Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:59 AM EST

PDB ID	:	3JB1
EMDB ID	:	EMD-6375
Title	:	Atomic model of cytoplasmic polyhedrosis virus with SAM
Authors	:	Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on	:	2015-07-06
Resolution	:	3.10 Å(reported)

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

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

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

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

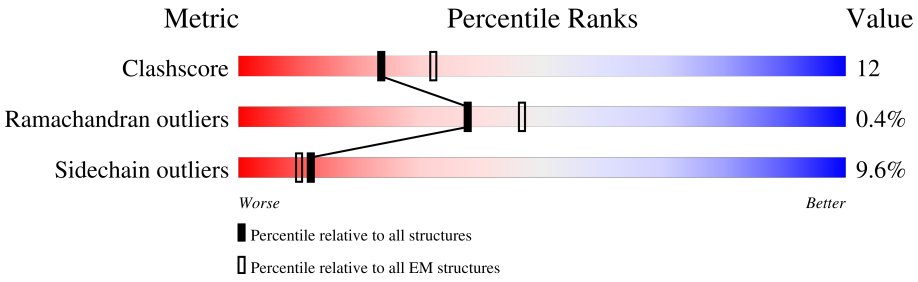
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1058	29% 64% 31% 5%
2	B	1333	59% 28% • 11%
2	C	1333	64% 26% • 6%
3	D	448	43% 19% • 35%
3	E	448	47% 16% • 35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32271 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		

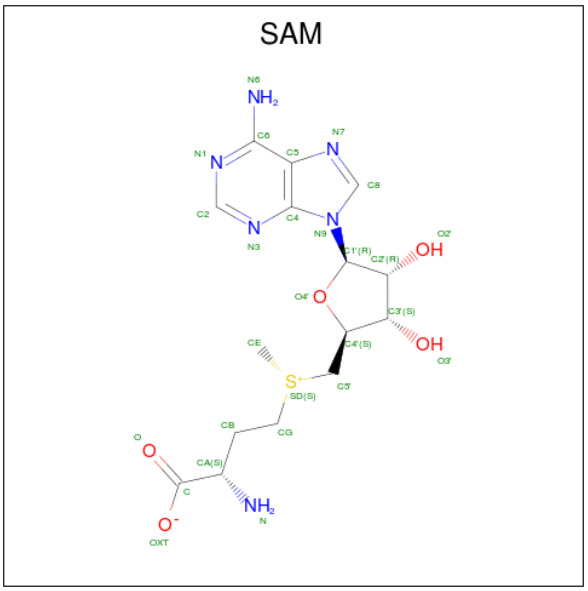
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	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: $C_{15}H_{22}N_6O_5S$).



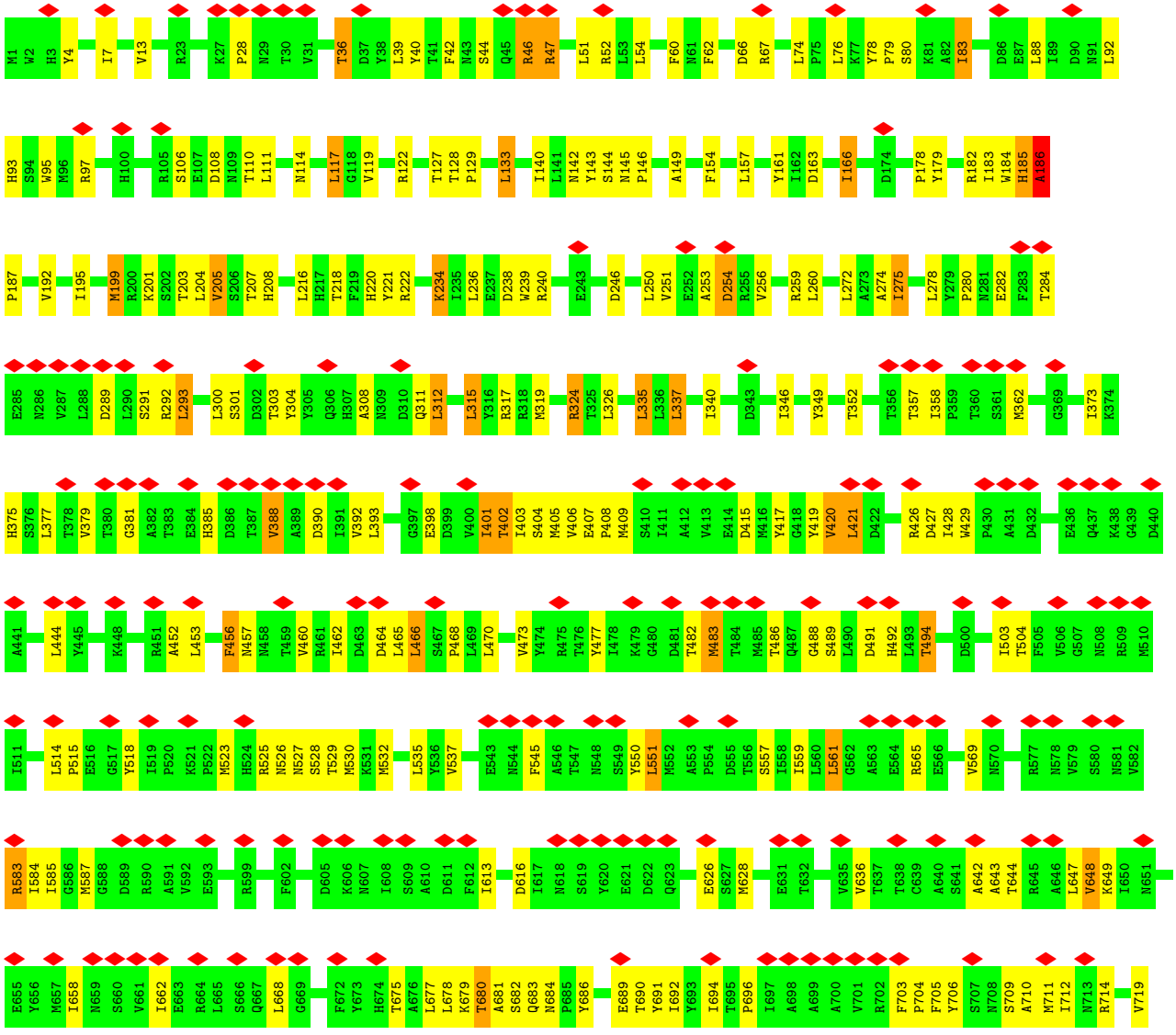
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
4	A	1	27	15	6	5	1	0

