Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:30 AM EST

PDB ID	:	3JAZ
EMDB ID	:	EMD-6371
Title	:	Atomic model of cytoplasmic polyhedrosis virus with 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:

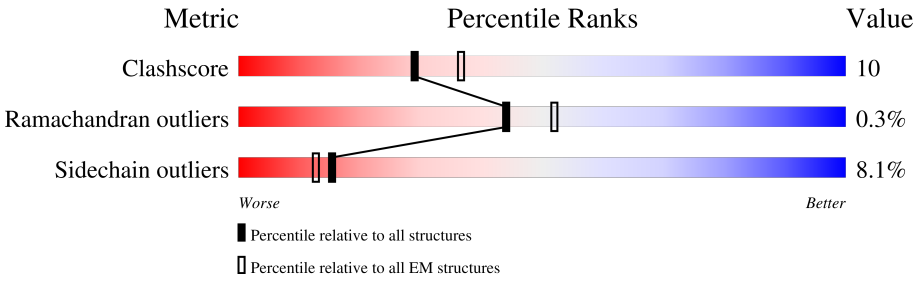
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	12% 68% 28% ·
2	B	1333	· 63% 24% · 11%
2	C	1333	· 69% 23% · 6%
3	D	448	· 45% 17% · 35%
3	E	448	· 46% 17% · 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32244 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
			Total	C	N	O	S		
1	A	1057	8434	5345	1457	1587	45	0	0

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1191	9397	5937	1634	1789	37	0	0
			Total	C	N	O	S		
2	C	1250	9851	6219	1712	1882	38	0	0

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

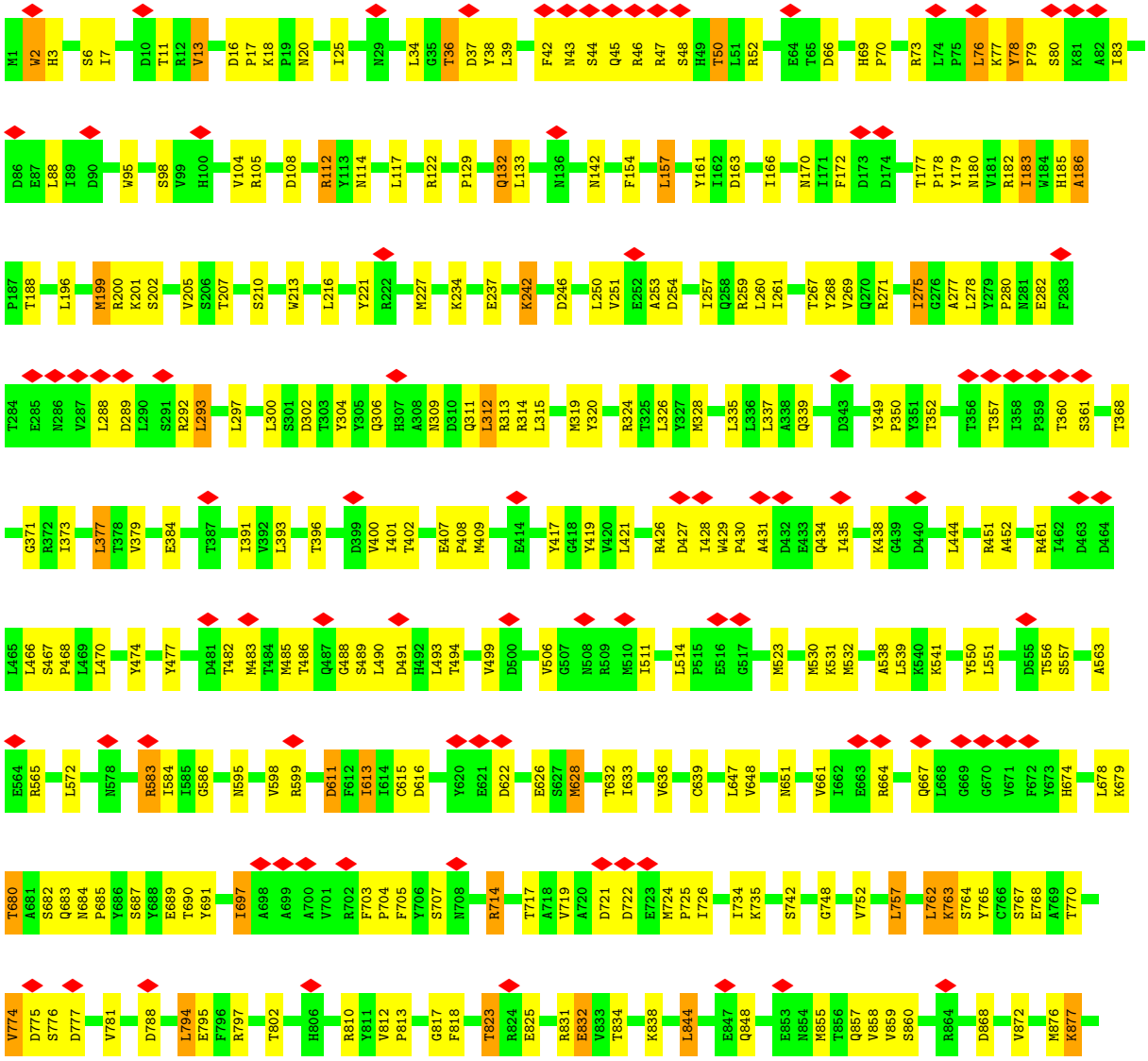
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	292	2281	1449	399	425	8	0	0
			Total	C	N	O	S		
3	E	292	2281	1449	399	425	8	0	0

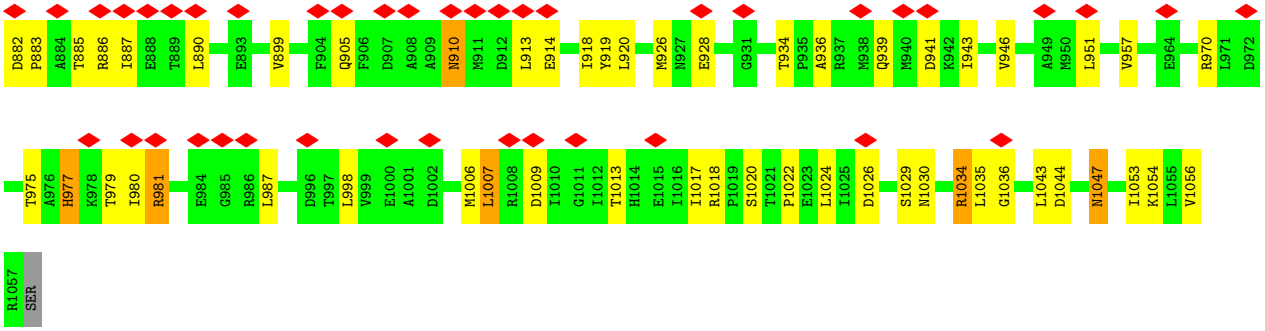
3 Residue-property plots (i)

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

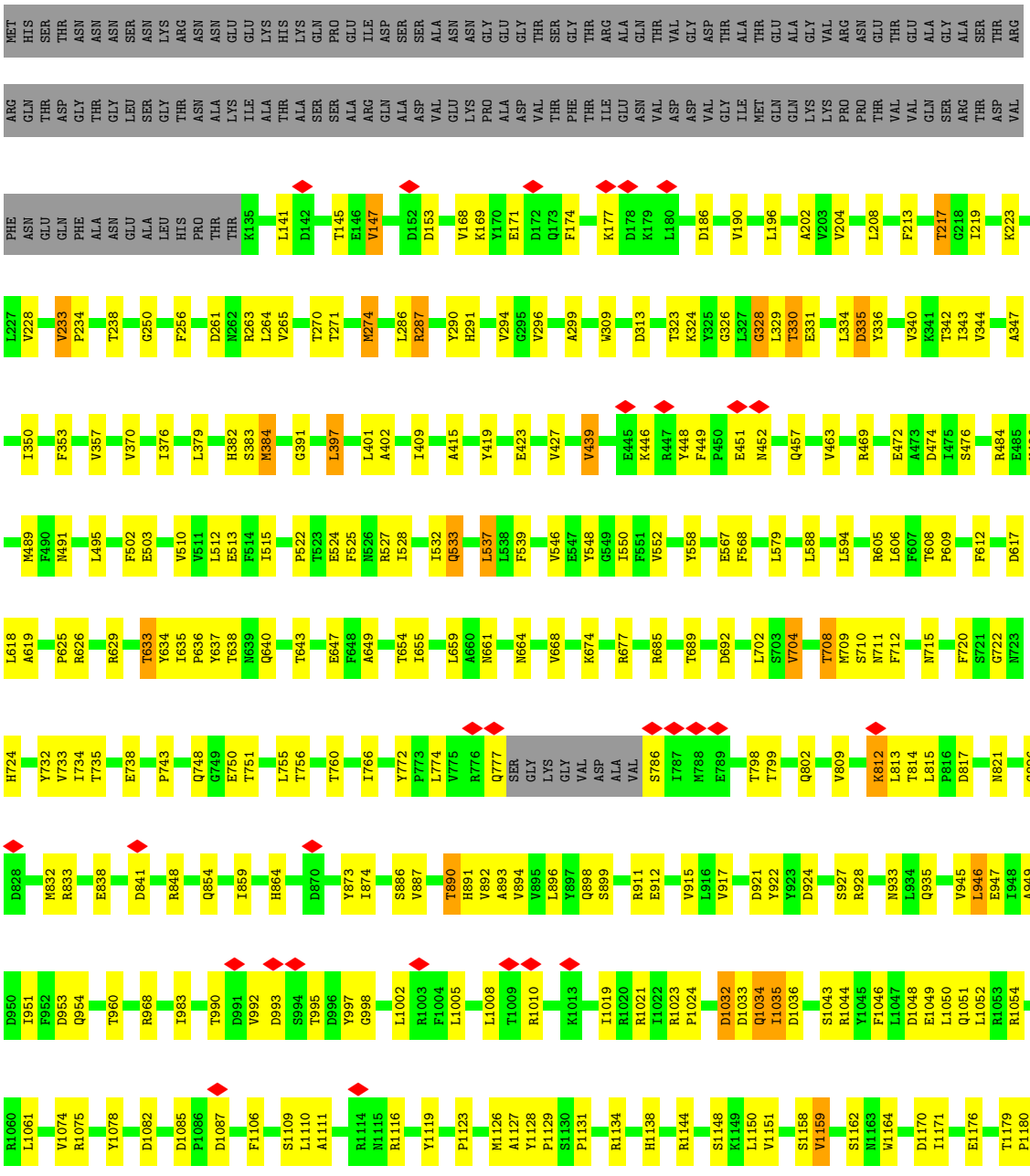
Chain A:

