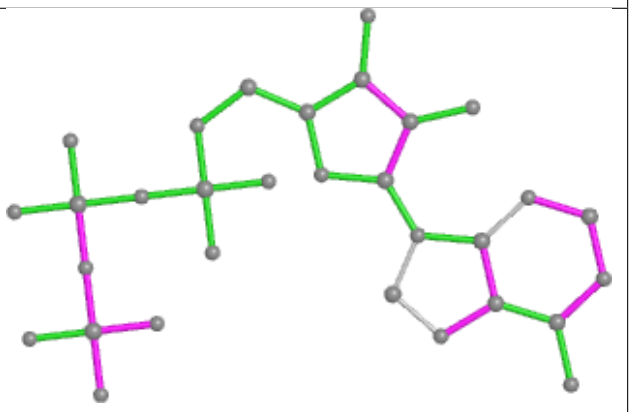


Rings

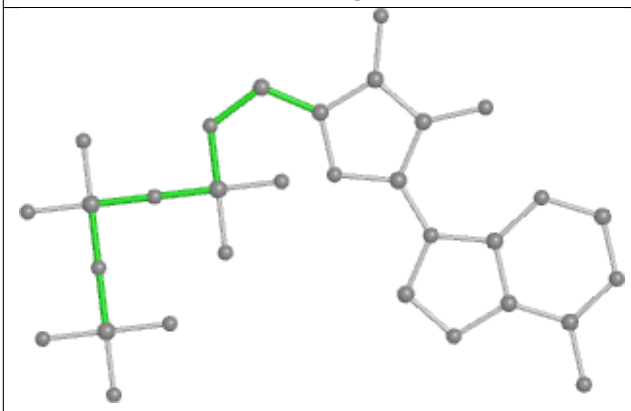
Ligand ATP A 1103



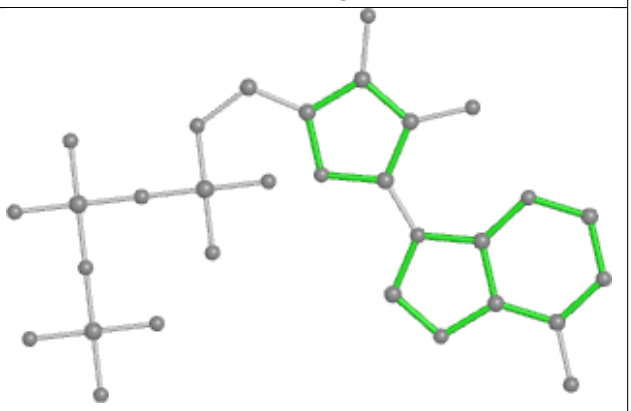
Bond lengths



Bond angles

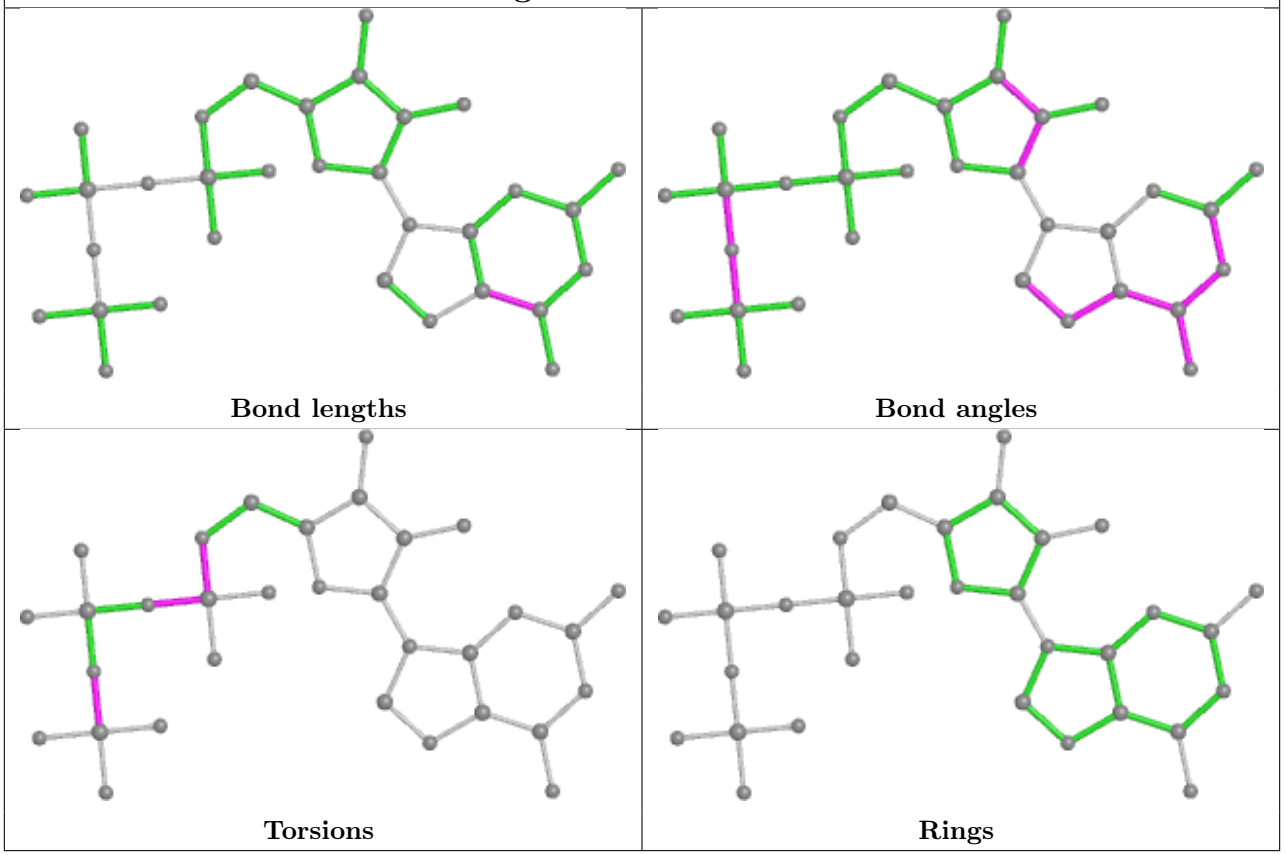


Torsions



Rings

Ligand GTP A 1104



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.

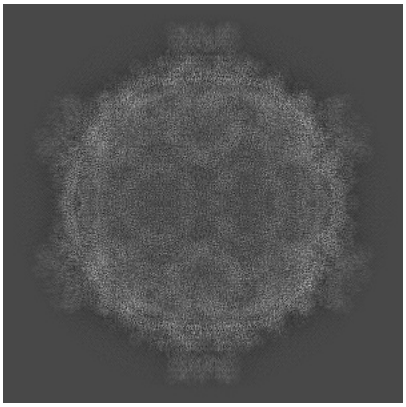