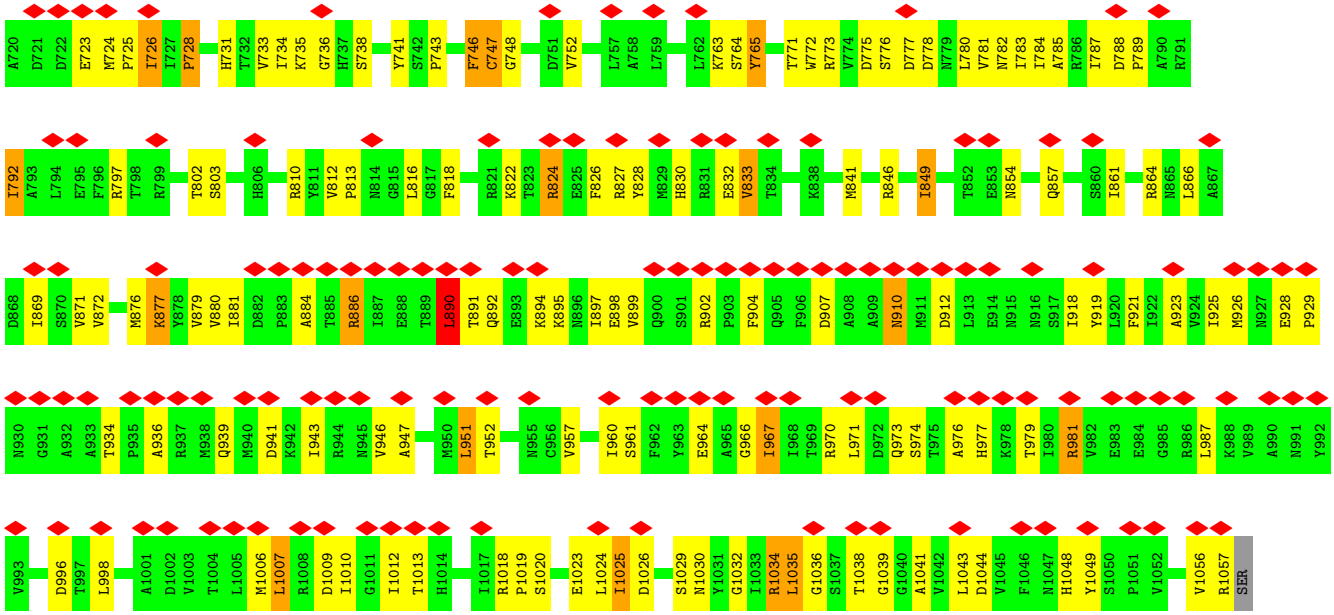
3 Residue-property plots (i)

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

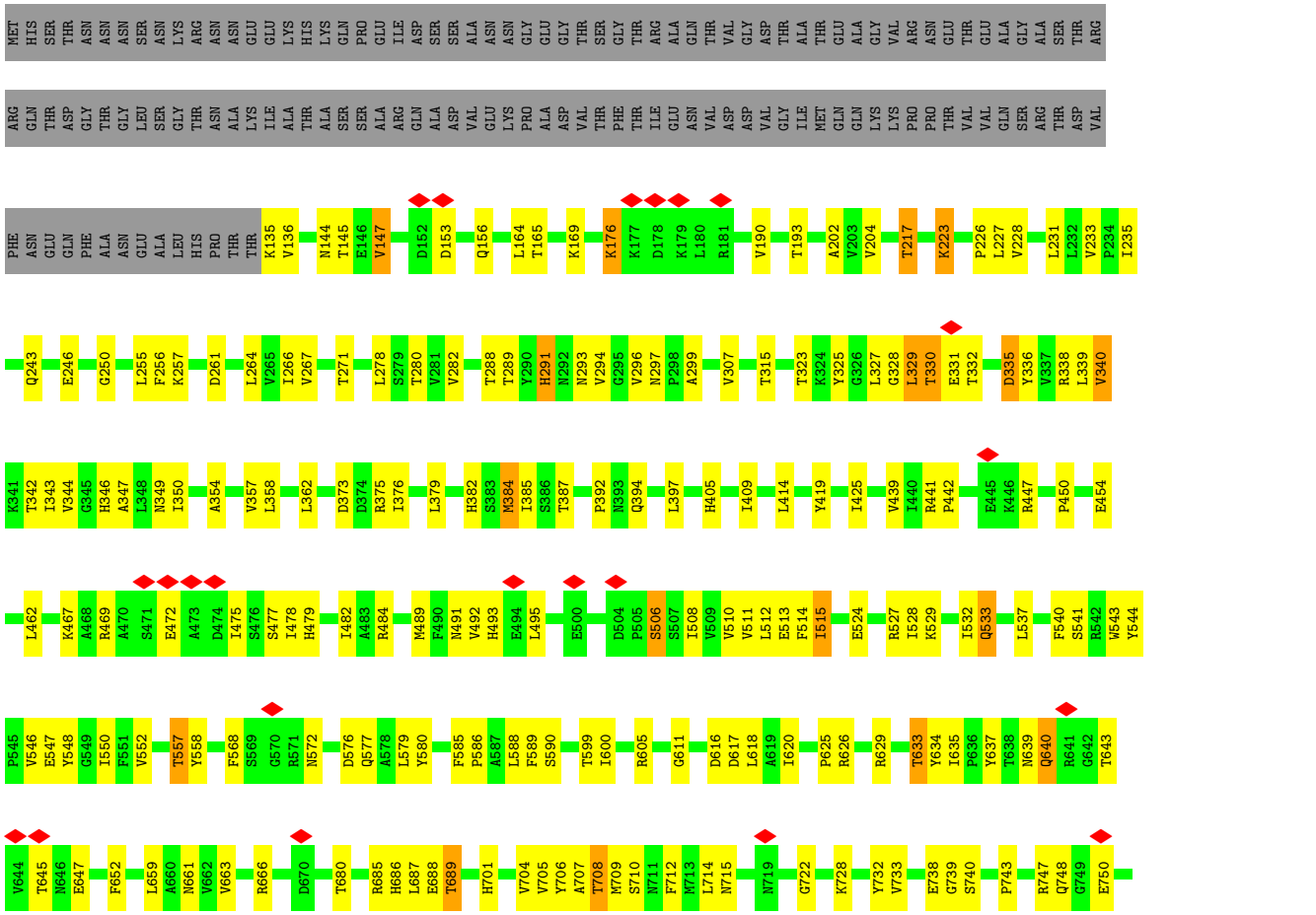
Chain A:

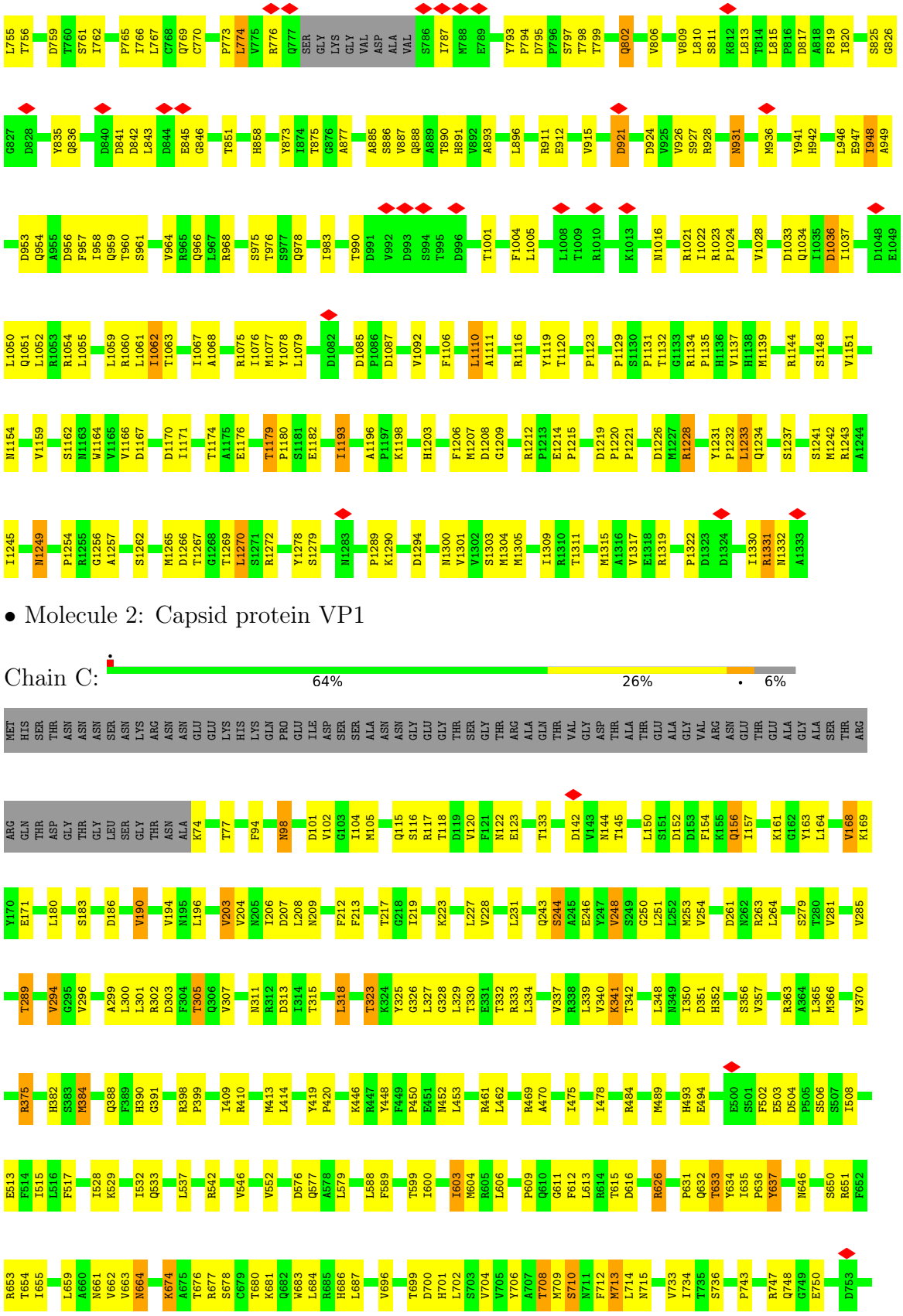




• Molecule 2: Capsid protein VP1

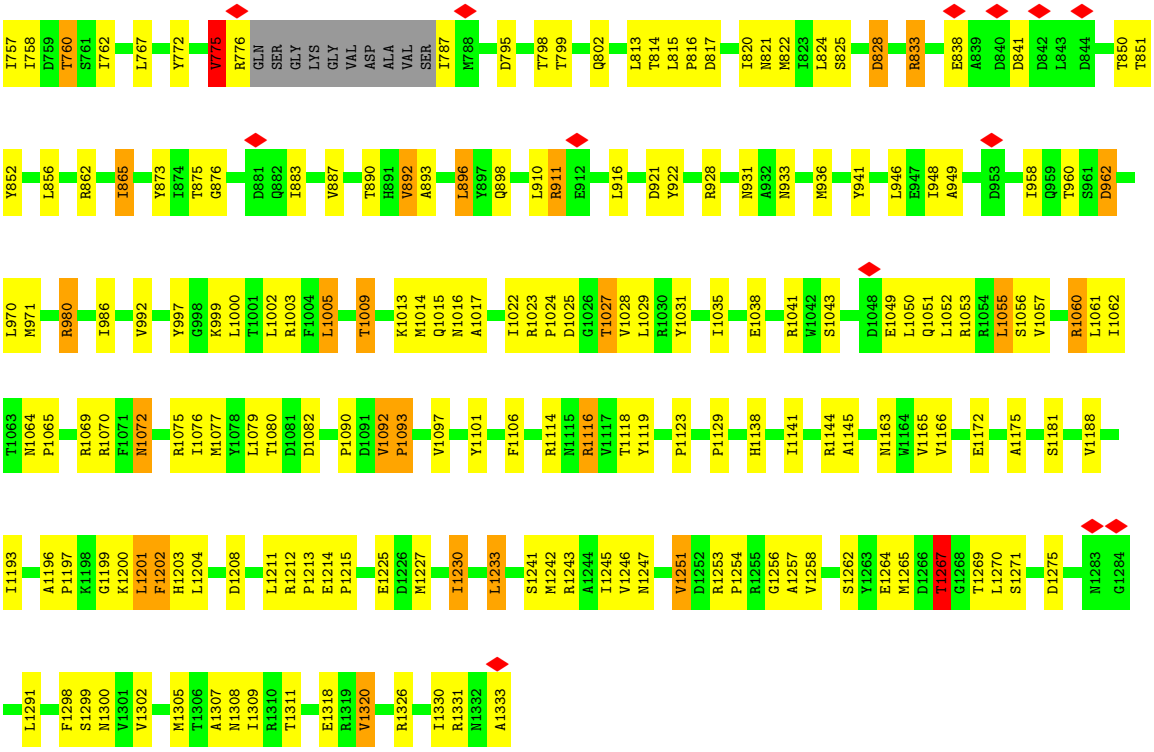
Chain B:





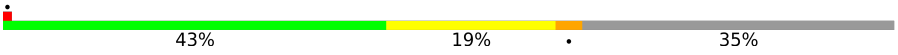
• Molecule 2: Capsid protein VP1

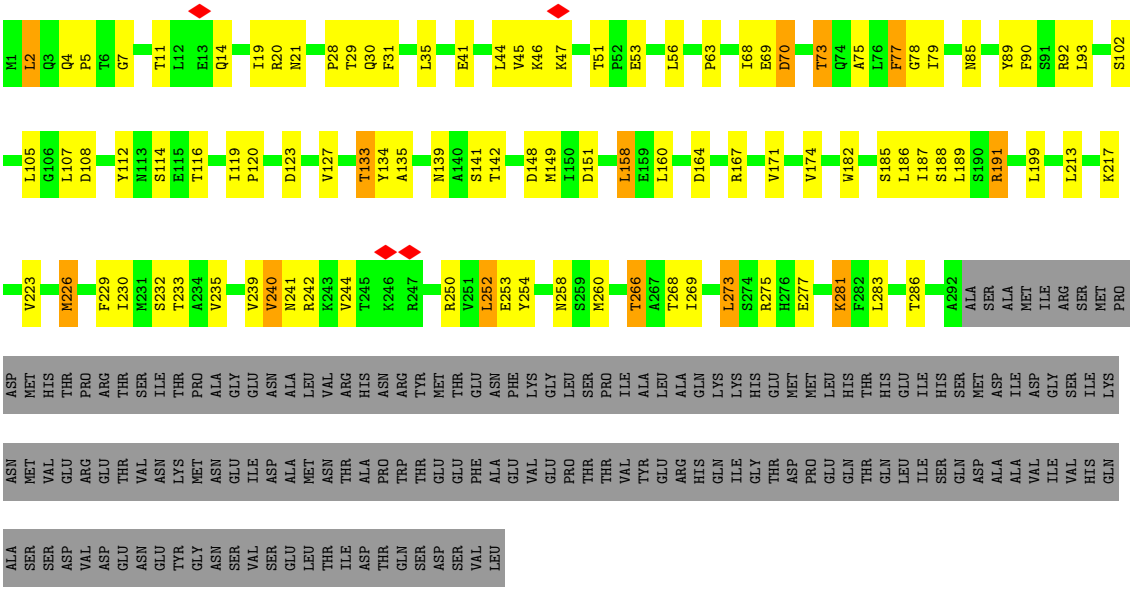
Chain C:



• Molecule 3: Viral structural protein 5

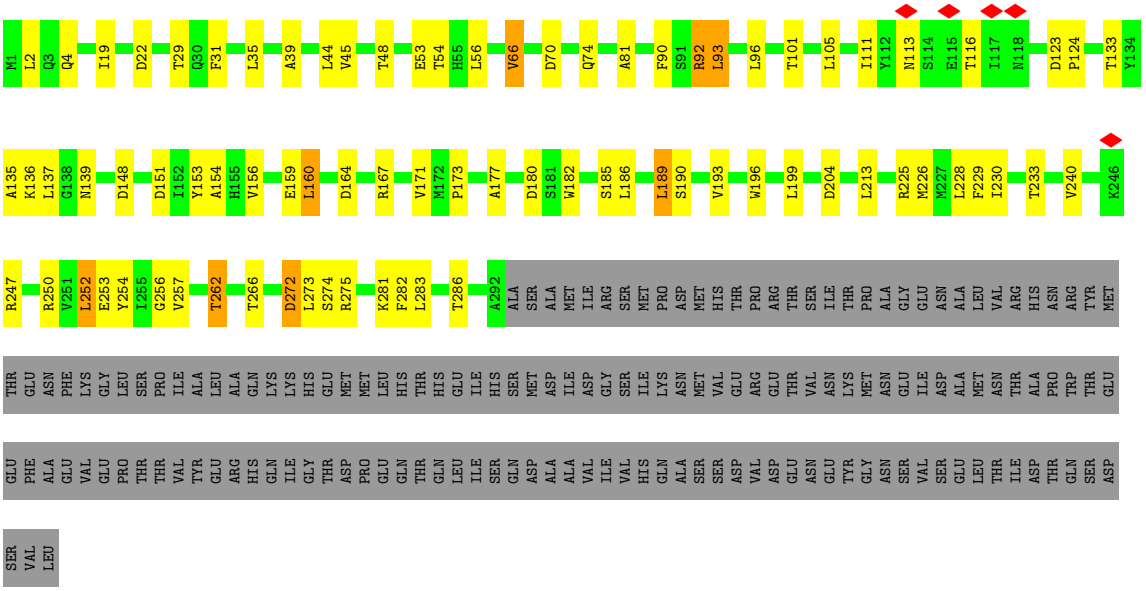
Chain D:





• Molecule 3: Viral structural protein 5

Chain E:


M1 L2 Q3 Q4 I19 D22 T29 Q30 F31 L35 A39 L44 V45 T48 E53 T54 H55 L56 V66 D70 Q74 A81 F90 S91 R92 L93 L96 T101 L105 I111 Y112 N113 S114 E115 T116 I117 N118 D123 P124 T133 Y134
A135 K136 L137 G138 N139 D148 D151 I152 Y153 A154 H155 V156 E159 L160 D164 R167 V171 M172 P173 A177 D180 S181 W182 S185 L186 L189 S190 V193 W196 L199 D204 L213 R225 M226 M227 L228 F229 I230 T233 V240 K246
R247 R250 V251 L252 E253 Y254 I255 G256 V257 T262 T266 D272 L273 S274 R275 K281 F282 L283 T286 A292 ALA SER ALA MET ILE ARG SER MET PRO ASP MET HIS THR PRO ARG THR SER ILE THR PRO ALA GLY GLU ASN ALA LEU VAL ARG HIS ASN ARG TYR MET
THR GLU ASN PHE LYS GLY LEU SER PRO ILE ALA LEU ALA GLN LYS LYS HIS GLU MET MET LEU HIS THR HIS GLU ILE HIS SER MET ASP ILE ASP GLY SER ILE LYS ASN MET VAL GLU ARG GLU THR VAL ASN LYS MET ASN GLU ILE ASP ALA MET ASN THR ALA PRO TRP THR GLU
GLU PHE ALA GLU VAL GLU PRO THR THR VAL TYR 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	44908	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	27.021	Depositor
Minimum map value	-18.914	Depositor
Average map value	0.066	Depositor
Map value standard deviation	1.604	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: SAM