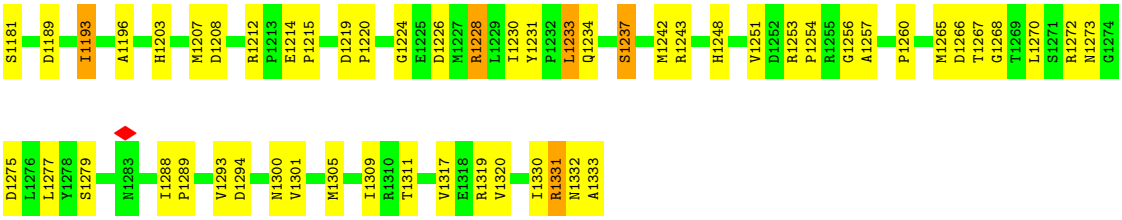




• Molecule 2: Capsid protein VP1

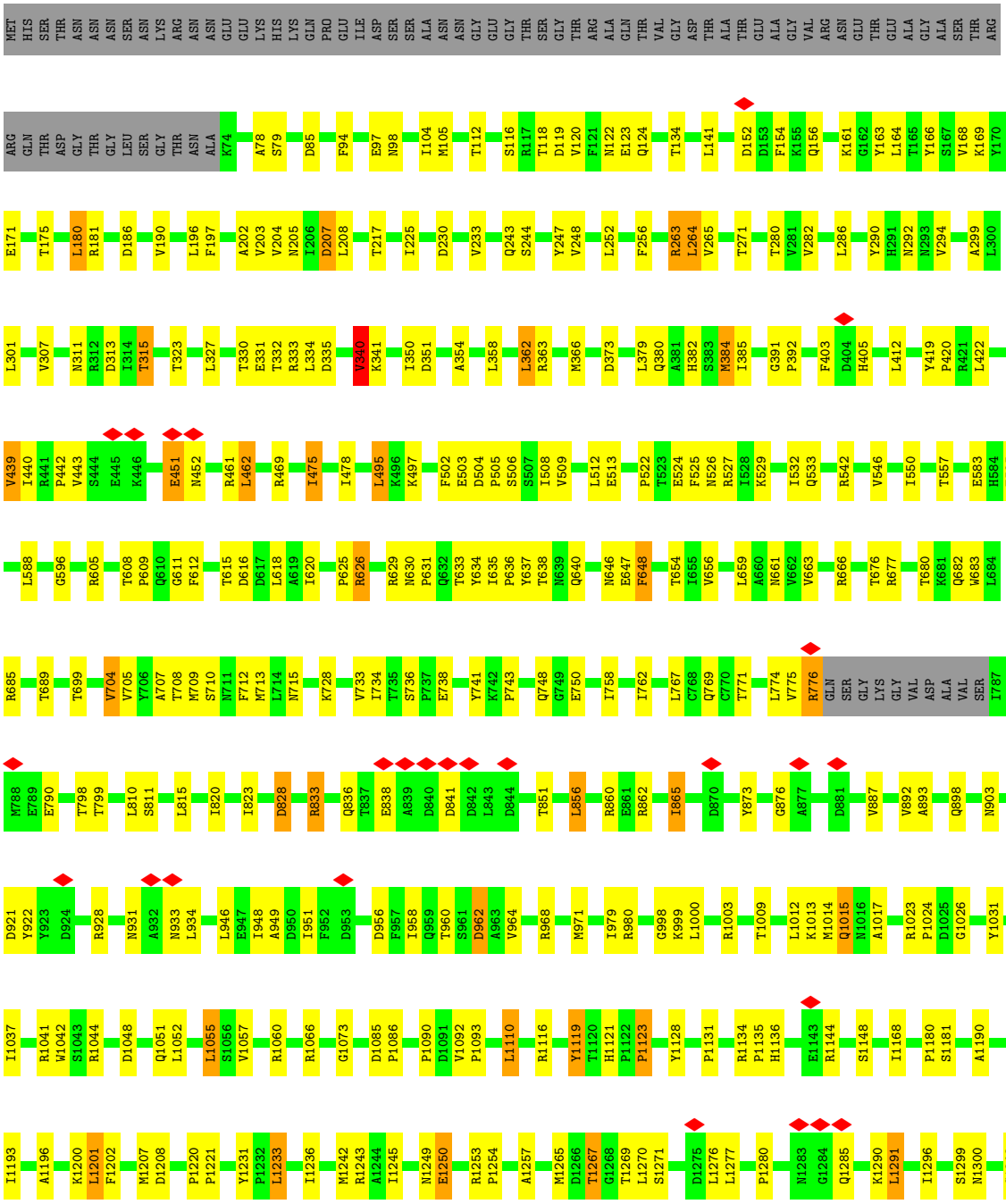
Chain B:

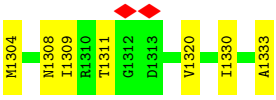




• Molecule 2: Capsid protein VP1

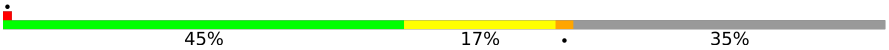
Chain C:

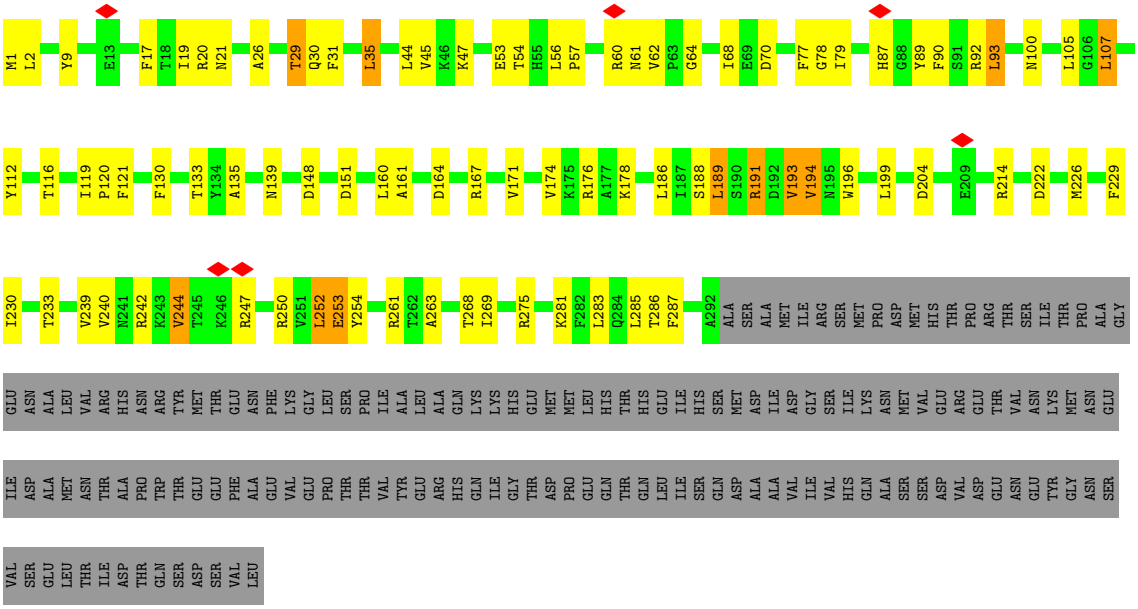




• Molecule 3: Viral structural protein 5

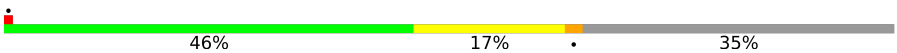
Chain D:

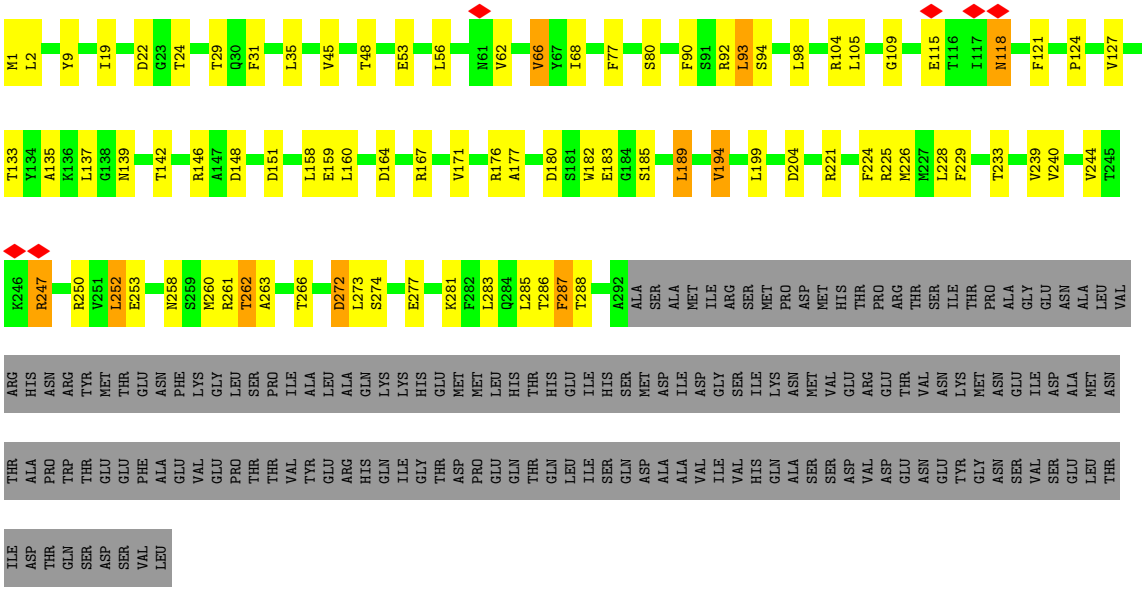




• Molecule 3: Viral structural protein 5

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19447	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	26.030	Depositor
Minimum map value	-16.162	Depositor
Average map value	0.072	Depositor
Map value standard deviation	1.603	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

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	0.29	0/8619	0.52	3/11737 (0.0%)
2	B	0.34	0/9590	0.55	1/13056 (0.0%)
2	C	0.33	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.55	0/3163
3	E	0.31	0/2327	0.53	0/3163
All	All	0.32	0/32915	0.55	4/44806 (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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ALA	C-N-CD	-8.47	101.96	120.60
1	A	186	ALA	C-N-CA	5.95	146.99	122.00
1	A	78	TYR	C-N-CD	-5.78	107.88	120.60
2	B	274	MET	CG-SD-CE	5.07	108.32	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	328	GLY	Peptide