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6378. These allow visual inspection of the internal detail of the map and identification of artifacts.

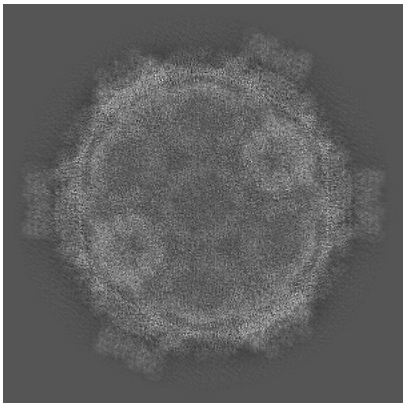
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

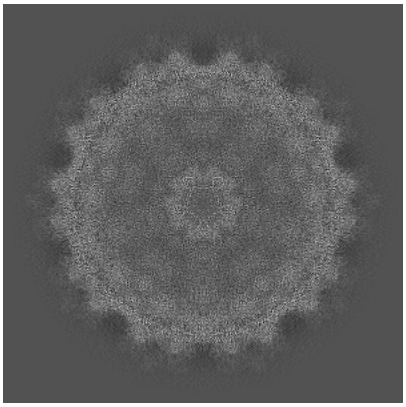
6.1.1 Primary map



X



Y

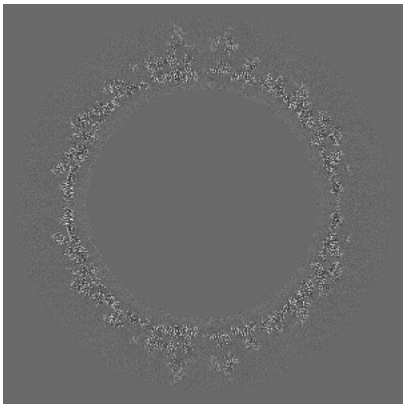


Z

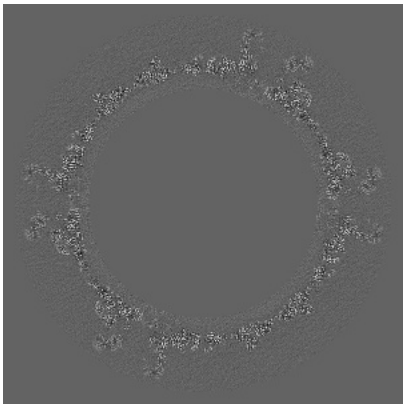
The images above show the map projected in three orthogonal directions.