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	0.52	3/11737 (0.0%)
2	B	0.33	0/9590	0.54	0/13056
2	C	0.34	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.54	0/3163
3	E	0.30	0/2327	0.52	0/3163
All	All	0.32	0/32915	0.54	3/44806 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ALA	C-N-CD	-8.20	102.57	120.60
1	A	186	ALA	C-N-CA	5.69	145.91	122.00
1	A	890	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8399	219	0
2	B	9397	0	9315	255	0
2	C	9851	0	9762	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2281	0	2282	62	0
3	E	2281	0	2282	47	0
4	A	27	0	22	5	0
All	All	32271	0	32062	785	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (785) 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:C:709:MET:O	2:C:715:ASN:ND2	2.09	0.85
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.60	0.83
3:D:44:LEU:HG	3:D:174:VAL:HG22	1.64	0.79
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.65	0.78
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.64	0.78
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.67	0.76
2:B:1134:ARG:NH1	2:B:1154:ASN:OD1	2.16	0.76
2:C:1208:ASP:OD2	2:C:1243:ARG:NH2	2.20	0.75
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.68	0.74
1:A:111:LEU:HD13	1:A:142:ASN:HB3	1.70	0.74
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.69	0.74
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.70	0.74
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.21	0.74
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.21	0.73
3:D:164:ASP:OD2	3:D:167:ARG:NH2	2.21	0.73
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.22	0.72
2:B:339:LEU:HD21	3:D:63:PRO:HB2	1.71	0.72
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.71	0.72
1:A:773:ARG:NH2	1:A:778:ASP:O	2.22	0.72
1:A:680:THR:HG23	1:A:683:GLN:HB2	1.71	0.72
2:C:332:THR:HG22	2:C:334:LEU:H	1.54	0.71
2:B:739:GLY:HA2	2:C:653:ARG:HD3	1.73	0.71
1:A:583:ARG:HH11	1:A:583:ARG:H	1.39	0.70
3:D:85:ASN:HB3	3:D:141:SER:HB3	1.72	0.70
2:B:576:ASP:H	2:B:579:LEU:HD12	1.56	0.70
2:C:704:VAL:HB	2:C:1330:ILE:HD11	1.74	0.70
1:A:857:GLN:OE1	1:A:877:LYS:NZ	2.24	0.70
2:C:674:LYS:HE3	2:C:677:ARG:HE	1.58	0.69
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.25	0.69
2:B:704:VAL:HA	2:B:1330:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:ASN:ND2	2:B:750:GLU:O	2.26	0.69
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.22	0.69
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.26	0.68
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.26	0.68
3:E:81:ALA:HB3	3:E:275:ARG:HD3	1.76	0.68
2:B:1171:ILE:HD13	2:B:1193:ILE:HD12	1.74	0.68
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.76	0.68
2:B:795:ASP:OD2	2:B:1319:ARG:NH1	2.26	0.67
1:A:127:THR:HG21	2:B:640:GLN:HA	1.77	0.67
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.75	0.67
2:C:244:SER:HA	2:C:1201:LEU:HD22	1.75	0.67
2:C:313:ASP:OD1	2:C:1253:ARG:NH2	2.27	0.67
1:A:880:VAL:HB	1:A:899:VAL:HG13	1.77	0.67
2:C:772:TYR:HB2	2:C:775:VAL:HG23	1.76	0.66
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.28	0.66
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.29	0.66
2:C:183:SER:OG	2:C:186:ASP:OD2	2.14	0.66
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.77	0.66
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.77	0.65
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.79	0.65
1:A:192:VAL:HG22	1:A:216:LEU:HD22	1.78	0.65
1:A:735:LYS:O	1:A:765:TYR:OH	2.14	0.65
2:B:484:ARG:O	2:B:527:ARG:NH2	2.29	0.65
1:A:203:THR:HG22	1:A:204:LEU:HG	1.77	0.65
1:A:559:ILE:HG22	1:A:585:ILE:HB	1.76	0.65
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.15	0.65
3:E:272:ASP:OD2	3:E:274:SER:OG	2.12	0.65
2:B:442:PRO:HB3	2:B:475:ILE:HG21	1.77	0.65
1:A:178:PRO:HB2	1:A:179:TYR:HD2	1.61	0.65
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.79	0.64
1:A:861:ILE:HG13	1:A:881:ILE:HB	1.78	0.64
3:D:46:LYS:HD3	3:D:158:LEU:HD23	1.79	0.64
1:A:254:ASP:OD1	1:A:254:ASP:N	2.30	0.64
1:A:532:MET:HA	1:A:535:LEU:HD12	1.79	0.64
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.78	0.64
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.21	0.64
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.29	0.63
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.81	0.63
1:A:462:ILE:HG13	1:A:466:LEU:HD22	1.80	0.63
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.25	0.63
1:A:427:ASP:HA	1:A:703:PHE:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.82	0.62
2:B:626:ARG:NH2	2:B:712:PHE:O	2.33	0.62
1:A:66:ASP:HB3	1:A:95:TRP:HE1	1.64	0.62
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.81	0.62
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.33	0.62
2:C:1305:MET:HE2	2:C:1309:ILE:HD11	1.80	0.62
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.31	0.62
1:A:1020:SER:OG	1:A:1023:GLU:OE2	2.16	0.62
2:B:325:TYR:OH	2:B:349:ASN:OD1	2.14	0.62
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.18	0.62
2:C:163:TYR:N	2:C:351:ASP:OD1	2.32	0.62
1:A:426:ARG:NH1	1:A:428:ILE:O	2.32	0.62
1:A:514:LEU:HD12	1:A:515:PRO:HD2	1.82	0.62
1:A:236:LEU:HD13	1:A:293:LEU:HD21	1.81	0.62
1:A:690:THR:HG21	1:A:711:MET:HB3	1.82	0.62
2:B:450:PRO:HG3	2:B:686:HIS:HB2	1.82	0.62
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.82	0.61
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.33	0.61
1:A:879:VAL:HG22	1:A:898:GLU:HB3	1.81	0.61
1:A:797:ARG:NH2	1:A:876:MET:O	2.30	0.61
3:D:2:LEU:HD12	3:D:107:LEU:HD21	1.82	0.61
1:A:178:PRO:HB2	1:A:179:TYR:CD2	2.36	0.61
2:C:370:VAL:HG12	2:C:398:ARG:HB2	1.83	0.61
2:C:713:MET:HG2	2:C:714:LEU:HG	1.83	0.61
2:B:961:SER:HB3	2:B:964:VAL:HG23	1.82	0.61
1:A:477:TYR:HA	1:A:482:THR:HG22	1.83	0.61
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.83	0.60
2:B:1085:ASP:OD2	2:B:1243:ARG:NH2	2.27	0.60
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.83	0.60
2:B:776:ARG:HD3	2:B:787:ILE:HB	1.81	0.60
2:C:341:LYS:HD2	2:C:1307:ALA:HB3	1.84	0.60
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.83	0.60