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	184	0
2	B	9397	0	9315	209	0
2	C	9851	0	9762	195	0
3	D	2281	0	2282	53	0
3	E	2281	0	2282	48	0
All	All	32244	0	32040	660	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 (660) 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)
2:B:812:LYS:NZ	2:B:812:LYS:HB3	1.55	1.12
2:B:812:LYS:NZ	2:B:812:LYS:CB	2.12	1.11
2:B:812:LYS:HB3	2:B:812:LYS:HZ3	0.95	1.10
1:A:277:ALA:HB3	1:A:319:MET:HE1	1.54	0.89
2:B:812:LYS:CB	2:B:812:LYS:HZ2	1.86	0.88
2:B:328:GLY:H	2:B:347:ALA:HB3	1.41	0.85
1:A:797:ARG:NH2	1:A:876:MET:O	2.09	0.85
2:B:812:LYS:HZ2	2:B:812:LYS:HB2	1.44	0.82
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.14	0.81
2:C:1116:ARG:HH11	2:C:1116:ARG:HG2	1.47	0.79
1:A:685:PRO:O	1:A:714:ARG:NH2	2.19	0.76
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.69	0.75
1:A:680:THR:HG22	1:A:683:GLN:HG3	1.69	0.75
3:E:77:PHE:HB2	3:E:194:VAL:HG23	1.69	0.75
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.19	0.74
2:C:161:LYS:O	2:C:263:ARG:NH2	2.20	0.74
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.69	0.74
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.20	0.74
2:C:815:LEU:HD11	2:C:1051:GLN:HE22	1.53	0.74
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.20	0.73
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.21	0.73
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HG2	1:A:324:ARG:HE	1.52	0.73
2:C:384:MET:HA	2:C:708:THR:HG21	1.71	0.73
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.21	0.72
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.70	0.72
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.71	0.72
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.23	0.72
2:B:1131:PRO:O	2:B:1162:SER:OG	2.07	0.72
1:A:563:ALA:O	1:A:565:ARG:NH1	2.23	0.72
3:E:283:LEU:HA	3:E:286:THR:HG22	1.72	0.72
2:C:1057:VAL:HG22	2:C:1291:LEU:HD21	1.72	0.71
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.24	0.71
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.72	0.71
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.26	0.69
2:B:469:ARG:NH1	2:B:472:GLU:OE1	2.27	0.68
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.26	0.68
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.75	0.68
1:A:680:THR:HG23	1:A:682:SER:H	1.59	0.67
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.27	0.67
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.27	0.67
1:A:489:SER:OG	1:A:491:ASP:OD1	2.10	0.67
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.74	0.67
2:B:1021:ARG:NE	2:B:1036:ASP:OD1	2.28	0.67
2:B:817:ASP:HA	2:B:983:ILE:HG12	1.77	0.66
3:E:164:ASP:OD2	3:E:167:ARG:NH2	2.28	0.66
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.27	0.66
2:C:366:MET:HG2	3:E:266:THR:HG21	1.77	0.66
1:A:36:THR:OG1	1:A:37:ASP:N	2.27	0.66
1:A:674:HIS:HB2	1:A:697:ILE:HD12	1.78	0.66
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	1.77	0.66
1:A:242:LYS:NZ	1:A:246:ASP:OD2	2.26	0.65
3:D:193:VAL:HG11	3:D:230:ILE:HG13	1.79	0.65
1:A:13:VAL:HG23	1:A:213:TRP:CD1	2.31	0.65
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.62	0.64
1:A:427:ASP:HA	1:A:703:PHE:HA	1.80	0.64
3:E:272:ASP:OD2	3:E:274:SER:OG	2.14	0.64
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.30	0.64
2:B:1085:ASP:OD2	2:B:1243:ARG:NH2	2.31	0.64
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.80	0.64
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.80	0.63
2:C:169:LYS:O	2:C:202:ALA:N	2.31	0.63
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.31	0.63
3:E:180:ASP:OD1	3:E:247:ARG:NH1	2.32	0.63
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.79	0.62
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.31	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.16	0.62
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.32	0.62
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.33	0.62
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.35	0.62
2:B:921:ASP:O	2:B:928:ARG:NH1	2.32	0.61
2:B:1048:ASP:HB3	2:B:1051:GLN:HG3	1.80	0.61
2:C:626:ARG:NH2	2:C:712:PHE:O	2.26	0.61
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.36	0.61
1:A:419:TYR:HE1	1:A:421:LEU:HD23	1.65	0.61
2:C:615:THR:H	2:C:1333:ALA:HA	1.64	0.61
2:C:163:TYR:N	2:C:351:ASP:OD2	2.32	0.61
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.83	0.61
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.81	0.61
2:C:78:ALA:HB2	2:C:1181:SER:HB2	1.81	0.61
2:C:443:VAL:HB	2:C:771:THR:HG23	1.81	0.61
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.26	0.61
1:A:161:TYR:CE2	2:B:1333:ALA:HB1	2.36	0.61
1:A:477:TYR:HA	1:A:482:THR:HG22	1.82	0.61
2:C:704:VAL:O	2:C:708:THR:HG23	2.00	0.61
2:C:709:MET:O	2:C:715:ASN:ND2	2.34	0.61
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.34	0.60
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.18	0.60
2:B:992:VAL:HG12	2:B:992:VAL:O	2.01	0.60
2:B:709:MET:O	2:B:715:ASN:ND2	2.33	0.60
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.34	0.60
2:B:1126:MET:HE1	3:E:146:ARG:HB3	1.83	0.60
2:B:626:ARG:NH2	2:B:712:PHE:O	2.34	0.60
3:D:261:ARG:NH1	3:D:263:ALA:O	2.35	0.60
3:E:148:ASP:OD1	3:E:151:ASP:N	2.32	0.60
1:A:409:MET:HE1	1:A:1036:GLY:HA2	1.83	0.60
1:A:288:LEU:HD22	1:A:368:THR:HG22	1.84	0.59
2:B:384:MET:HA	2:B:708:THR:HG21	1.84	0.59
1:A:129:PRO:HB2	2:B:1332:ASN:HD22	1.67	0.59
1:A:227:MET:HG2	1:A:269:VAL:HG21	1.84	0.59
1:A:957:VAL:HG22	1:A:1056:VAL:HG23	1.85	0.59
2:B:342:THR:OG1	2:B:343:ILE:N	2.36	0.59
1:A:47:ARG:NH1	1:A:80:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.35	0.59
2:B:640:GLN:OE1	2:B:647:GLU:N	2.33	0.58
1:A:114:ASN:ND2	1:A:117:LEU:HB2	2.17	0.58
1:A:848:GLN:OE1	1:A:1054:LYS:NZ	2.35	0.58
2:B:335:ASP:OD1	2:B:340:VAL:N	2.33	0.58
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.38	0.58
1:A:234:LYS:NZ	1:A:237:GLU:OE2	2.37	0.58
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.86	0.58
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.86	0.57
2:B:226:PRO:HB2	2:B:250:GLY:HA3	1.85	0.57
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.86	0.57
1:A:129:PRO:HG2	2:B:1332:ASN:HB2	1.85	0.57
2:B:537:LEU:HD13	2:B:548:TYR:HE1	1.69	0.57
1:A:292:ARG:NH1	1:A:777:ASP:OD1	2.35	0.57
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.86	0.57
2:B:528:ILE:HG13	2:B:532:ILE:HD12	1.85	0.57
2:C:207:ASP:OD1	2:C:207:ASP:N	2.37	0.57
2:C:533:GLN:HG3	2:C:588:LEU:HD12	1.85	0.57
2:C:1119:TYR:HH	2:C:1121:HIS:HD1	1.51	0.57
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.87	0.57
2:C:741:TYR:OH	2:C:1026:GLY:O	2.21	0.57
2:B:704:VAL:O	2:B:708:THR:HG23	2.05	0.57
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.23	0.57
2:C:550:ILE:HD13	2:C:596:GLY:HA3	1.87	0.57
2:C:244:SER:HA	2:C:1201:LEU:HD22	1.85	0.56
1:A:651:ASN:HA	1:A:689:GLU:HG3	1.88	0.56
2:C:104:ILE:HG12	2:C:1311:THR:HG23	1.88	0.56
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.69	0.56
2:B:1032:ASP:HB3	2:B:1035:ILE:HG23	1.87	0.56
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.87	0.56
1:A:687:SER:OG	1:A:689:GLU:OE1	2.21	0.56
1:A:163:ASP:OD1	1:A:182:ARG:NE	2.32	0.56
1:A:257:ILE:HG21	1:A:326:LEU:HD11	1.87	0.56
2:B:606:LEU:HD13	2:B:655:ILE:HG23	1.88	0.56
1:A:565:ARG:NH2	1:A:616:ASP:OD2	2.37	0.56
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.39	0.56
2:C:931:ASN:HB3	2:C:934:LEU:HD23	1.87	0.56
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.87	0.56
2:B:147:VAL:HG22	2:B:379:LEU:HD11	1.88	0.55
1:A:36:THR:OG1	1:A:37:ASP:OD1	2.24	0.55
1:A:541:LYS:HD3	1:A:550:TYR:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:THR:HG21	2:B:710:SER:HB3	1.87	0.55
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.89	0.55
1:A:714:ARG:NH1	1:A:1044:ASP:OD1	2.40	0.55
2:B:474:ASP:OD2	2:B:476:SER:OG	2.24	0.55
2:B:1171:ILE:HD11	2:B:1193:ILE:HG23	1.88	0.55
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.39	0.55
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.88	0.55
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.88	0.55
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.39	0.55
2:C:1048:ASP:HB3	2:C:1051:GLN:HG3	1.88	0.55
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.89	0.55
2:C:180:LEU:HD12	2:C:181:ARG:H	1.72	0.54
2:B:1109:SER:HB2	3:E:262:THR:HG21	1.88	0.54
2:C:203:VAL:HG12	2:C:1243:ARG:HG3	1.89	0.54
2:C:230:ASP:HA	2:C:233:VAL:HG11	1.89	0.54
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.42	0.54
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.40	0.54
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.88	0.54
1:A:78:TYR:CE2	1:A:83:ILE:HA	2.42	0.54
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.35	0.54
1:A:664:ARG:HD2	1:A:667:GLN:HE21	1.72	0.54
1:A:928:GLU:HG2	1:A:934:THR:HG22	1.89	0.54
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.35	0.54
2:C:451:GLU:OE2	2:C:452:ASN:ND2	2.41	0.54
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.89	0.54
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.89	0.54
3:E:239:VAL:HG12	3:E:250:ARG:HD2	1.90	0.54
1:A:882:ASP:OD2	1:A:885:THR:OG1	2.24	0.54
2:B:748:GLN:HA	2:C:682:GLN:HE22	1.73	0.54
2:C:504:ASP:OD2	2:C:506:SER:OG	2.26	0.53
3:D:60:ARG:NH2	3:D:87:HIS:O	2.41	0.53
2:C:505:PRO:HG2	2:C:677:ARG:HB2	1.89	0.53
2:B:892:VAL:HG12	2:B:894:VAL:HB	1.91	0.53
2:C:640:GLN:HB2	2:C:646:ASN:HD22	1.71	0.53
1:A:572:LEU:HB3	1:A:584:ILE:HD13	1.89	0.53
2:C:611:GLY:HA3	2:C:635:ILE:O	2.08	0.53
1:A:44:SER:O	1:A:45:GLN:HB2	2.09	0.53
1:A:170:ASN:OD1	1:A:172:PHE:N	2.42	0.53
2:B:674:LYS:HA	2:B:677:ARG:HD3	1.90	0.53
2:C:252:LEU:HD22	2:C:823:ILE:HD13	1.90	0.53
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.90	0.53
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.91	0.53
3:E:176:ARG:HG3	3:E:253:GLU:HB3	1.90	0.53
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.90	0.53
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.90	0.52
1:A:541:LYS:HG2	1:A:975:THR:HG21	1.90	0.52
2:B:217:THR:HB	2:B:219:ILE:HG13	1.91	0.52
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.91	0.52
2:C:865:ILE:HG12	2:C:1041:ARG:HG2	1.91	0.52
1:A:161:TYR:CD2	2:B:1333:ALA:HB1	2.45	0.52
2:B:261:ASP:OD1	2:B:263:ARG:NE	2.41	0.52
2:B:813:LEU:HD11	2:B:1008:LEU:HD13	1.91	0.52
3:E:66:VAL:HG11	3:E:92:ARG:HG3	1.91	0.52
1:A:486:THR:HB	1:A:489:SER:HB3	1.92	0.52
2:C:439:VAL:HG11	2:C:705:VAL:HG21	1.92	0.52
3:D:229:PHE:CE1	3:D:252:LEU:HD11	2.44	0.52
2:C:707:ALA:HB2	2:C:1330:ILE:HG23	1.92	0.52
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.45	0.52
2:B:328:GLY:HA3	2:B:347:ALA:H	1.74	0.52
2:C:495:LEU:HD13	2:C:532:ILE:HG13	1.92	0.52
2:C:156:GLN:HE22	2:C:1309:ILE:H	1.58	0.52
1:A:775:ASP:OD1	1:A:776:SER:N	2.42	0.51
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.91	0.51
1:A:267:THR:OG1	1:A:320:TYR:OH	2.26	0.51
1:A:379:VAL:HG21	1:A:794:LEU:HD13	1.90	0.51
2:C:828:ASP:OD2	2:C:862:ARG:NH2	2.44	0.51
2:C:633:THR:HG21	2:C:710:SER:CB	2.40	0.51
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.92	0.51
2:C:1116:ARG:HG2	2:C:1116:ARG:NH1	2.23	0.51
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.45	0.51
2:B:299:ALA:HB2	2:B:1265:MET:HB3	1.92	0.51
2:B:1134:ARG:NH1	2:B:1158:SER:OG	2.40	0.51
2:C:676:THR:O	2:C:680:THR:HG23	2.11	0.51
3:D:233:THR:HB	3:D:268:THR:HG21	1.93	0.51
1:A:831:ARG:NH1	1:A:832:GLU:OE2	2.44	0.51
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.44	0.50
2:B:550:ILE:HG22	2:B:594:LEU:HD21	1.93	0.50
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.26	0.50
2:B:1288:ILE:HG12	3:D:20:ARG:NH2	2.26	0.50
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.46	0.50
1:A:860:SER:HA	1:A:920:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.94	0.50
1:A:887:ILE:HG13	1:A:899:VAL:HG21	1.93	0.50
2:B:357:VAL:HG13	2:B:1054:ARG:HG2	1.92	0.50
2:B:513:GLU:OE2	2:B:760:THR:OG1	2.23	0.50
2:B:1087:ASP:OD2	2:B:1237:SER:OG	2.28	0.50
1:A:539:LEU:HG	1:A:647:LEU:HD12	1.93	0.50
2:B:766:ILE:O	2:B:772:TYR:OH	2.25	0.50
2:B:874:ILE:HD11	2:B:917:VAL:HG13	1.93	0.50
2:C:382:HIS:HE2	2:C:713:MET:H	1.60	0.50
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.94	0.50
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.12	0.50
3:D:19:ILE:HD12	3:D:19:ILE:O	2.12	0.50
1:A:18:LYS:HA	1:A:112:ARG:HA	1.94	0.50
2:C:748:GLN:HG3	2:C:1000:LEU:HD22	1.92	0.50
2:C:828:ASP:OD1	2:C:828:ASP:N	2.45	0.50
1:A:42:PHE:CE1	1:A:47:ARG:HA	2.47	0.49
1:A:371:GLY:N	1:A:818:PHE:O	2.42	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.93	0.49
3:D:176:ARG:HD3	3:D:253:GLU:HB3	1.94	0.49
3:E:1:MET:HB2	3:E:121:PHE:CE2	2.48	0.49
3:E:221:ARG:O	3:E:225:ARG:HG3	2.11	0.49
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.93	0.49
2:B:990:THR:O	2:B:992:VAL:HG23	2.12	0.49
2:C:522:PRO:HB3	2:C:609:PRO:HB3	1.93	0.49
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.94	0.49
1:A:391:ILE:HD11	1:A:757:LEU:HD22	1.95	0.49
1:A:939:GLN:HB2	1:A:998:LEU:HD21	1.95	0.49
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.12	0.49
1:A:275:ILE:HA	1:A:278:LEU:HD12	1.95	0.49
1:A:557:SER:N	1:A:611:ASP:OD1	2.29	0.49
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	1.93	0.49
2:C:633:THR:HG21	2:C:710:SER:HB2	1.94	0.49
2:C:865:ILE:HD12	2:C:1042:TRP:HE3	1.77	0.49
2:C:1042:TRP:HD1	2:C:1044:ARG:HG2	1.77	0.49
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.94	0.49
3:D:148:ASP:OD2	3:D:151:ASP:N	2.41	0.49
3:E:159:GLU:O	3:E:225:ARG:HG2	2.13	0.49
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.13	0.49
2:C:225:ILE:HB	2:C:247:TYR:HD1	1.78	0.49
2:C:354:ALA:O	2:C:358:LEU:HG	2.12	0.49
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1230:ILE:HG12	2:C:119:ASP:HA	1.95	0.49
2:C:164:LEU:HD23	2:C:208:LEU:HA	1.95	0.49
2:B:1150:LEU:HD23	2:C:141:LEU:HD22	1.95	0.49
2:C:503:GLU:O	2:C:666:ARG:NH2	2.39	0.48
1:A:163:ASP:HB3	1:A:180:ASN:ND2	2.28	0.48
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.48
2:B:558:TYR:HB3	2:B:568:PHE:CD2	2.47	0.48
2:B:1214:GLU:HG2	2:B:1215:PRO:HD2	1.95	0.48
3:D:57:PRO:HD3	3:D:139:ASN:ND2	2.28	0.48
2:C:85:ASP:HB2	2:C:161:LYS:HE2	1.96	0.48
2:C:248:VAL:HG11	2:C:971:MET:HG2	1.95	0.48
2:C:525:PHE:CE1	2:C:532:ILE:HD13	2.48	0.48
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.69	0.48
2:C:862:ARG:O	2:C:865:ILE:HG22	2.13	0.48
2:B:330:THR:OG1	2:B:331:GLU:N	2.47	0.48
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.95	0.48
2:B:1189:ASP:HA	2:C:118:THR:HG22	1.96	0.48
2:C:168:VAL:HG11	2:C:196:LEU:HG	1.94	0.48
2:B:419:TYR:HB3	2:B:1005:LEU:HD22	1.95	0.48
1:A:717:THR:HB	1:A:1020:SER:HB2	1.96	0.48
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.95	0.48
2:C:286:LEU:HD11	2:C:290:TYR:HB3	1.96	0.48
2:C:616:ASP:O	2:C:620:ILE:HG13	2.13	0.48
1:A:2:TRP:HD1	1:A:3:HIS:H	1.57	0.48
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.27	0.48
2:C:526:ASN:OD1	2:C:529:LYS:NZ	2.42	0.48
2:C:1090:PRO:HD3	2:C:1231:TYR:CD2	2.49	0.48
2:B:213:PHE:HB3	2:B:219:ILE:HD12	1.96	0.48
2:B:634:TYR:CE1	2:B:722:GLY:HA3	2.49	0.48
2:B:995:THR:O	2:B:998:GLY:N	2.45	0.48
2:C:422:LEU:HD13	2:C:810:LEU:HD11	1.96	0.48
3:D:26:ALA:HB1	3:D:30:GLN:HG3	1.96	0.48
1:A:377:LEU:HB3	1:A:763:LYS:HB3	1.96	0.48
2:C:704:VAL:HB	2:C:1330:ILE:HD11	1.96	0.48
1:A:43:ASN:HD21	1:A:46:ARG:HD2	1.77	0.47
1:A:724:MET:HG3	1:A:725:PRO:HD2	1.95	0.47
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.96	0.47
2:B:1159:VAL:HA	2:B:1164:TRP:HB2	1.97	0.47
2:C:626:ARG:HG2	2:C:631:PRO:HB3	1.96	0.47
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.14	0.47
1:A:426:ARG:HG3	1:A:707:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:THR:HG23	1:A:980:ILE:HG12	1.97	0.47
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.48	0.47
1:A:43:ASN:ND2	1:A:46:ARG:HD2	2.29	0.47
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.96	0.47
1:A:39:LEU:HD11	1:A:52:ARG:HH11	1.79	0.47
2:C:380:GLN:HB3	2:C:618:LEU:HD22	1.97	0.47
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.46	0.47
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	1.97	0.47
2:C:1073:GLY:HA2	2:C:1168:ILE:O	2.13	0.47
3:E:229:PHE:O	3:E:233:THR:HG23	2.15	0.47
1:A:6:SER:HB2	1:A:251:VAL:O	2.15	0.47
1:A:275:ILE:HD11	1:A:300:LEU:HD22	1.97	0.47
1:A:531:LYS:HD3	1:A:683:GLN:HG2	1.97	0.47
2:B:313:ASP:OD2	2:B:1253:ARG:NH1	2.48	0.47