6.2 Central slices

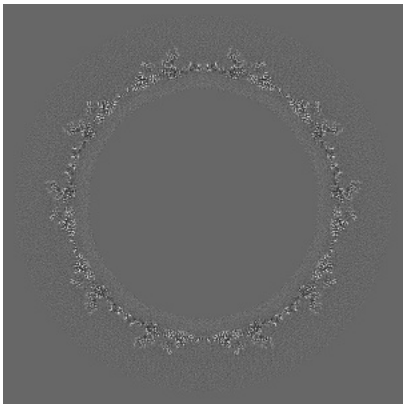
6.2.1 Primary map



X Index: 350



Y Index: 350

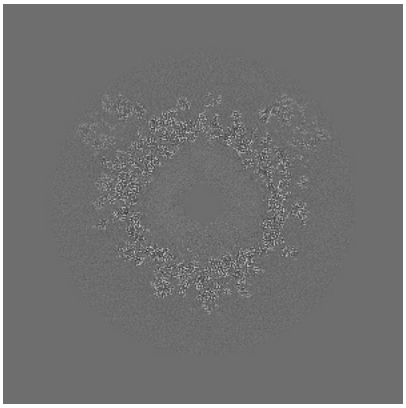


Z Index: 350

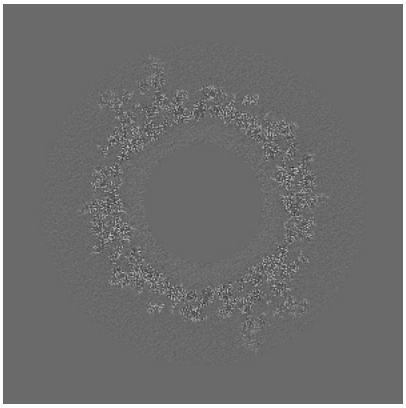
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

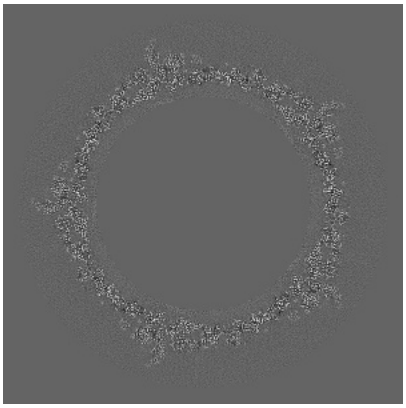
6.3.1 Primary map



X Index: 153



Y Index: 521



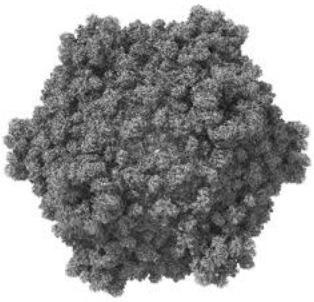
Z Index: 278

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.