2:C:712:PHE:HB2	2:C:715:ASN:ND2	2.15	0.60
2:B:1226:ASP:OD2	2:C:122:ASN:ND2	2.33	0.60
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.67	0.60
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.83	0.59
2:C:382:HIS:ND1	2:C:799:THR:HG23	2.17	0.59
1:A:385:HIS:NE2	1:A:803:SER:OG	2.34	0.59
2:C:817:ASP:O	2:C:821:ASN:ND2	2.27	0.59
2:C:980:ARG:NH2	2:C:997:TYR:O	2.35	0.59
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HD21	1:A:530:MET:HE2	1.84	0.59
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.83	0.59
1:A:828:TYR:HB3	1:A:1034:ARG:HB3	1.84	0.59
2:B:153:ASP:OD1	2:B:153:ASP:N	2.35	0.59
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.36	0.59
1:A:565:ARG:NH2	1:A:616:ASP:OD2	2.35	0.59
2:C:748:GLN:HG3	2:C:1000:LEU:HD22	1.85	0.59
2:C:1211:LEU:HD21	2:C:1246:VAL:HG21	1.84	0.59
1:A:957:VAL:HG22	1:A:1056:VAL:HG23	1.84	0.59
2:B:817:ASP:HA	2:B:983:ILE:HG12	1.85	0.59
1:A:208:HIS:HE1	1:A:234:LYS:HG2	1.68	0.58
2:B:1266:ASP:OD2	2:B:1279:SER:N	2.29	0.58
1:A:409:MET:HE2	1:A:465:LEU:HD22	1.85	0.58
2:B:439:VAL:HG11	2:B:705:VAL:HG21	1.85	0.58
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.38	0.58
2:B:329:LEU:HB2	2:B:346:HIS:CE1	2.37	0.58
2:C:776:ARG:HB3	2:C:787:ILE:HD12	1.84	0.58
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.37	0.58
1:A:686:TYR:CZ	1:A:1035:LEU:HB2	2.39	0.58
1:A:923:ALA:N	1:A:961:SER:OG	2.35	0.58
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.39	0.58
2:C:115:GLN:HB3	2:C:117:ARG:HD3	1.84	0.58
1:A:833:VAL:HG12	1:A:1043:LEU:HD23	1.86	0.58
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.85	0.58
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.86	0.58
1:A:129:PRO:HD2	2:B:1332:ASN:HB2	1.84	0.58
1:A:78:TYR:HE1	1:A:83:ILE:HG23	1.69	0.57
2:B:384:MET:HA	2:B:708:THR:HG21	1.86	0.57
2:B:806:VAL:HG22	2:B:1001:THR:HG21	1.85	0.57
2:B:462:LEU:HD13	2:B:680:THR:HG22	1.86	0.57
2:C:503:GLU:OE2	2:C:542:ARG:NH2	2.32	0.57
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.87	0.57
1:A:951:LEU:HD13	1:A:1057:ARG:HH12	1.69	0.57
2:C:414:LEU:HD23	2:C:814:THR:HB	1.87	0.57
2:C:450:PRO:HG3	2:C:686:HIS:HB2	1.87	0.57
2:C:504:ASP:OD2	2:C:506:SER:OG	2.23	0.57
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.69	0.57
2:B:558:TYR:CZ	2:B:585:PHE:HB2	2.39	0.57
1:A:163:ASP:OD1	1:A:182:ARG:NE	2.33	0.57
2:B:335:ASP:OD2	2:B:340:VAL:N	2.38	0.56
1:A:317:ARG:NH1	3:D:41:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD11	1:A:973:GLN:HB2	1.87	0.56
1:A:420:VAL:HA	1:A:974:SER:HB2	1.88	0.56
2:C:1023:ARG:HB3	2:C:1025:ASP:OD1	2.06	0.56
2:C:1214:GLU:HG2	2:C:1215:PRO:HD2	1.86	0.56
2:B:1131:PRO:O	2:B:1162:SER:OG	2.14	0.56
3:D:233:THR:HB	3:D:268:THR:HG21	1.86	0.56
1:A:275:ILE:HG13	1:A:301:SER:HA	1.88	0.56
1:A:775:ASP:OD1	1:A:776:SER:N	2.38	0.56
2:B:328:GLY:HA3	2:B:347:ALA:H	1.71	0.56
2:B:479:HIS:HA	2:B:482:ILE:HD12	1.87	0.56
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.39	0.55
2:C:161:LYS:HD2	2:C:212:PHE:HB2	1.88	0.55
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.89	0.55
1:A:373:ILE:HG21	1:A:375:HIS:CE1	2.41	0.55
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.89	0.55
1:A:526:ASN:OD1	1:A:529:THR:OG1	2.17	0.55
2:C:169:LYS:HB2	2:C:203:VAL:HG23	1.87	0.55
2:C:576:ASP:OD1	2:C:747:ARG:NH2	2.40	0.55
1:A:904:PHE:H	4:A:1101:SAM:H2	1.71	0.55
2:B:439:VAL:HG12	2:B:701:HIS:NE2	2.22	0.55
2:B:958:ILE:HG22	2:B:960:THR:HG23	1.88	0.55
3:E:4:GLN:NE2	3:E:204:ASP:OD2	2.39	0.55
1:A:274:ALA:HA	1:A:319:MET:HE2	1.89	0.55
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.06	0.55
2:C:1013:LYS:HE2	2:C:1015:GLN:NE2	2.21	0.55
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.87	0.55
1:A:144:SER:OG	1:A:145:ASN:N	2.40	0.55
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.89	0.55
1:A:404:SER:HB2	1:A:826:PHE:HD1	1.72	0.54
2:B:643:THR:HG22	2:B:645:THR:H	1.72	0.54
2:B:1289:PRO:HG2	3:D:191:ARG:NH2	2.22	0.54
2:C:1002:LEU:HD12	2:C:1005:LEU:HB2	1.87	0.54
1:A:939:GLN:HB2	1:A:998:LEU:HD21	1.89	0.54
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.90	0.54
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.71	0.54
2:C:611:GLY:HA3	2:C:635:ILE:O	2.08	0.54
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.89	0.54
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.89	0.54
2:B:652:PHE:HE2	2:B:688:GLU:HA	1.72	0.54
1:A:488:GLY:H	1:A:492:HIS:HD1	1.55	0.54
2:B:261:ASP:HB3	2:B:357:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:LEU:HA	2:B:1309:ILE:HD13	1.89	0.54
2:B:1076:ILE:HG22	2:B:1159:VAL:HG11	1.90	0.54
1:A:525:ARG:HG2	1:A:529:THR:HG21	1.91	0.53
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.42	0.53
2:B:145:THR:HB	2:B:1317:VAL:HG23	1.90	0.53
2:B:1249:ASN:OD1	2:B:1249:ASN:N	2.33	0.53
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.43	0.53
2:C:261:ASP:OD1	2:C:263:ARG:NH1	2.41	0.53
3:D:283:LEU:HA	3:D:286:THR:HG22	1.90	0.53
2:B:409:ILE:HD13	2:B:625:PRO:HB2	1.89	0.53
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.74	0.53
1:A:569:VAL:HG13	1:A:584:ILE:HG22	1.89	0.53
2:C:294:VAL:HG11	2:C:327:LEU:HD21	1.91	0.53
2:C:450:PRO:HD2	2:C:453:LEU:HD22	1.91	0.53
1:A:528:SER:OG	1:A:565:ARG:NH1	2.41	0.53
3:D:108:ASP:OD1	3:D:112:TYR:OH	2.24	0.53
2:C:1114:ARG:HH21	2:C:1116:ARG:CZ	2.22	0.53
2:B:335:ASP:OD1	2:B:340:VAL:HG22	2.09	0.52
2:C:332:THR:HG23	2:C:1270:LEU:HD12	1.92	0.52
3:E:190:SER:HA	3:E:230:ILE:HD12	1.91	0.52
1:A:929:PRO:HA	4:A:1101:SAM:H2'	1.91	0.52
2:C:384:MET:HA	2:C:708:THR:HG21	1.91	0.52
2:C:448:TYR:CZ	2:C:470:ALA:HB1	2.44	0.52
2:B:425:ILE:HG13	2:B:1004:PHE:CD2	2.44	0.52
2:B:558:TYR:HB3	2:B:568:PHE:CD1	2.44	0.52
2:C:824:LEU:HD23	2:C:971:MET:HE1	1.91	0.52
1:A:406:VAL:HG11	1:A:460:VAL:HG13	1.90	0.52
1:A:40:TYR:HB2	1:A:51:LEU:HD13	1.90	0.52
1:A:689:GLU:N	1:A:689:GLU:OE1	2.42	0.52
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.45	0.52
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.92	0.52
2:C:980:ARG:HH11	2:C:980:ARG:HB2	1.75	0.52
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.43	0.52
1:A:133:LEU:HD11	1:A:140:ILE:HD13	1.91	0.52