2:B:886:SER:O	2:B:890:THR:HG23	2.14	0.47
2:B:992:VAL:O	2:B:993:ASP:HB2	2.15	0.47
2:C:119:ASP:OD1	2:C:119:ASP:N	2.47	0.47
2:C:197:PHE:HB2	2:C:301:LEU:HD21	1.96	0.47
3:D:78:GLY:O	3:D:275:ARG:NH2	2.47	0.47
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.97	0.47
2:B:1268:GLY:HA3	2:B:1277:LEU:O	2.14	0.47
2:C:629:ARG:HA	2:C:1037:ILE:HG22	1.96	0.47
1:A:289:ASP:OD1	1:A:368:THR:OG1	2.30	0.47
2:B:270:THR:HG22	2:B:291:HIS:HA	1.97	0.47
2:B:512:LEU:HD13	2:B:659:LEU:HD12	1.97	0.47
2:B:522:PRO:HB3	2:B:609:PRO:HB3	1.96	0.47
2:B:612:PHE:CD1	2:B:638:THR:HG22	2.49	0.47
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.49	0.47
2:C:713:MET:HB2	2:C:713:MET:HE2	1.75	0.47
3:D:93:LEU:HD12	3:D:93:LEU:HA	1.74	0.47
2:B:153:ASP:OD1	2:B:153:ASP:N	2.43	0.46
2:B:720:PHE:CE2	2:B:722:GLY:HA2	2.50	0.46
3:D:17:PHE:HB3	3:D:196:TRP:CE2	2.50	0.46
1:A:302:ASP:O	1:A:306:GLN:HB2	2.16	0.46
1:A:812:VAL:HA	1:A:813:PRO:HA	1.70	0.46
2:B:141:LEU:HD22	2:B:391:GLY:HA3	1.97	0.46
2:B:287:ARG:NH2	2:B:326:GLY:HA3	2.30	0.46
2:C:856:LEU:HD23	2:C:860:ARG:HD3	1.98	0.46
3:D:45:VAL:HG13	3:D:171:VAL:HG12	1.98	0.46
2:B:1180:PRO:HA	2:B:1207:MET:SD	2.55	0.46
2:C:1180:PRO:HD3	2:C:1208:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:281:LYS:O	3:D:285:LEU:HG	2.15	0.46
2:B:347:ALA:HA	2:B:1301:VAL:HA	1.97	0.46
2:B:832:MET:SD	2:B:946:LEU:HG	2.55	0.46
2:C:495:LEU:HD23	2:C:497:LYS:HA	1.98	0.46
2:C:524:GLU:OE1	2:C:758:ILE:HG12	2.15	0.46
1:A:78:TYR:HB3	1:A:79:PRO:HA	1.98	0.46
2:C:332:THR:HG22	2:C:334:LEU:H	1.81	0.46
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.98	0.46
2:B:446:LYS:HB3	2:B:448:TYR:HD2	1.80	0.46
2:B:833:ARG:HG3	2:B:922:TYR:CZ	2.50	0.46
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.78	0.46
2:B:873:TYR:HA	2:B:896:LEU:O	2.16	0.46
2:B:949:ALA:HB1	2:B:960:THR:HG22	1.98	0.46
2:B:1106:PHE:CE2	2:B:1119:TYR:HB2	2.51	0.46
2:B:1176:GLU:HB2	2:B:1203:HIS:HE2	1.81	0.46
2:B:854:GLN:NE2	2:C:647:GLU:OE1	2.48	0.46
2:C:1031:TYR:CE2	2:C:1041:ARG:HG3	2.51	0.46
1:A:438:LYS:NZ	1:A:626:GLU:OE2	2.47	0.45
2:B:196:LEU:HD22	2:B:296:VAL:HG11	1.98	0.45
2:B:525:PHE:CE1	2:B:532:ILE:HD13	2.51	0.45
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.97	0.45
1:A:129:PRO:CG	2:B:1332:ASN:HB2	2.46	0.45
2:B:489:MET:SD	2:B:527:ARG:HD2	2.56	0.45
2:B:515:ILE:HD12	2:B:659:LEU:HD11	1.97	0.45
2:C:615:THR:HB	2:C:1333:ALA:HB1	1.97	0.45
3:D:29:THR:HG22	3:D:222:ASP:HB2	1.98	0.45
3:E:137:LEU:HD23	3:E:281:LYS:HG3	1.98	0.45
2:B:384:MET:HA	2:B:708:THR:CG2	2.45	0.45
2:B:510:VAL:O	2:B:513:GLU:HB3	2.16	0.45
2:B:1075:ARG:HB2	2:B:1233:LEU:HD11	1.98	0.45
2:C:979:ILE:HD13	2:C:1013:LYS:HB2	1.98	0.45
3:D:53:GLU:CD	3:D:53:GLU:H	2.20	0.45
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.99	0.45
1:A:201:LYS:O	2:B:629:ARG:HG2	2.16	0.45
1:A:613:ILE:HG21	1:A:639:CYS:HB3	1.98	0.45
2:B:309:TRP:CZ2	2:B:1257:ALA:HB1	2.50	0.45
3:E:146:ARG:NH1	3:E:277:GLU:OE2	2.49	0.45
1:A:735:LYS:O	1:A:765:TYR:OH	2.24	0.45
1:A:1020:SER:OG	1:A:1022:PRO:HD2	2.15	0.45
2:B:609:PRO:HD3	2:B:724:HIS:CD2	2.52	0.45
1:A:428:ILE:HG23	1:A:430:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ALA:HB2	1:A:725:PRO:HB3	1.99	0.45
2:B:1176:GLU:HB2	2:B:1203:HIS:NE2	2.32	0.45
2:C:311:ASN:O	2:C:315:THR:HB	2.16	0.45
1:A:474:TYR:HD1	1:A:499:VAL:HG22	1.81	0.45
1:A:722:ASP:OD1	1:A:722:ASP:N	2.44	0.45
2:B:287:ARG:HB2	2:B:329:LEU:O	2.16	0.45
2:C:405:HIS:ND1	2:C:625:PRO:HA	2.31	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:777:GLN:O	2:B:786:SER:N	2.49	0.45
2:C:1110:LEU:HD23	2:C:1110:LEU:HA	1.76	0.45
1:A:268:TYR:O	1:A:271:ARG:HG2	2.17	0.45
2:B:370:VAL:HG21	2:B:402:ALA:HB2	1.98	0.45
2:B:449:PHE:CE1	2:B:463:VAL:HG22	2.51	0.45
2:C:585:PHE:CE1	2:C:728:LYS:HE2	2.52	0.45
2:C:775:VAL:HA	2:C:776:ARG:HA	1.72	0.45
1:A:42:PHE:HE1	1:A:47:ARG:HA	1.82	0.45
1:A:280:PRO:HB3	1:A:304:TYR:CE2	2.52	0.45
1:A:1007:LEU:HD12	1:A:1007:LEU:HA	1.86	0.45
2:B:502:PHE:CE1	2:B:539:PHE:HB2	2.52	0.45
2:B:619:ALA:HB2	2:B:711:ASN:HA	1.98	0.45
2:B:813:LEU:HG	2:B:1010:ARG:HH11	1.82	0.45
2:C:264:LEU:HD21	2:C:362:LEU:HA	1.99	0.45
1:A:25:ILE:HD12	1:A:25:ILE:HA	1.82	0.44
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.52	0.44
1:A:857:GLN:HB3	1:A:877:LYS:HG3	1.98	0.44
1:A:1007:LEU:HD21	1:A:1053:ILE:HG21	1.99	0.44
2:C:999:LYS:HG2	2:C:1009:THR:HA	1.99	0.44
1:A:315:LEU:O	1:A:319:MET:HG3	2.17	0.44
2:C:332:THR:HG23	2:C:1270:LEU:HD12	2.00	0.44
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.49	0.44
2:C:605:ARG:O	2:C:608:THR:HG23	2.18	0.44
2:C:1249:ASN:HB3	2:C:1250:GLU:H	1.65	0.44
2:C:186:ASP:O	2:C:190:VAL:HB	2.17	0.44
2:C:962:ASP:OD1	2:C:962:ASP:N	2.48	0.44
1:A:7:ILE:HD11	1:A:250:LEU:HD21	1.98	0.44
1:A:417:TYR:CD2	1:A:490:LEU:HD22	2.52	0.44
2:B:347:ALA:HB2	2:B:1301:VAL:HG22	1.98	0.44
2:C:1085:ASP:HA	2:C:1086:PRO:HD3	1.88	0.44
1:A:50:THR:HA	1:A:170:ASN:ND2	2.33	0.44
1:A:491:ASP:HA	1:A:494:THR:HG22	1.99	0.44
2:B:933:ASN:HB3	2:B:935:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.16	0.44
1:A:43:ASN:HB3	1:A:48:SER:OG	2.16	0.44
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.52	0.44
1:A:154:PHE:CD2	1:A:185:HIS:HA	2.52	0.44
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.49	0.44
1:A:470:LEU:HD21	1:A:530:MET:HE2	2.00	0.44
1:A:485:MET:HB2	1:A:491:ASP:OD1	2.18	0.44
2:B:649:ALA:HB1	2:B:692:ASP:OD1	2.17	0.44
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.80	0.44
3:E:68:ILE:HA	3:E:68:ILE:HD12	1.89	0.44
1:A:196:LEU:HD13	1:A:349:TYR:CE1	2.52	0.44
2:B:186:ASP:O	2:B:190:VAL:HB	2.17	0.44
1:A:400:VAL:HG22	1:A:774:VAL:HG21	1.99	0.44
1:A:680:THR:HG23	1:A:682:SER:N	2.30	0.44
2:B:169:LYS:O	2:B:202:ALA:N	2.47	0.44
2:B:685:ARG:O	2:B:689:THR:HG23	2.18	0.44
2:B:953:ASP:OD1	2:B:960:THR:OG1	2.34	0.44
2:C:478:ILE:HG13	2:C:762:ILE:HD11	1.98	0.44
2:C:1236:ILE:HD13	2:C:1236:ILE:HA	1.85	0.44
3:E:53:GLU:CD	3:E:53:GLU:H	2.21	0.44
3:E:104:ARG:NH2	3:E:115:GLU:OE2	2.50	0.44
1:A:11:THR:OG1	1:A:254:ASP:OD2	2.36	0.44
1:A:328:MET:HB2	1:A:328:MET:HE2	1.81	0.44
1:A:913:LEU:HD22	1:A:919:TYR:CZ	2.53	0.44
3:E:258:ASN:ND2	3:E:260:MET:SD	2.90	0.44
1:A:154:PHE:HZ	1:A:183:ILE:HB	1.82	0.43
1:A:467:SER:N	1:A:468:PRO:HD2	2.33	0.43
1:A:823:THR:OG1	1:A:825:GLU:OE1	2.36	0.43
3:E:283:LEU:O	3:E:287:PHE:HB2	2.17	0.43
1:A:615:CYS:HB2	1:A:639:CYS:SG	2.58	0.43
2:B:171:GLU:OE2	2:B:174:PHE:N	2.51	0.43
2:C:502:PHE:O	2:C:542:ARG:HG2	2.18	0.43
1:A:844:LEU:HD11	1:A:1017:ILE:HD12	2.00	0.43
2:B:826:GLY:HA3	2:B:949:ALA:HB2	2.00	0.43
2:B:893:ALA:HB1	2:B:915:VAL:HA	2.00	0.43
2:C:152:ASP:OD1	2:C:152:ASP:N	2.50	0.43
2:C:439:VAL:HG23	2:C:440:ILE:HG22	2.01	0.43
2:C:865:ILE:CG1	2:C:1041:ARG:HG2	2.49	0.43
2:C:1015:GLN:H	2:C:1015:GLN:HG2	1.44	0.43
2:C:1121:HIS:CD2	2:C:1123:PRO:HG2	2.53	0.43
1:A:1043:LEU:O	1:A:1047:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.70	0.43
3:D:60:ARG:O	3:D:62:VAL:HG23	2.18	0.43
1:A:532:MET:HG3	1:A:565:ARG:HD2	2.01	0.43
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.99	0.43
3:D:178:LYS:HA	3:D:250:ARG:O	2.19	0.43
3:D:253:GLU:HA	3:D:254:TYR:HA	1.58	0.43
3:D:283:LEU:HA	3:D:286:THR:HG22	2.00	0.43
1:A:485:MET:HG2	1:A:511:ILE:HD11	1.99	0.43
2:B:617:ASP:OD1	2:B:618:LEU:N	2.51	0.43
2:B:1059:LEU:HD23	2:B:1059:LEU:HA	1.81	0.43
2:C:865:ILE:HD12	2:C:1042:TRP:CE3	2.52	0.43
1:A:95:TRP:O	1:A:98:SER:HB3	2.18	0.43
1:A:734:ILE:HD13	1:A:762:LEU:HD13	2.00	0.43
1:A:882:ASP:OD1	1:A:882:ASP:N	2.52	0.43
2:B:409:ILE:HD13	2:B:625:PRO:HB2	2.01	0.43
2:C:265:VAL:HB	2:C:1304:MET:HB3	2.00	0.43
2:C:340:VAL:HG23	2:C:341:LYS:HG2	2.00	0.43
2:C:685:ARG:O	2:C:689:THR:HG23	2.18	0.43
2:C:811:SER:O	2:C:815:LEU:HB2	2.19	0.43
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.00	0.43
1:A:312:LEU:HD11	1:A:361:SER:HB3	2.00	0.43
1:A:767:SER:N	1:A:788:ASP:OD1	2.52	0.43
2:C:736:SER:HB2	2:C:738:GLU:OE1	2.19	0.43
2:C:1116:ARG:HH22	2:C:1131:PRO:HD2	1.84	0.43
3:E:176:ARG:NH1	3:E:253:GLU:OE2	2.45	0.43
1:A:34:LEU:HG	1:A:38:TYR:CZ	2.54	0.43
1:A:289:ASP:H	1:A:368:THR:HG23	1.84	0.43
1:A:377:LEU:HD22	1:A:768:GLU:HA	2.01	0.43
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	2.01	0.43
2:C:442:PRO:HD2	2:C:475:ILE:HG23	2.00	0.43
3:D:68:ILE:HG12	3:D:93:LEU:HD13	2.00	0.43
1:A:261:ILE:HD11	1:A:326:LEU:HD13	2.01	0.42
1:A:586:GLY:HA3	1:A:595:ASN:OD1	2.19	0.42
2:B:286:LEU:HD11	2:B:290:TYR:CD1	2.54	0.42
2:B:484:ARG:HE	2:B:524:GLU:CD	2.13	0.42
2:B:892:VAL:HG13	2:B:951:ILE:HG22	2.01	0.42
2:B:145:THR:HB	2:B:1317:VAL:HG23	2.00	0.42
2:C:154:PHE:HB3	2:C:264:LEU:HB2	2.02	0.42
2:C:504:ASP:N	2:C:504:ASP:OD1	2.48	0.42
2:C:1085:ASP:HA	2:C:1243:ARG:HH22	1.85	0.42
3:E:261:ARG:NH1	3:E:263:ALA:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LYS:HE2	1:A:690:THR:HG22	2.01	0.42
2:B:439:VAL:HG11	2:B:702:LEU:HD13	2.01	0.42
2:B:484:ARG:O	2:B:527:ARG:NH2	2.53	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.84	0.42
2:C:334:LEU:HA	2:C:334:LEU:HD23	1.77	0.42
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.59	0.42
3:D:77:PHE:HB2	3:D:194:VAL:HG23	2.02	0.42
3:D:283:LEU:O	3:D:287:PHE:HB2	2.20	0.42
1:A:556:THR:HB	1:A:611:ASP:OD2	2.20	0.42
2:B:171:GLU:HG2	2:B:1181:SER:OG	2.19	0.42
2:B:515:ILE:HG21	2:B:655:ILE:HG21	2.02	0.42
2:B:1242:MET:HG2	2:B:1260:PRO:HD3	2.01	0.42
2:C:1066:ARG:HD2	2:C:1296:ILE:HG13	2.02	0.42
2:C:1267:THR:HB	2:C:1299:SER:HB3	2.01	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.77	0.42
1:A:628:MET:O	1:A:632:THR:HG22	2.20	0.42
2:B:814:THR:HA	2:B:1010:ARG:HH12	1.84	0.42
2:B:859:ILE:H	2:B:859:ILE:HG13	1.68	0.42
1:A:565:ARG:HD3	1:A:565:ARG:HA	1.73	0.42
2:B:331:GLU:O	2:B:344:VAL:HA	2.20	0.42
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.55	0.42
2:B:838:GLU:C	2:B:935:GLN:HG2	2.40	0.42
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.34	0.42
2:B:1043:SER:HB2	2:B:1046:PHE:CE2	2.55	0.42
2:B:1128:TYR:HB3	2:B:1134:ARG:HG2	2.01	0.42
2:C:1190:ALA:O	2:C:1193:ILE:HG22	2.20	0.42
1:A:251:VAL:HG12	1:A:253:ALA:H	1.84	0.42
1:A:373:ILE:HG12	1:A:817:GLY:N	2.35	0.42
1:A:595:ASN:HD22	1:A:595:ASN:H	1.66	0.42
1:A:936:ALA:HB1	1:A:998:LEU:HD23	2.02	0.42
2:B:664:ASN:O	2:B:668:VAL:HG13	2.20	0.42
2:B:887:VAL:O	2:B:891:HIS:N	2.51	0.42
2:B:924:ASP:O	2:B:927:SER:OG	2.33	0.42
3:D:188:SER:O	3:D:191:ARG:HG3	2.19	0.42
3:E:118:ASN:ND2	3:E:118:ASN:H	2.17	0.42
1:A:259:ARG:NH1	1:A:277:ALA:HB2	2.35	0.42
2:B:382:HIS:HD1	2:B:799:THR:HG23	1.84	0.42
2:B:491:ASN:ND2	2:B:750:GLU:O	2.53	0.42
2:C:385:ILE:HD13	2:C:385:ILE:HA	1.75	0.42
2:B:336:TYR:HA	3:D:64:GLY:HA3	2.01	0.41
2:B:533:GLN:HB2	2:B:588:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	2.01	0.41
2:C:379:LEU:HD23	2:C:379:LEU:HA	1.86	0.41
1:A:20:ASN:OD1	1:A:20:ASN:N	2.53	0.41
1:A:834:THR:O	1:A:838:LYS:HG2	2.20	0.41
2:B:1305:MET:H	2:B:1305:MET:HG2	1.65	0.41
2:C:405:HIS:CE1	2:C:625:PRO:HA	2.55	0.41
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.55	0.41
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.84	0.41
2:C:828:ASP:OD1	2:C:960:THR:OG1	2.32	0.41
3:D:1:MET:HB2	3:D:121:PHE:CZ	2.55	0.41
3:D:87:HIS:CE1	3:D:89:TYR:H	2.38	0.41
3:D:160:LEU:HB3	3:D:161:ALA:H	1.77	0.41
1:A:384:GLU:HA	1:A:802:THR:HG22	2.01	0.41
1:A:538:ALA:HB1	1:A:678:LEU:HD11	2.02	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.18	0.41
2:B:147:VAL:HG13	2:B:379:LEU:HD21	2.01	0.41
2:B:233:VAL:HA	2:B:234:PRO:HD2	1.80	0.41
2:B:814:THR:HA	2:B:1010:ARG:NH1	2.36	0.41
2:B:1224:GLY:HA2	2:C:124:GLN:HG2	2.02	0.41
2:C:256:PHE:CE2	2:C:815:LEU:HD22	2.55	0.41
2:C:451:GLU:O	2:C:452:ASN:HB2	2.20	0.41
2:C:823:ILE:O	2:C:968:ARG:HD3	2.20	0.41
3:E:182:TRP:CE3	3:E:182:TRP:N	2.88	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.20	0.41
1:A:178:PRO:HB2	1:A:179:TYR:CD1	2.55	0.41
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.90	0.41
2:B:208:LEU:HD22	2:B:213:PHE:CE2	2.55	0.41
2:B:376:ILE:HD13	2:B:379:LEU:HD12	2.01	0.41
2:B:537:LEU:HD22	2:B:537:LEU:HA	1.93	0.41
2:C:264:LEU:HD22	2:C:264:LEU:HA	1.87	0.41
2:C:659:LEU:O	2:C:663:VAL:HG23	2.20	0.41
1:A:132:GLN:H	1:A:132:GLN:HG2	1.70	0.41
1:A:309:ASN:OD1	1:A:311:GLN:HG3	2.20	0.41
1:A:461:ARG:HH21	1:A:684:ASN:CG	2.23	0.41
1:A:882:ASP:HA	1:A:883:PRO:HD3	1.95	0.41
2:B:397:LEU:HA	2:B:1309:ILE:HD13	2.02	0.41
2:B:640:GLN:HE22	2:B:647:GLU:HB3	1.86	0.41
2:C:382:HIS:ND1	2:C:799:THR:HG23	2.35	0.41
2:C:1233:LEU:HD13	2:C:1233:LEU:HA	1.77	0.41
3:E:281:LYS:O	3:E:285:LEU:HG	2.21	0.41
1:A:684:ASN:HA	1:A:685:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:O	2:B:1267:THR:HG22	2.21	0.41
2:C:412:LEU:HD23	2:C:412:LEU:HA	1.80	0.41
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.92	0.41
2:C:635:ILE:HA	2:C:636:PRO:HD3	1.89	0.41
2:C:836:GLN:N	2:C:836:GLN:OE1	2.54	0.41
3:E:9:TYR:H	3:E:204:ASP:CG	2.24	0.41
3:E:93:LEU:HA	3:E:93:LEU:HD23	1.69	0.41
3:E:182:TRP:NE1	3:E:185:SER:HA	2.35	0.41
1:A:73:ARG:O	1:A:76:LEU:HB3	2.21	0.41
1:A:557:SER:HB3	1:A:583:ARG:HB2	2.01	0.41
2:B:1050:LEU:HA	2:B:1050:LEU:HD23	1.83	0.41
2:B:1219:ASP:HA	2:B:1220:PRO:HD3	1.86	0.41
2:C:648:PHE:HB2	2:C:699:THR:HG21	2.03	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.83	0.41
1:A:177:THR:HA	1:A:178:PRO:HD3	1.93	0.41
1:A:271:ARG:HE	1:A:271:ARG:HB3	1.66	0.41
1:A:583:ARG:HH11	1:A:583:ARG:H	1.68	0.41
1:A:647:LEU:HD22	1:A:691:TYR:HB3	2.03	0.41
2:B:353:PHE:CD2	2:B:1061:LEU:HD23	2.56	0.41
2:B:415:ALA:O	2:B:419:TYR:N	2.45	0.41
2:B:612:PHE:HZ	2:B:1330:ILE:HG22	1.86	0.41
2:B:635:ILE:HA	2:B:636:PRO:HD3	1.83	0.41
2:B:1074:VAL:HG22	2:B:1171:ILE:HD12	2.03	0.41
2:C:583:GLU:CD	2:C:583:GLU:H	2.24	0.41
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.56	0.41
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.95	0.41
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.21	0.41
3:D:9:TYR:H	3:D:204:ASP:CG	2.23	0.41
1:A:616:ASP:OD1	1:A:691:TYR:OH	2.31	0.41
1:A:633:ILE:HD13	1:A:633:ILE:HA	1.87	0.41
2:B:802:GLN:HB2	2:B:997:TYR:CE2	2.56	0.41
2:B:1002:LEU:HD23	2:B:1002:LEU:HA	1.87	0.41
2:C:403:PHE:CE2	2:C:625:PRO:HD3	2.56	0.41
2:C:876:GLY:O	2:C:903:ASN:ND2	2.51	0.41
3:D:19:ILE:H	3:D:19:ILE:HG13	1.66	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.87	0.40
2:B:817:ASP:OD1	2:B:821:ASN:ND2	2.55	0.40
2:B:1044:ARG:HH22	2:B:1049:GLU:CD	2.24	0.40
3:E:273:LEU:O	3:E:277:GLU:HG3	2.21	0.40
1:A:951:LEU:HD12	1:A:951:LEU:HA	1.94	0.40
2:C:475:ILE:H	2:C:475:ILE:HG13	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:833:ARG:HG3	2:C:922:TYR:CE1	2.56	0.40
2:C:1134:ARG:HB3	2:C:1135:PRO:HD2	2.03	0.40
3:E:109:GLY:HA2	3:E:199:LEU:HD12	2.02	0.40
1:A:431:ALA:O	1:A:435:ILE:HG12	2.22	0.40
2:B:177:LYS:HD3	2:B:177:LYS:O	2.22	0.40
2:C:166:TYR:HA	2:C:205:ASN:O	2.22	0.40
2:C:331:GLU:HA	2:C:335:ASP:OD2	2.22	0.40
2:C:956:ASP:O	2:C:1044:ARG:NH1	2.55	0.40
2:C:1271:SER:HB3	2:C:1277:LEU:HD21	2.03	0.40
3:E:124:PRO:HA	3:E:127:VAL:HG22	2.03	0.40
3:E:189:LEU:HD12	3:E:189:LEU:HA	1.85	0.40
1:A:293:LEU:HD22	1:A:297:LEU:HG	2.02	0.40
1:A:858:VAL:HG22	1:A:918:ILE:HB	2.03	0.40
2:B:605:ARG:O	2:B:608:THR:HG23	2.21	0.40
2:B:1228:ARG:HG2	2:B:1231:TYR:CE1	2.55	0.40
2:C:509:VAL:HG22	2:C:683:TRP:CH2	2.55	0.40
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.97	0.40
1:A:13:VAL:HG23	1:A:213:TRP:HD1	1.85	0.40
1:A:764:SER:HA	1:A:795:GLU:HG3	2.04	0.40
1:A:859:VAL:HB	1:A:919:TYR:CD1	2.56	0.40
1:A:977:HIS:HB2	1:A:981:ARG:HB3	2.03	0.40
2:B:832:MET:SD	2:B:848:ARG:HB3	2.61	0.40
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.04	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%)	1011 (96%)	41 (4%)	3 (0%)	41	73
2	B	1187/1333 (89%)	1133 (96%)	49 (4%)	5 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	1246/1333 (94%)	1180 (95%)	63 (5%)	3 (0%)	47 79
3	D	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	22 57
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	41 73
All	All	4068/4620 (88%)	3889 (96%)	165 (4%)	14 (0%)	44 73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	B	1123	PRO
2	C	1267	THR
3	D	61	ASN
3	E	80	SER
2	C	1123	PRO
1	A	483	MET
2	B	503	GLU
2	B	738	GLU
1	A	350	PRO
2	C	340	VAL
2	B	1034	GLN
3	D	244	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%)	852 (90%)	90 (10%)	8 31
2	B	1038/1153 (90%)	967 (93%)	71 (7%)	16 45
2	C	1089/1153 (94%)	1011 (93%)	78 (7%)	14 44
3	D	240/379 (63%)	218 (91%)	22 (9%)	9 33
3	E	240/379 (63%)	214 (89%)	26 (11%)	6 25
All	All	3549/4007 (89%)	3262 (92%)	287 (8%)	15 39