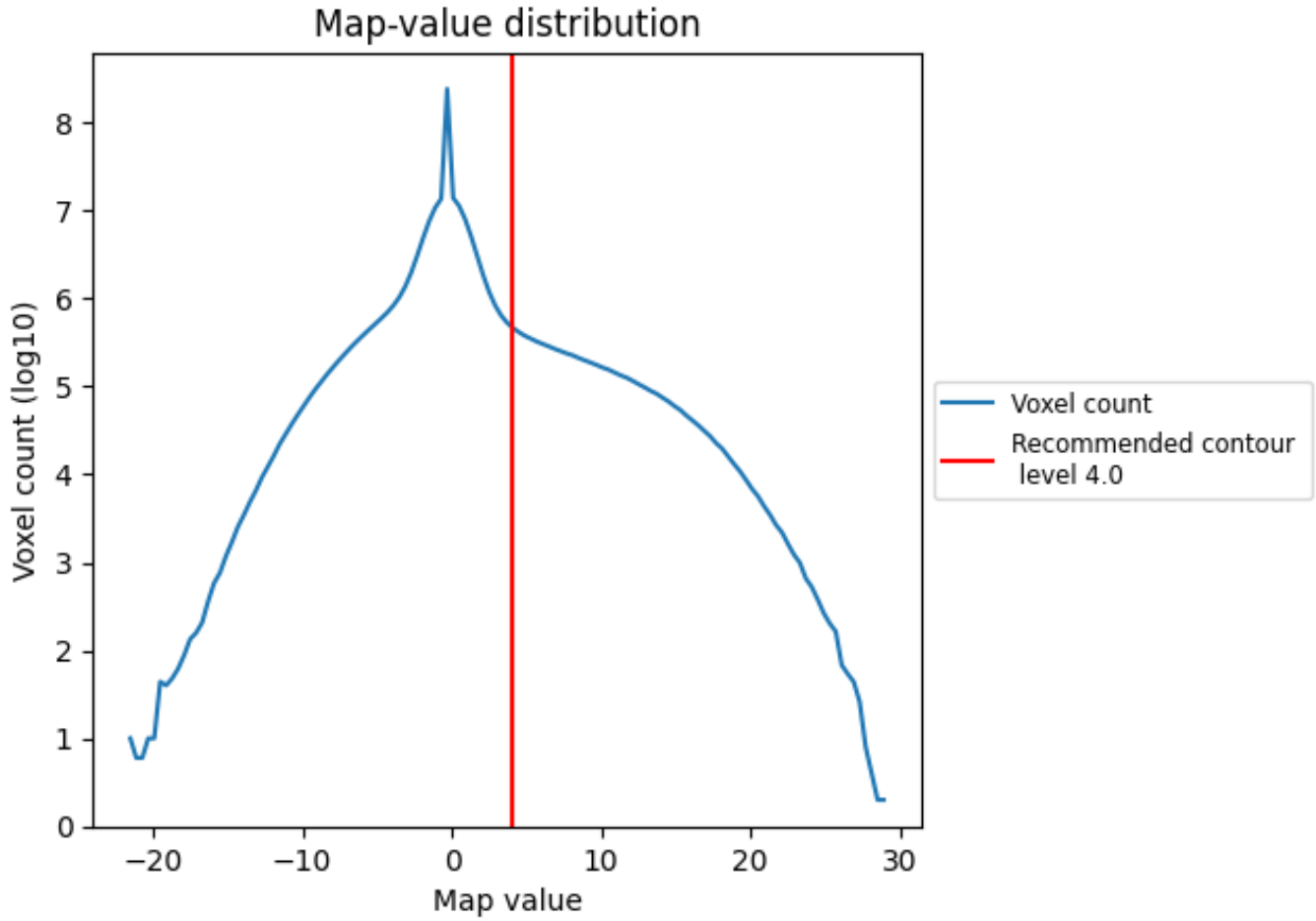
6.5 Mask visualisation (i)