1:A:385:HIS:HB3	1:A:388:VAL:HG13	1.92	0.52
2:B:611:GLY:HA3	2:B:635:ILE:O	2.10	0.52
1:A:812:VAL:HG22	1:A:816:LEU:HD11	1.92	0.52
2:B:704:VAL:O	2:B:708:THR:HG23	2.09	0.52
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.91	0.52
2:C:213:PHE:HB3	2:C:219:ILE:HD12	1.90	0.52
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.92	0.52
2:B:616:ASP:OD2	2:B:710:SER:OG	2.28	0.52
1:A:1039:GLY:O	1:A:1043:LEU:HB2	2.10	0.51
2:B:887:VAL:HG22	2:B:893:ALA:HA	1.91	0.51
2:B:1036:ASP:N	2:B:1036:ASP:OD1	2.43	0.51
2:C:104:ILE:HG12	2:C:1311:THR:HG23	1.92	0.51
2:C:962:ASP:OD1	2:C:962:ASP:N	2.42	0.51
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	1.92	0.51
1:A:675:THR:HG22	1:A:694:ILE:HG12	1.90	0.51
1:A:199:MET:HE3	1:A:220:HIS:HE1	1.75	0.51
1:A:964:GLU:HG3	1:A:966:GLY:H	1.75	0.51
2:B:469:ARG:NH1	2:B:472:GLU:OE1	2.43	0.51
2:C:161:LYS:O	2:C:263:ARG:NH2	2.43	0.51
3:E:92:ARG:NH2	3:E:113:ASN:HB2	2.25	0.51
1:A:13:VAL:HG21	1:A:146:PRO:HB3	1.93	0.51
1:A:649:LYS:HB2	1:A:691:TYR:CE1	2.44	0.51
2:B:975:SER:N	2:B:978:GLN:OE1	2.42	0.51
2:B:1135:PRO:O	2:B:1137:VAL:HG23	2.10	0.51
2:B:342:THR:OG1	2:B:343:ILE:N	2.44	0.51
2:B:1180:PRO:HA	2:B:1207:MET:SD	2.51	0.51
2:C:1077:MET:HG3	2:C:1165:VAL:HG22	1.91	0.51
1:A:771:THR:HG22	1:A:783:ILE:HG12	1.93	0.51
2:B:544:TYR:HB3	2:B:547:GLU:HB2	1.93	0.51
2:B:586:PRO:HB2	2:B:589:PHE:HD2	1.75	0.51
2:B:558:TYR:CE1	2:B:590:SER:HB3	2.46	0.51
2:C:204:VAL:HG11	2:C:1242:MET:HE2	1.92	0.51
1:A:527:ASN:HD21	1:A:684:ASN:HD21	1.58	0.51
1:A:557:SER:HB3	1:A:583:ARG:HB2	1.91	0.51
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.92	0.51
2:B:1179:THR:HG23	2:B:1182:GLU:HG2	1.92	0.51
2:C:606:LEU:HA	2:C:651:ARG:HH21	1.76	0.51
3:D:53:GLU:CD	3:D:53:GLU:H	2.14	0.51
2:B:469:ARG:NH2	2:B:513:GLU:OE2	2.43	0.51
2:C:228:VAL:HG21	2:C:253:MET:HG2	1.93	0.51
2:C:875:THR:OG1	2:C:876:GLY:N	2.43	0.51
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.27	0.51
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.46	0.51
1:A:420:VAL:HA	1:A:974:SER:CB	2.41	0.50
2:B:307:VAL:HG21	2:B:1245:ILE:HG22	1.93	0.50
1:A:420:VAL:HG13	1:A:976:ALA:HB3	1.91	0.50
2:B:585:PHE:CE1	2:B:728:LYS:HE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:SER:HB2	2:B:1016:ASN:HD21	1.77	0.50
2:C:528:ILE:HG13	2:C:532:ILE:HD12	1.93	0.50
2:C:533:GLN:HG3	2:C:588:LEU:HD12	1.92	0.50
2:C:799:THR:HA	2:C:802:GLN:HG2	1.92	0.50
2:C:1118:THR:HA	2:C:1129:PRO:HA	1.92	0.50
1:A:280:PRO:HB3	1:A:304:TYR:CE1	2.46	0.50
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.92	0.50
2:B:1062:ILE:HG22	2:B:1063:THR:HG23	1.92	0.50
2:C:357:VAL:HG23	2:C:1057:VAL:HG11	1.94	0.50
3:E:182:TRP:NE1	3:E:185:SER:HA	2.26	0.50
1:A:381:GLY:H	1:A:802:THR:HB	1.76	0.50
2:B:156:GLN:HB3	2:B:266:ILE:HD11	1.93	0.50
2:B:441:ARG:HH22	2:B:773:PRO:HB3	1.77	0.50
2:B:1144:ARG:NH1	2:B:1170:ASP:OD2	2.44	0.50
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	1.94	0.50
2:C:334:LEU:HD22	2:C:337:VAL:HG21	1.92	0.50
2:C:616:ASP:OD1	2:C:710:SER:OG	2.25	0.50
1:A:239:TRP:CZ2	1:A:280:PRO:HD2	2.46	0.50
1:A:452:ALA:HB2	1:A:725:PRO:HB3	1.94	0.50
2:B:299:ALA:HB2	2:B:1265:MET:HB3	1.93	0.50
2:C:390:HIS:HB2	2:C:1318:GLU:HB3	1.94	0.50
3:E:45:VAL:HG13	3:E:171:VAL:HG12	1.94	0.50
1:A:402:THR:HG23	1:A:824:ARG:HB3	1.94	0.49
1:A:417:TYR:HB3	1:A:537:VAL:HG11	1.94	0.49
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.94	0.49
1:A:830:HIS:HB2	1:A:1034:ARG:NH1	2.27	0.49
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.94	0.49
2:C:504:ASP:OD1	2:C:504:ASP:N	2.44	0.49
3:D:253:GLU:HB2	3:D:254:TYR:CD1	2.46	0.49
2:B:508:ILE:HG21	2:B:663:VAL:HG21	1.93	0.49
1:A:907:ASP:HB2	1:A:910:ASN:HD21	1.77	0.49
2:B:1206:PHE:CE1	2:B:1232:PRO:HD3	2.48	0.49
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.12	0.49
1:A:303:THR:HG21	1:A:813:PRO:HD3	1.94	0.49
2:B:169:LYS:NZ	2:B:1182:GLU:OE2	2.37	0.49
2:C:323:THR:HG21	2:C:1262:SER:HB2	1.93	0.49
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.93	0.49
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.95	0.49
2:C:1080:THR:OG1	2:C:1082:ASP:OD1	2.29	0.49
3:E:283:LEU:HA	3:E:286:THR:HG22	1.95	0.49
1:A:892:GLN:HA	1:A:897:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.94	0.49
1:A:60:PHE:HA	1:A:119:VAL:HG11	1.95	0.49
1:A:457:ASN:HA	1:A:686:TYR:HB2	1.93	0.49
2:B:921:ASP:OD1	2:B:921:ASP:N	2.44	0.49
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.24	0.49
2:C:206:ILE:HD13	2:C:1298:PHE:HE2	1.77	0.49
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.94	0.49
1:A:292:ARG:NH2	1:A:777:ASP:OD1	2.46	0.49
1:A:377:LEU:HD12	1:A:377:LEU:H	1.77	0.49
1:A:773:ARG:HG2	1:A:781:VAL:HG22	1.94	0.49
2:B:338:ARG:HH11	2:B:397:LEU:HD23	1.77	0.49
2:C:828:ASP:OD2	2:C:828:ASP:N	2.46	0.49
2:C:1106:PHE:CE1	2:C:1119:TYR:HB2	2.48	0.49
1:A:404:SER:HB2	1:A:826:PHE:CD1	2.48	0.49
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.94	0.49
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	1.95	0.49
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.94	0.49
2:C:980:ARG:HB2	2:C:980:ARG:NH1	2.28	0.49
2:C:865:ILE:HD11	2:C:1041:ARG:O	2.12	0.48
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.46	0.48
2:B:712:PHE:HB2	2:B:715:ASN:OD1	2.13	0.48
2:B:193:THR:HG21	2:B:297:ASN:O	2.13	0.48
2:B:373:ASP:HA	2:B:1315:MET:HE1	1.94	0.48
2:B:957:PHE:CE1	2:B:1016:ASN:HB3	2.48	0.48
2:C:388:GLN:HB3	2:C:1320:VAL:HG13	1.96	0.48
1:A:947:ALA:HB3	1:A:1010:ILE:HD13	1.95	0.48
2:B:1110:LEU:HD13	3:E:272:ASP:HB3	1.94	0.48
2:B:1144:ARG:HH11	2:B:1170:ASP:HB3	1.78	0.48
2:C:326:GLY:H	2:C:1267:THR:HG21	1.77	0.48
3:E:186:LEU:HD22	3:E:233:THR:HG21	1.94	0.48
1:A:967:ILE:HB	1:A:1049:TYR:HB3	1.95	0.48
2:B:387:THR:HG22	2:B:1322:PRO:HD3	1.95	0.48
2:C:223:LYS:NZ	2:C:1203:HIS:HB2	2.28	0.48
1:A:392:VAL:HG22	1:A:733:VAL:HG12	1.95	0.48
2:B:558:TYR:CE1	2:B:585:PHE:HB2	2.48	0.48
2:C:302:ARG:HD2	2:C:318:LEU:HD12	1.95	0.48
2:B:634:TYR:CE1	2:B:722:GLY:HA3	2.49	0.48
1:A:199:MET:CE	1:A:220:HIS:HE1	2.26	0.48
2:B:732:TYR:CE1	2:B:1021:ARG:HG2	2.49	0.48
2:C:613:LEU:HD11	2:C:632:GLN:HB3	1.96	0.48