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	13	VAL
1	A	36	THR
1	A	50	THR
1	A	76	LEU
1	A	77	LYS
1	A	88	LEU
1	A	104	VAL
1	A	105	ARG
1	A	108	ASP
1	A	112	ARG
1	A	132	GLN
1	A	133	LEU
1	A	142	ASN
1	A	157	LEU
1	A	166	ILE
1	A	183	ILE
1	A	188	THR
1	A	199	MET
1	A	202	SER
1	A	207	THR
1	A	210	SER
1	A	216	LEU
1	A	242	LYS
1	A	260	LEU
1	A	275	ILE
1	A	293	LEU
1	A	312	LEU
1	A	313	ARG
1	A	314	ARG
1	A	337	LEU
1	A	339	GLN
1	A	357	THR
1	A	360	THR
1	A	377	LEU
1	A	396	THR
1	A	401	ILE
1	A	402	THR
1	A	444	LEU
1	A	451	ARG
1	A	466	LEU
1	A	493	LEU

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	514	LEU
1	A	523	MET
1	A	583	ARG
1	A	598	VAL
1	A	599	ARG
1	A	611	ASP
1	A	613	ILE
1	A	622	ASP
1	A	628	MET
1	A	648	VAL
1	A	680	THR
1	A	697	ILE
1	A	714	ARG
1	A	719	VAL
1	A	721	ASP
1	A	742	SER
1	A	757	LEU
1	A	762	LEU
1	A	763	LYS
1	A	770	THR
1	A	774	VAL
1	A	794	LEU
1	A	823	THR
1	A	832	GLU
1	A	844	LEU
1	A	855	MET
1	A	868	ASP
1	A	872	VAL
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	905	GLN
1	A	910	ASN
1	A	914	GLU
1	A	926	MET
1	A	941	ASP
1	A	970	ARG
1	A	977	HIS
1	A	981	ARG
1	A	987	LEU
1	A	1007	LEU