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

7 Map analysis

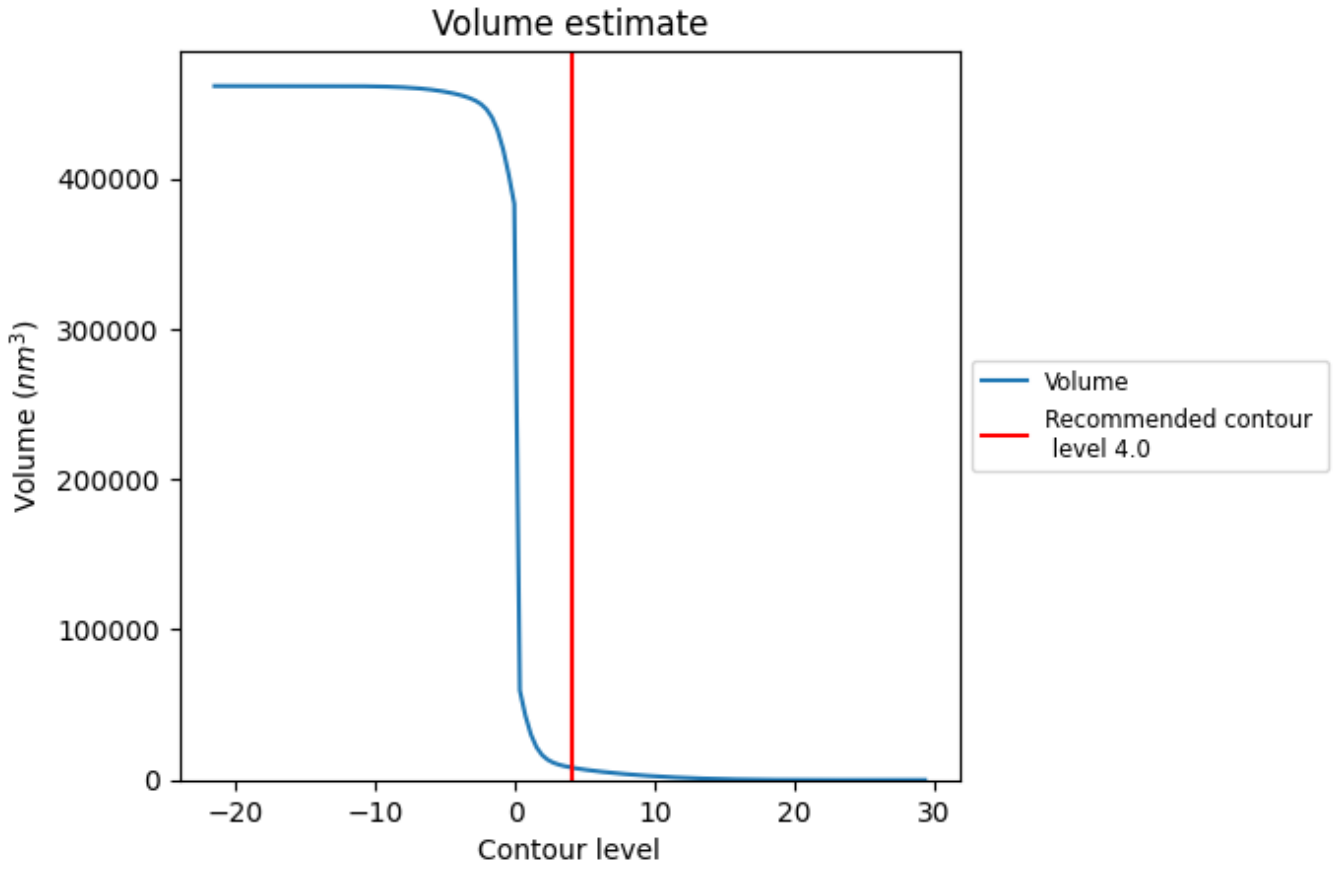
This section contains the results of statistical analysis of the map.

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.

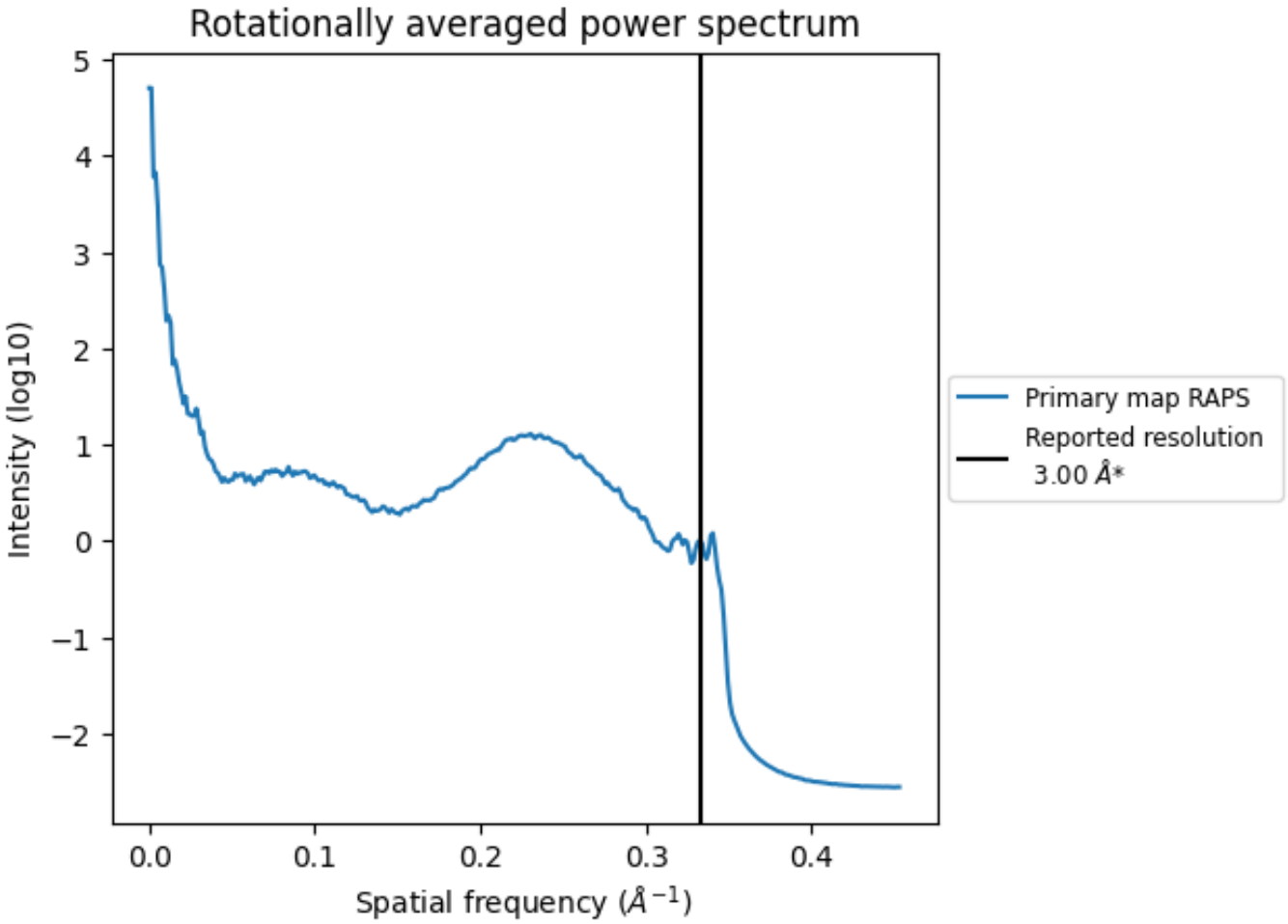
7.2 Volume estimate



The volume at the recommended contour level is 8307 nm^3; this corresponds to an approximate mass of 7504 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 0.333 Å^{-1}

8 Fourier-Shell correlation

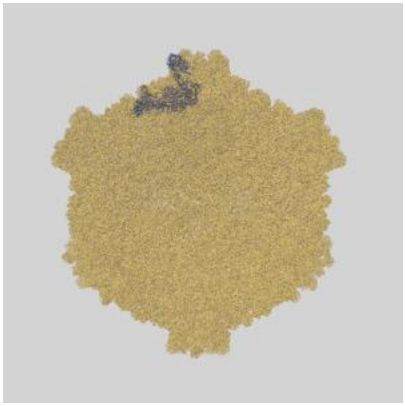
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

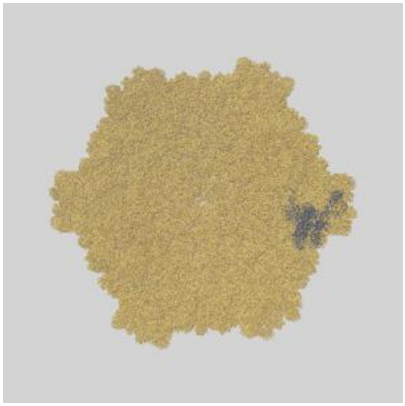
This section contains information regarding the fit between EMDB map EMD-6378 and PDB model 3JAY. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