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Mol	Chain	Res	Type
1	A	1013	THR
1	A	1018	ARG
1	A	1024	LEU
1	A	1034	ARG
1	A	1035	LEU
1	A	1047	ASN
2	B	147	VAL
2	B	168	VAL
2	B	217	THR
2	B	223	LYS
2	B	233	VAL
2	B	238	THR
2	B	264	LEU
2	B	265	VAL
2	B	271	THR
2	B	274	MET
2	B	287	ARG
2	B	294	VAL
2	B	323	THR
2	B	330	THR
2	B	334	LEU
2	B	335	ASP
2	B	383	SER
2	B	384	MET
2	B	397	LEU
2	B	439	VAL
2	B	451	GLU
2	B	452	ASN
2	B	457	GLN
2	B	495	LEU
2	B	533	GLN
2	B	537	LEU
2	B	546	VAL
2	B	552	VAL
2	B	567	GLU
2	B	579	LEU
2	B	633	THR
2	B	637	TYR
2	B	643	THR
2	B	654	THR
2	B	661	ASN
2	B	704	VAL

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Mol	Chain	Res	Type
2	B	708	THR
2	B	735	THR
2	B	751	THR
2	B	755	LEU
2	B	774	LEU
2	B	798	THR
2	B	809	VAL
2	B	812	LYS
2	B	815	LEU
2	B	864	HIS
2	B	890	THR
2	B	899	SER
2	B	912	GLU
2	B	945	VAL
2	B	946	LEU
2	B	1032	ASP
2	B	1052	LEU
2	B	1082	ASP
2	B	1110	LEU
2	B	1138	HIS
2	B	1159	VAL
2	B	1179	THR
2	B	1193	ILE
2	B	1212	ARG
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1237	SER
2	B	1270	LEU
2	B	1293	VAL
2	B	1294	ASP
2	B	1311	THR
2	B	1319	ARG
2	B	1320	VAL
2	B	1331	ARG
2	C	79	SER
2	C	97	GLU
2	C	98	ASN
2	C	112	THR
2	C	116	SER
2	C	120	VAL
2	C	134	THR

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Mol	Chain	Res	Type
2	C	175	THR
2	C	180	LEU
2	C	207	ASP
2	C	217	THR
2	C	243	GLN
2	C	263	ARG
2	C	264	LEU
2	C	280	THR
2	C	282	VAL
2	C	294	VAL
2	C	315	THR
2	C	323	THR
2	C	327	LEU
2	C	330	THR
2	C	340	VAL
2	C	362	LEU
2	C	373	ASP
2	C	384	MET
2	C	439	VAL
2	C	451	GLU
2	C	462	LEU
2	C	475	ILE
2	C	495	LEU
2	C	508	ILE
2	C	512	LEU
2	C	527	ARG
2	C	546	VAL
2	C	557	THR
2	C	626	ARG
2	C	630	ASN
2	C	637	TYR
2	C	638	THR
2	C	648	PHE
2	C	654	THR
2	C	656	VAL
2	C	661	ASN
2	C	704	VAL
2	C	767	LEU
2	C	769	GLN
2	C	774	LEU
2	C	776	ARG
2	C	790	GLU

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Mol	Chain	Res	Type
2	C	798	THR
2	C	828	ASP
2	C	833	ARG
2	C	851	THR
2	C	856	LEU
2	C	865	ILE
2	C	892	VAL
2	C	946	LEU
2	C	948	ILE
2	C	951	ILE
2	C	962	ASP
2	C	964	VAL
2	C	980	ARG
2	C	1014	MET
2	C	1015	GLN
2	C	1052	LEU
2	C	1055	LEU
2	C	1110	LEU
2	C	1119	TYR
2	C	1136	HIS
2	C	1148	SER
2	C	1200	LYS
2	C	1201	LEU
2	C	1202	PHE
2	C	1233	LEU
2	C	1250	GLU
2	C	1269	THR
2	C	1291	LEU
2	C	1320	VAL
3	D	2	LEU
3	D	21	ASN
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	54	THR
3	D	92	ARG
3	D	93	LEU
3	D	100	ASN
3	D	107	LEU
3	D	116	THR
3	D	130	PHE
3	D	133	THR

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Mol	Chain	Res	Type
3	D	189	LEU
3	D	191	ARG
3	D	193	VAL
3	D	194	VAL
3	D	214	ARG
3	D	226	MET
3	D	239	VAL
3	D	252	LEU
3	D	253	GLU
3	E	2	LEU
3	E	24	THR
3	E	29	THR
3	E	35	LEU
3	E	48	THR
3	E	66	VAL
3	E	93	LEU
3	E	94	SER
3	E	98	LEU
3	E	118	ASN
3	E	133	THR
3	E	139	ASN
3	E	142	THR
3	E	158	LEU
3	E	160	LEU
3	E	189	LEU
3	E	194	VAL
3	E	226	MET
3	E	240	VAL
3	E	244	VAL
3	E	247	ARG
3	E	252	LEU
3	E	262	THR
3	E	272	ASP
3	E	287	PHE
3	E	288	THR

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	49	HIS
1	A	114	ASN
1	A	595	ASN

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Mol	Chain	Res	Type
1	A	667	GLN
1	A	1030	ASN
2	B	491	ASN
2	B	1332	ASN
2	C	430	ASN
2	C	981	HIS
2	C	1051	GLN
2	C	1138	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

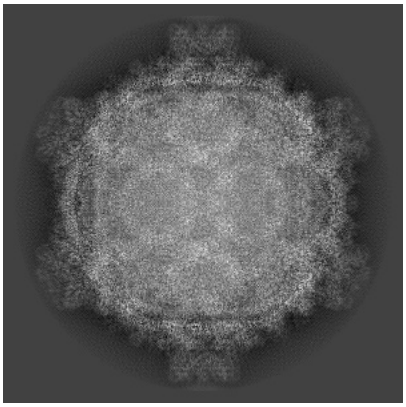
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6371. These allow visual inspection of the internal detail of the map and identification of artifacts.

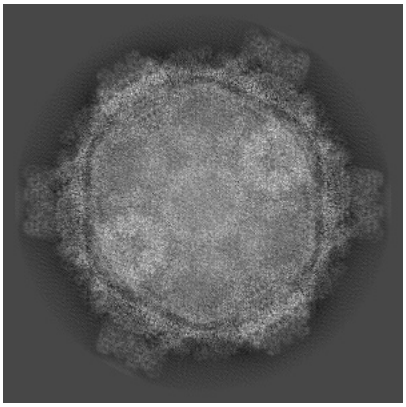
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

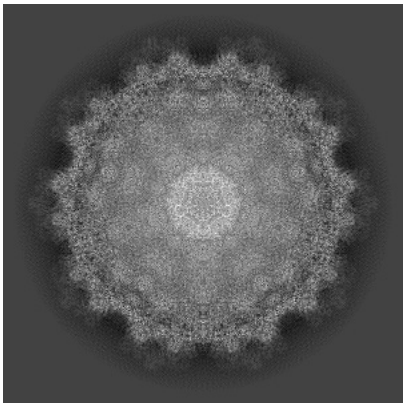
6.1.1 Primary map



X



Y

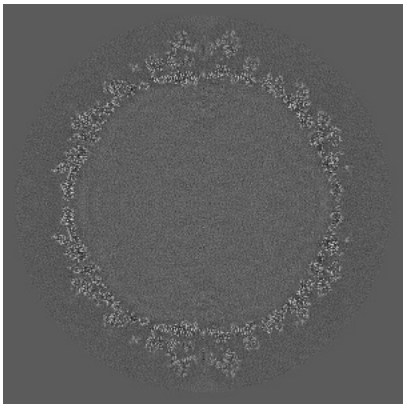


Z

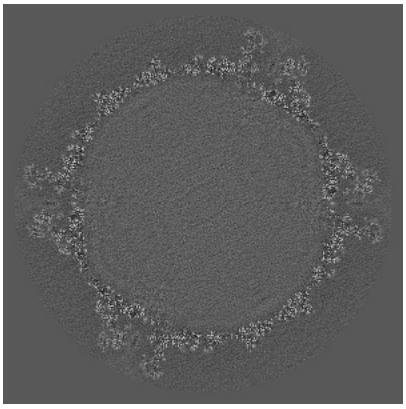
The images above show the map projected in three orthogonal directions.