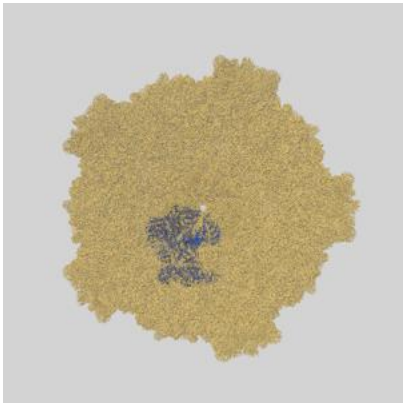
9.1.1 Map-model overlay



X

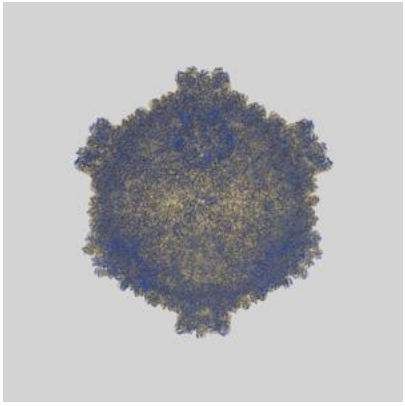


Y

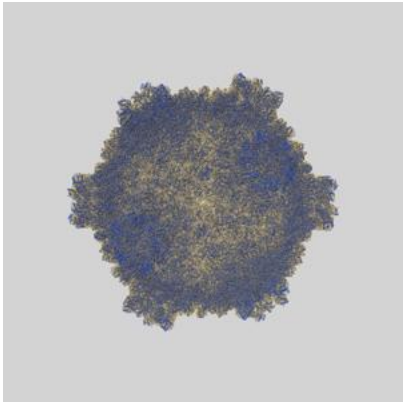


Z

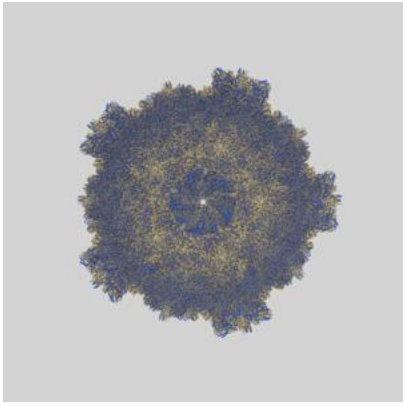
9.1.2 Map-model assembly overlay



X



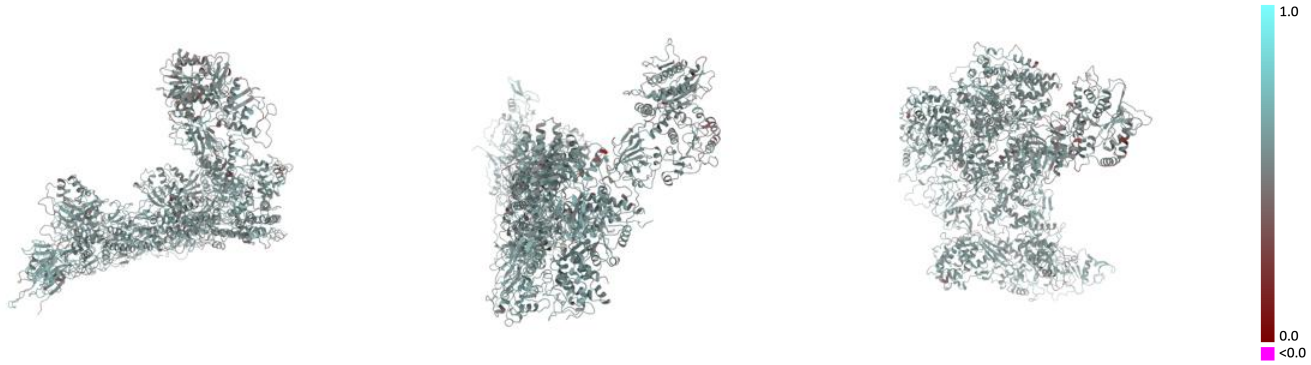
Y



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.

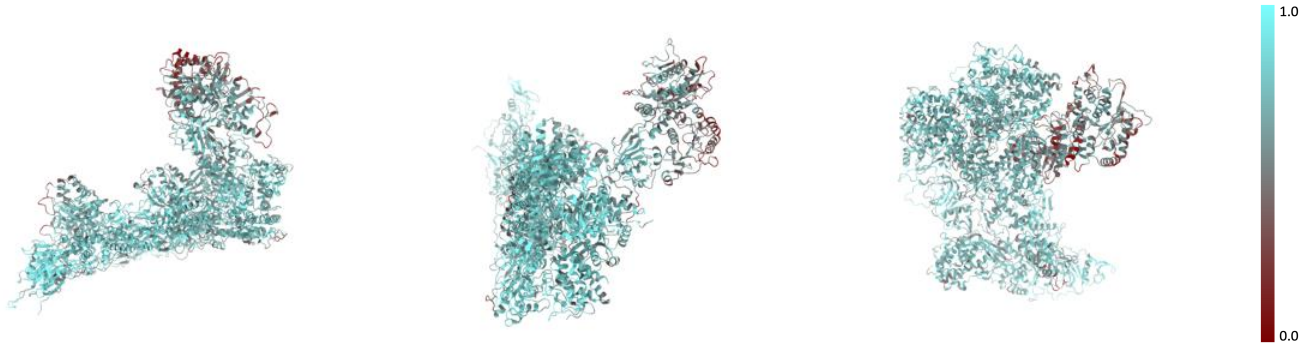
9.2 Q-score mapped to coordinate model (i)



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.

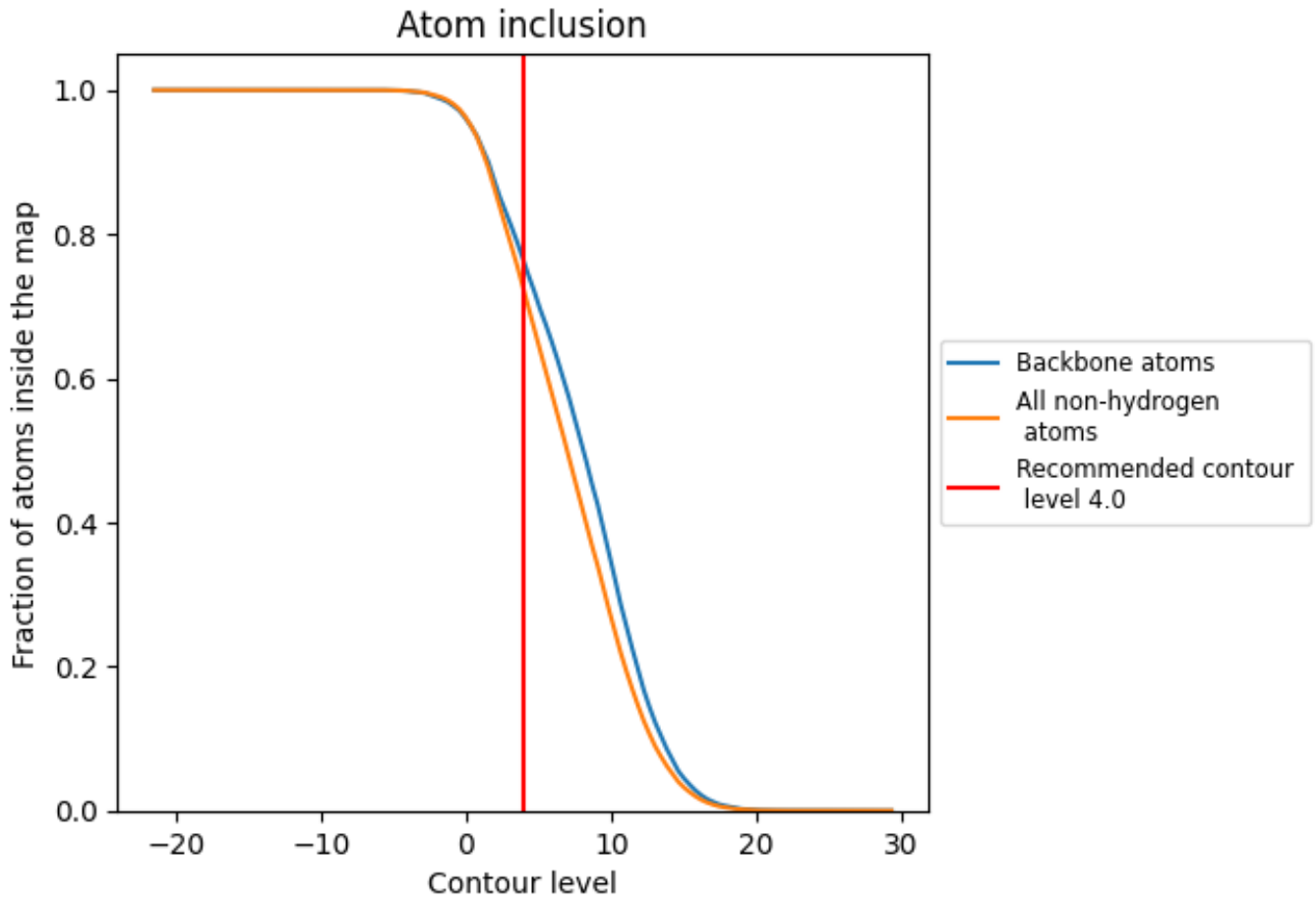
9.3 Atom inclusion mapped to coordinate model (i)



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, 76% of all backbone atoms, 72% 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	0.7200	0.5490
A	0.6155	0.5310
B	0.7553	0.5550
C	0.7633	0.5550
D	0.7589	0.5620
E	0.7400	0.5540