6.2 Central slices

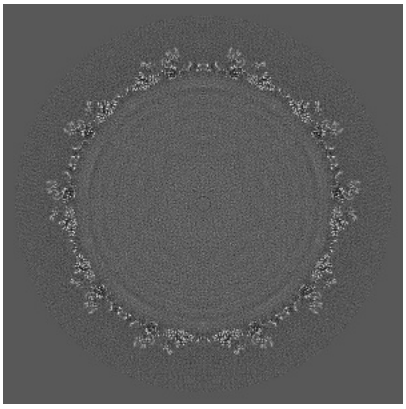
6.2.1 Primary map



X Index: 350



Y Index: 350

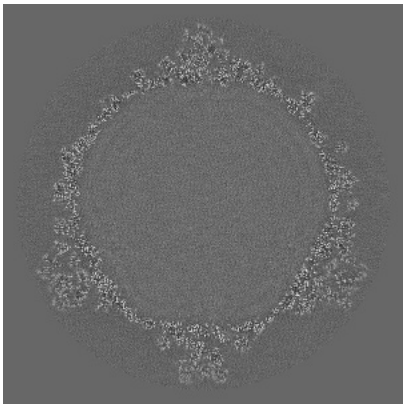


Z Index: 350

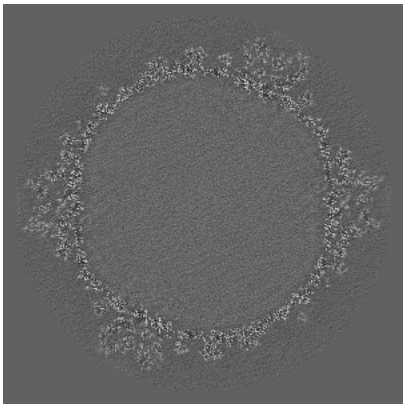
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

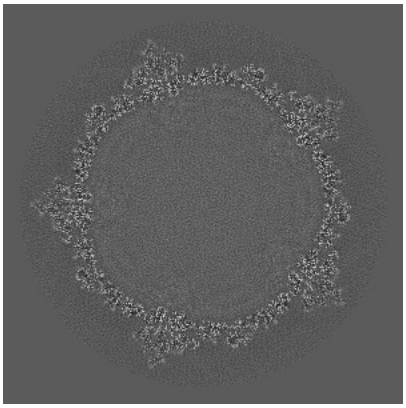
6.3.1 Primary map



X Index: 302



Y Index: 328

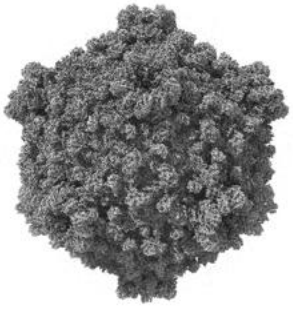


Z Index: 273

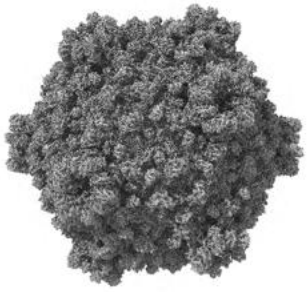
The images above show the largest variance slices of the map in three orthogonal directions.

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.

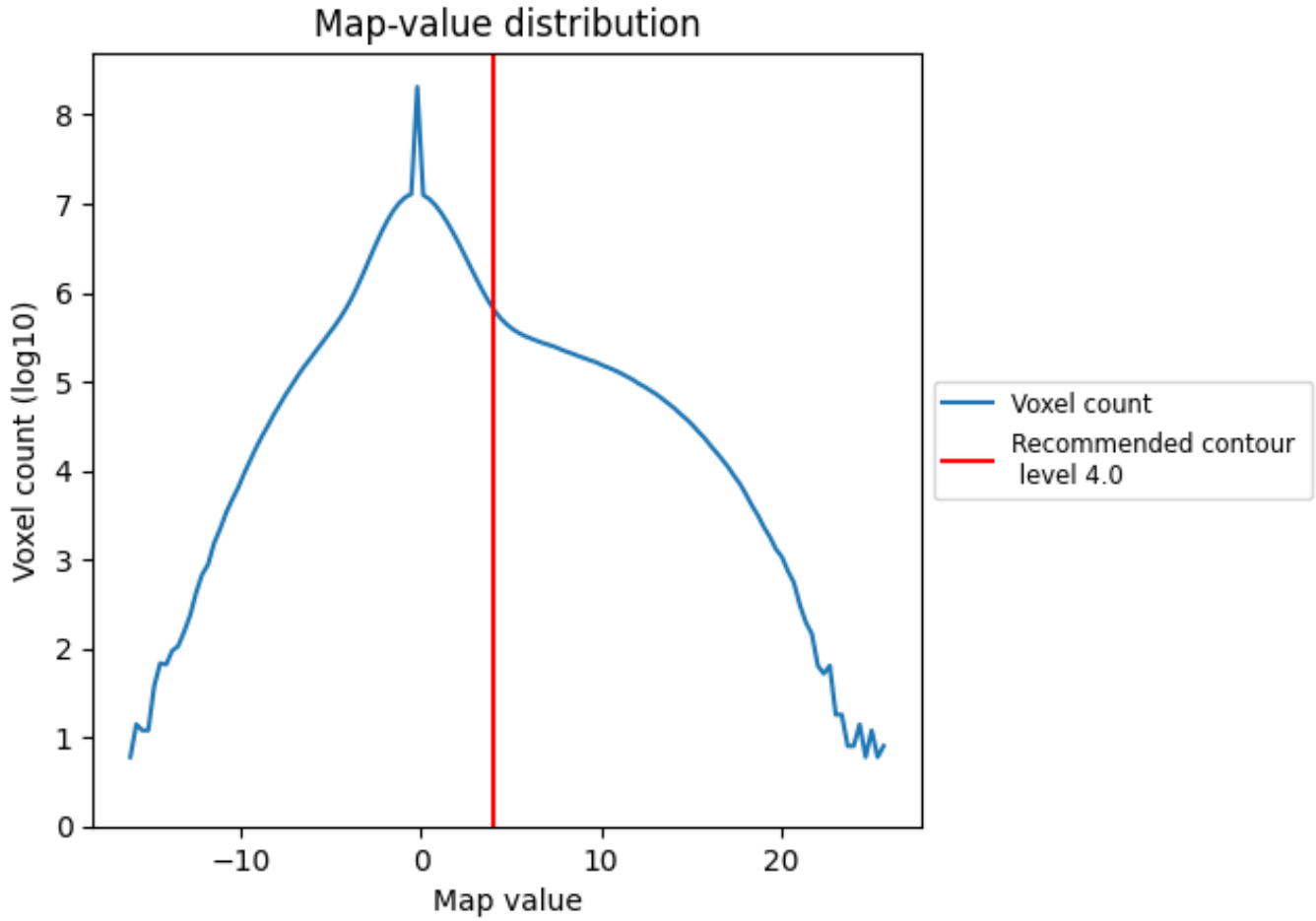
6.5 Mask visualisation (i)

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

7 Map analysis

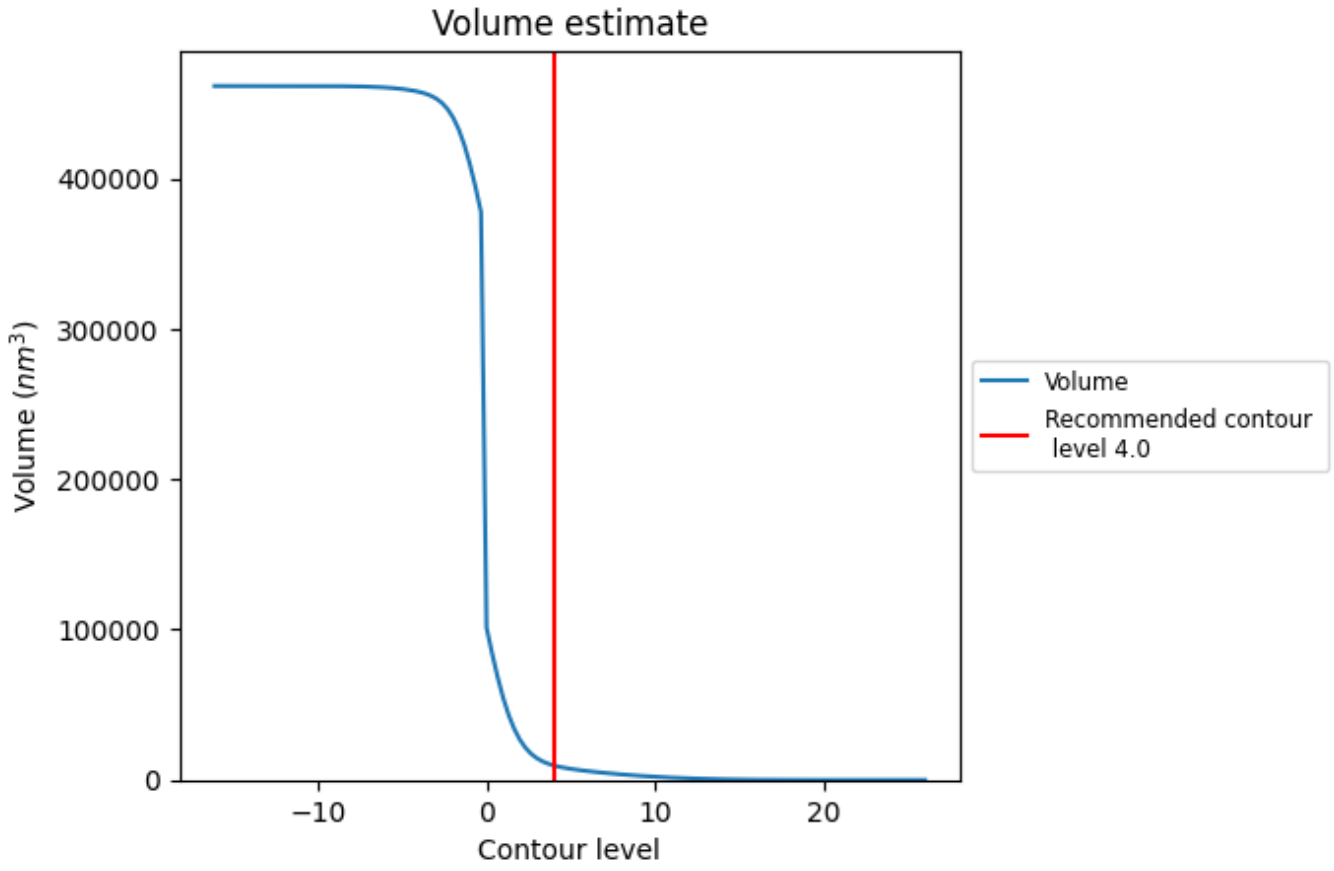
This section contains the results of statistical analysis of the map.

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.

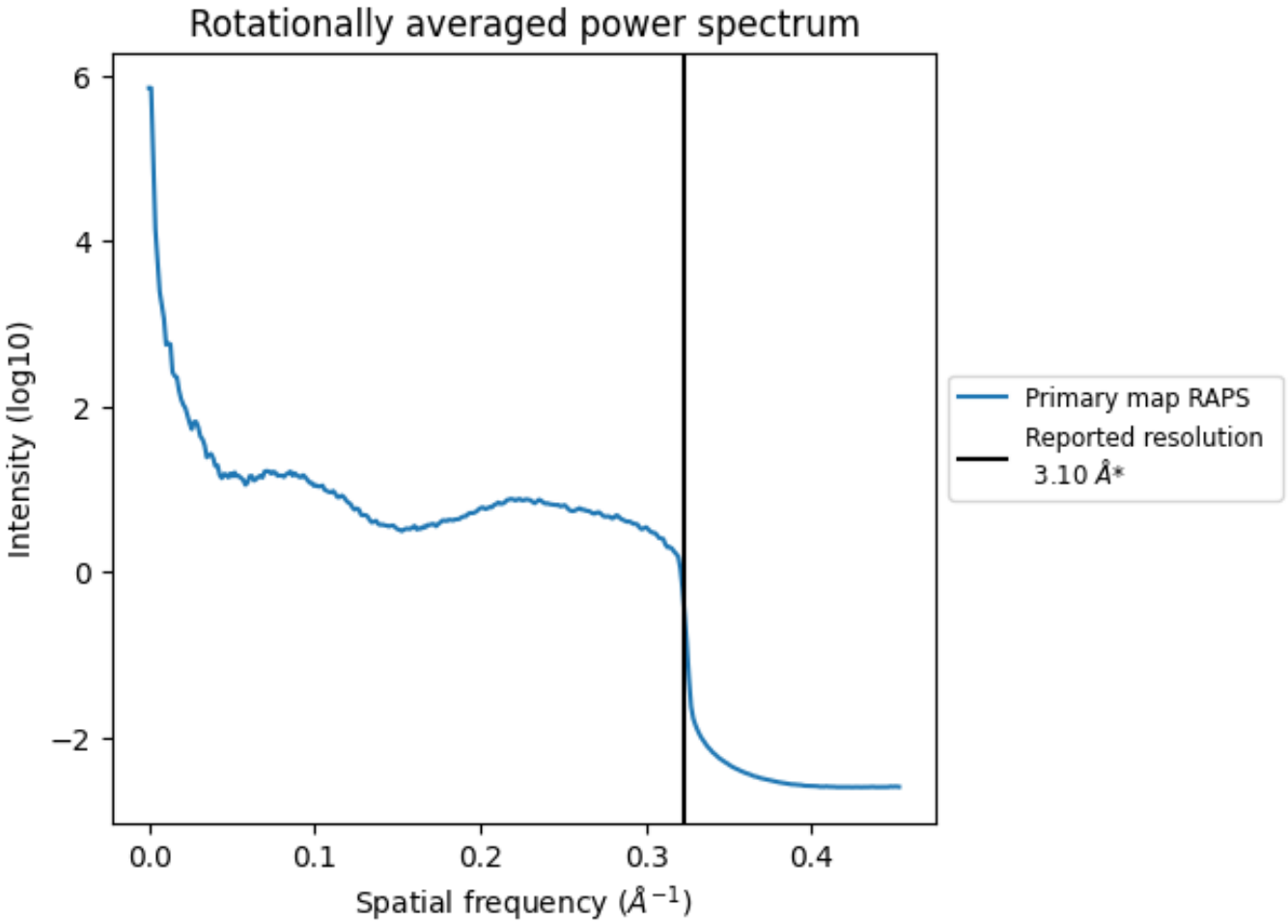
7.2 Volume estimate



The volume at the recommended contour level is 9600 nm^3; this corresponds to an approximate mass of 8672 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

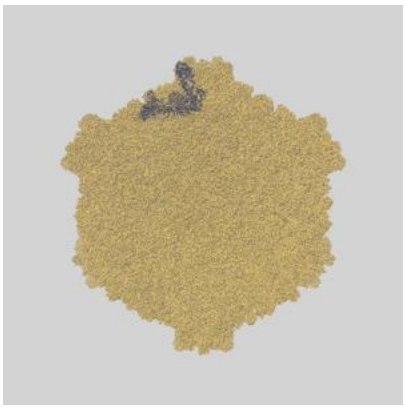
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

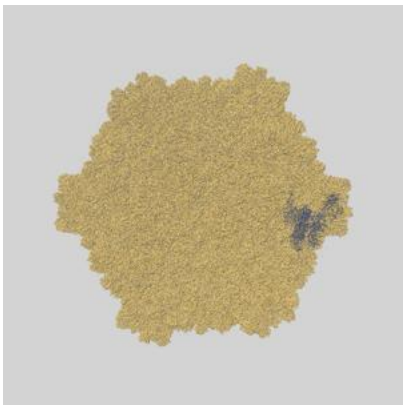
This section contains information regarding the fit between EMDB map EMD-6371 and PDB model 3JAZ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

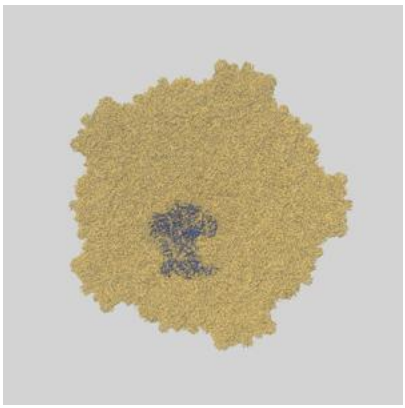
9.1.1 Map-model overlay



X

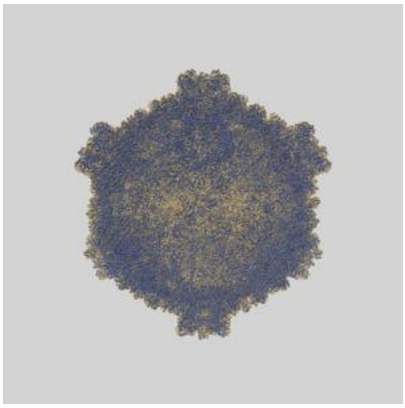


Y

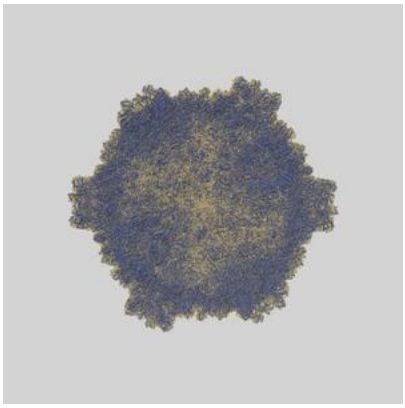


Z

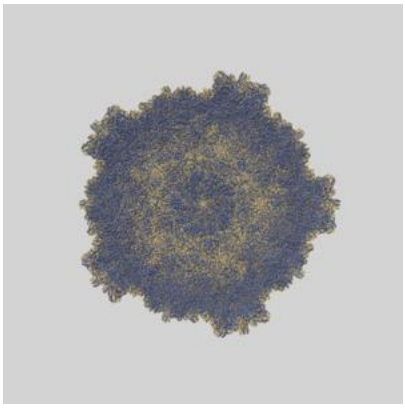
9.1.2 Map-model assembly overlay



X



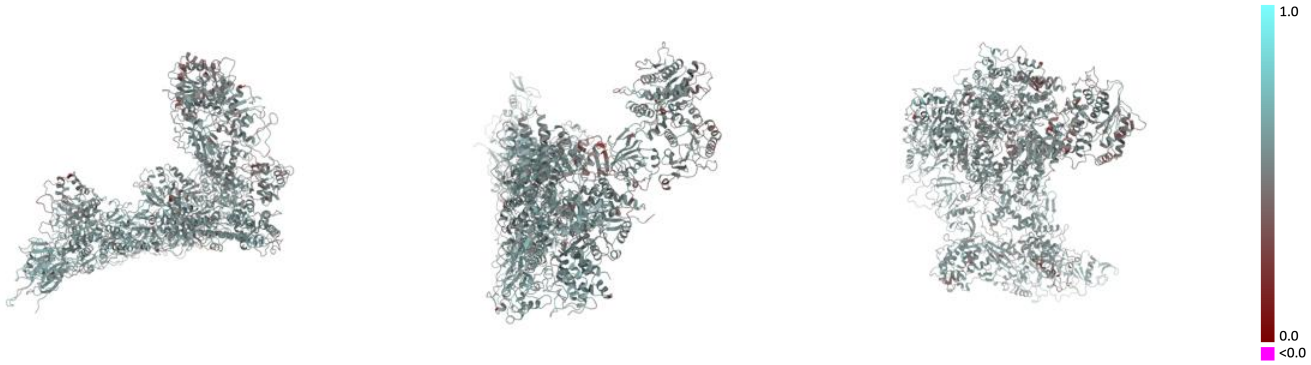
Y



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.

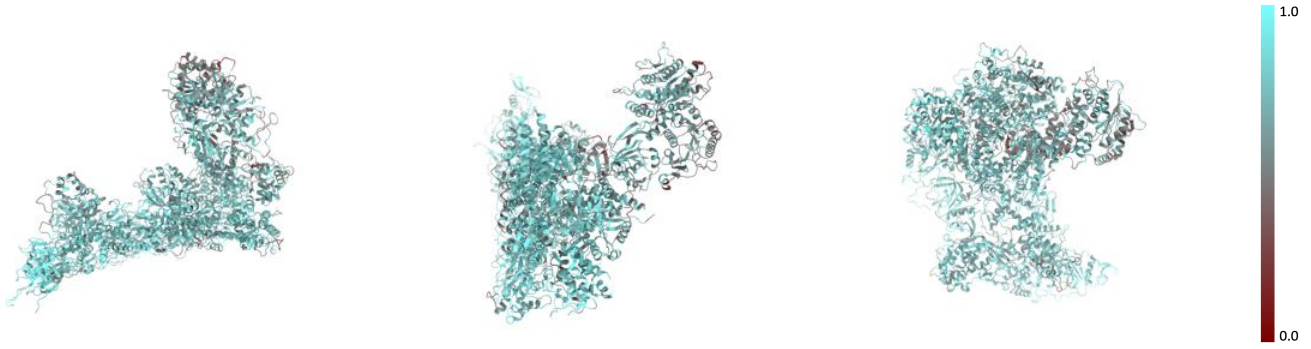
9.2 Q-score mapped to coordinate model



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.

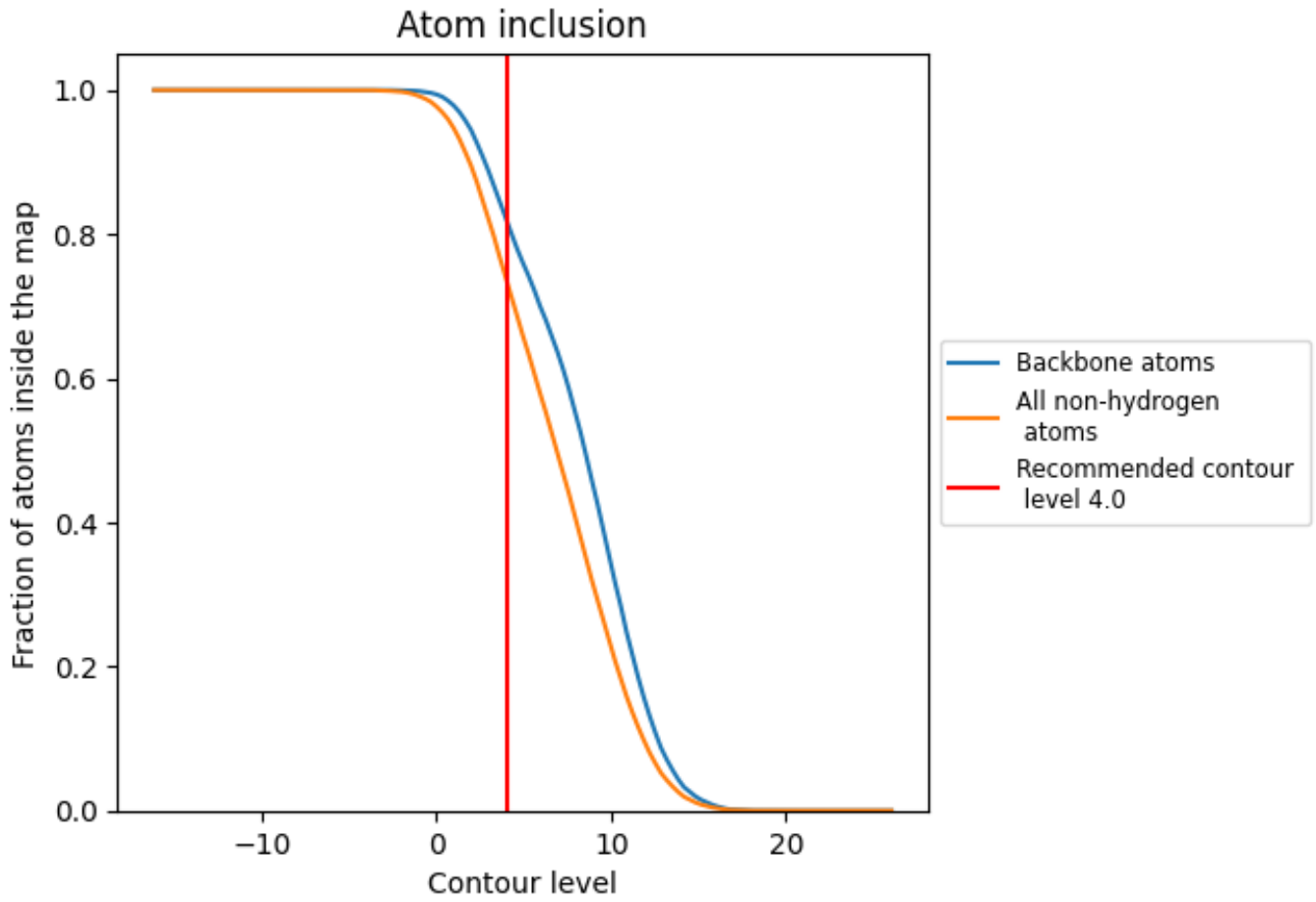
9.3 Atom inclusion mapped to coordinate model



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, 82% of all backbone atoms, 74% 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	0.7363	0.5370
A	0.6463	0.5100
B	0.7677	0.5470
C	0.7702	0.5480
D	0.7764	0.5510
E	0.7530	0.5390