1:A:4:TYR:OH	1:A:246:ASP:OD1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:CD2	1:A:185:HIS:HA	2.48	0.48
1:A:746:PHE:CE2	1:A:787:ILE:HD11	2.49	0.48
1:A:879:VAL:HA	1:A:898:GLU:O	2.14	0.48
2:C:1241:SER:OG	2:C:1264:GLU:OE2	2.25	0.48
1:A:201:LYS:O	2:B:629:ARG:HG2	2.14	0.48
1:A:462:ILE:HA	1:A:465:LEU:HD12	1.96	0.48
1:A:919:TYR:HB3	1:A:921:PHE:CE2	2.49	0.48
1:A:1026:ASP:O	1:A:1030:ASN:ND2	2.32	0.48
2:C:683:TRP:CZ2	2:C:687:LEU:HD11	2.49	0.48
1:A:822:LYS:HB3	1:A:822:LYS:HE2	1.69	0.47
2:B:776:ARG:HB3	2:B:787:ILE:H	1.79	0.47
2:C:493:HIS:HB3	2:C:758:ILE:HD13	1.96	0.47
2:C:813:LEU:HA	2:C:992:VAL:HG11	1.95	0.47
2:C:970:LEU:HD23	2:C:970:LEU:HA	1.72	0.47
3:E:39:ALA:HB1	3:E:173:PRO:HB2	1.96	0.47
2:B:217:THR:HG23	2:B:257:LYS:HD3	1.96	0.47
2:B:1106:PHE:CE1	2:B:1119:TYR:HB2	2.49	0.47
2:C:190:VAL:O	2:C:194:VAL:HG23	2.13	0.47
2:C:494:GLU:HB2	2:C:757:ILE:HD13	1.96	0.47
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.96	0.47
3:E:53:GLU:OE1	3:E:281:LYS:NZ	2.47	0.47
1:A:489:SER:OG	1:A:491:ASP:OD2	2.32	0.47
1:A:709:SER:HB2	1:A:712:ILE:HG13	1.96	0.47
2:B:327:LEU:HD12	2:B:327:LEU:HA	1.68	0.47
2:B:392:PRO:HG2	2:B:394:GLN:HG3	1.96	0.47
2:B:633:THR:HG21	2:B:710:SER:HB2	1.95	0.47
2:B:1087:ASP:OD2	2:B:1237:SER:OG	2.32	0.47
2:B:419:TYR:HB3	2:B:1005:LEU:HD22	1.95	0.47
2:B:552:VAL:HG22	2:B:572:ASN:HB2	1.96	0.47
2:C:999:LYS:HG2	2:C:1009:THR:HA	1.96	0.47
2:C:1031:TYR:OH	2:C:1038:GLU:HA	2.13	0.47
3:D:158:LEU:HD12	3:D:158:LEU:HA	1.64	0.47
1:A:919:TYR:HB3	1:A:921:PHE:HE2	1.79	0.47
2:B:255:LEU:HD11	2:B:1059:LEU:HD23	1.96	0.47
2:C:1072:ASN:HB3	2:C:1172:GLU:HG2	1.95	0.47
3:E:44:LEU:HD11	3:E:256:GLY:HA3	1.95	0.47
2:B:617:ASP:OD1	2:B:618:LEU:N	2.47	0.47
2:B:1330:ILE:HD13	2:B:1330:ILE:HA	1.68	0.47
2:C:164:LEU:HD23	2:C:208:LEU:HA	1.96	0.47
1:A:251:VAL:HG12	1:A:253:ALA:H	1.80	0.47
1:A:726:ILE:HD12	1:A:743:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:MET:SD	2:B:527:ARG:HD2	2.55	0.47
2:B:512:LEU:HD21	2:B:687:LEU:HD12	1.97	0.47
2:B:873:TYR:HA	2:B:896:LEU:O	2.14	0.47
2:C:517:PHE:CD1	2:C:760:THR:HG22	2.49	0.47
3:D:148:ASP:OD1	3:D:151:ASP:N	2.39	0.47
3:D:185:SER:O	3:D:189:LEU:HB2	2.15	0.47
1:A:904:PHE:H	4:A:1101:SAM:C2	2.27	0.47
2:B:338:ARG:HB3	2:B:340:VAL:HG13	1.97	0.47
2:C:828:ASP:OD2	2:C:960:THR:OG1	2.30	0.47
2:B:164:LEU:HD21	2:B:1067:ILE:HD11	1.96	0.47
3:D:213:LEU:HD11	3:D:217:LYS:HE3	1.97	0.47
3:D:273:LEU:O	3:D:277:GLU:HG3	2.14	0.47
3:E:56:LEU:HD23	3:E:136:LYS:HG3	1.96	0.47
1:A:106:SER:OG	1:A:108:ASP:OD1	2.20	0.46
2:B:482:ILE:HG23	2:B:706:TYR:OH	2.15	0.46
2:C:144:ASN:HD21	2:C:391:GLY:HA2	1.80	0.46
2:C:254:VAL:HB	2:C:1062:ILE:HD11	1.97	0.46
2:B:540:PHE:CE2	2:B:600:ILE:HG23	2.50	0.46
2:B:1278:TYR:CE1	2:B:1290:LYS:HA	2.50	0.46
3:D:253:GLU:HA	3:D:254:TYR:HA	1.46	0.46
3:E:96:LEU:HA	3:E:101:THR:HG21	1.98	0.46
1:A:895:LYS:HB2	1:A:897:ILE:HG12	1.96	0.46
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.96	0.46
3:D:28:PRO:CB	3:D:226:MET:HG3	2.45	0.46
2:B:949:ALA:HB1	2:B:960:THR:HG22	1.98	0.46
2:C:883:ILE:HD13	2:C:910:LEU:HD21	1.97	0.46
3:D:182:TRP:NE1	3:D:185:SER:HA	2.30	0.46
1:A:746:PHE:HB2	1:A:785:ALA:HB3	1.97	0.46
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.96	0.46
2:B:347:ALA:HA	2:B:1301:VAL:HA	1.97	0.46
2:B:495:LEU:HD22	2:B:532:ILE:HG13	1.96	0.46
2:B:1077:MET:HG2	2:B:1079:LEU:HD13	1.97	0.46
1:A:28:PRO:HA	1:A:97:ARG:HG2	1.96	0.46
1:A:401:ILE:HD12	1:A:747:CYS:SG	2.56	0.46
2:B:228:VAL:HG11	2:B:231:LEU:HD12	1.98	0.46
2:C:1243:ARG:HB3	2:C:1258:VAL:HG23	1.98	0.46
3:D:45:VAL:HG22	3:D:171:VAL:HG12	1.98	0.46
3:D:258:ASN:ND2	3:D:260:MET:SD	2.88	0.46
1:A:403:ILE:HG22	1:A:827:ARG:HG3	1.98	0.46
2:B:454:GLU:OE2	2:B:467:LYS:NZ	2.41	0.46
1:A:218:THR:OG1	1:A:220:HIS:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD13	1:A:337:LEU:HA	1.80	0.46
1:A:947:ALA:HB1	1:A:1012:ILE:HG21	1.97	0.46
2:B:357:VAL:HG13	2:B:1054:ARG:HD3	1.98	0.46
2:B:529:LYS:HD2	2:B:589:PHE:CD2	2.51	0.46
2:C:186:ASP:CG	2:C:279:SER:H	2.19	0.46
2:C:588:LEU:HD23	2:C:588:LEU:HA	1.81	0.46
3:D:56:LEU:HD23	3:D:56:LEU:HA	1.76	0.46
1:A:398:GLU:HG3	1:A:402:THR:HB	1.97	0.46
2:B:1209:GLY:O	2:B:1212:ARG:HG2	2.16	0.46
2:C:171:GLU:HB2	2:C:1211:LEU:HD13	1.97	0.46
2:C:1101:TYR:HB2	2:C:1141:ILE:HG12	1.98	0.46
2:C:1271:SER:N	2:C:1275:ASP:O	2.44	0.46
3:D:78:GLY:O	3:D:275:ARG:NH2	2.44	0.46
3:E:193:VAL:HG21	3:E:230:ILE:HG13	1.98	0.46
2:B:842:ASP:HB2	2:B:845:GLU:HG3	1.98	0.46
2:B:953:ASP:OD1	2:B:960:THR:OG1	2.27	0.46
2:C:409:ILE:O	2:C:413:MET:HG2	2.16	0.46
3:D:77:PHE:HB3	3:D:230:ILE:HG21	1.98	0.45
3:D:232:SER:HA	3:D:235:VAL:HG22	1.97	0.45
3:E:148:ASP:OD2	3:E:151:ASP:N	2.39	0.45
3:E:262:THR:HG22	3:E:272:ASP:HA	1.98	0.45
1:A:1034:ARG:HH21	1:A:1036:GLY:HA2	1.80	0.45
2:B:738:GLU:OE1	2:B:858:HIS:HD2	1.98	0.45
2:B:959:GLN:HG3	2:B:964:VAL:HG21	1.98	0.45
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.15	0.45
2:C:98:ASN:ND2	2:C:101:ASP:OD1	2.49	0.45
2:C:822:MET:O	2:C:825:SER:OG	2.33	0.45
1:A:864:ARG:HE	1:A:864:ARG:HB3	1.56	0.45
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.15	0.45
1:A:79:PRO:HA	1:A:80:SER:HA	1.58	0.45
2:B:226:PRO:HB2	2:B:250:GLY:HA3	1.99	0.45
2:B:891:HIS:CD2	3:D:240:VAL:HG21	2.52	0.45
2:B:1075:ARG:NH2	2:B:1167:ASP:OD1	2.45	0.45
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.73	0.45
1:A:613:ILE:HD11	1:A:642:ALA:HB3	1.98	0.45
2:B:759:ASP:OD2	2:B:761:SER:OG	2.35	0.45
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	1.97	0.45
1:A:734:ILE:HG12	1:A:746:PHE:CE1	2.52	0.45
2:C:190:VAL:HG23	2:C:300:LEU:HD22	1.99	0.45
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.99	0.45
2:C:529:LYS:HD2	2:C:589:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.51	0.45
2:C:700:ASP:HB3	2:C:1326:ARG:HG2	1.97	0.45
3:E:160:LEU:HD11	3:E:229:PHE:HA	1.98	0.45
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.99	0.45
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.68	0.45
1:A:1056:VAL:O	1:A:1057:ARG:HD2	2.17	0.45
3:E:229:PHE:O	3:E:233:THR:HG23	2.17	0.45
1:A:7:ILE:HG13	1:A:250:LEU:HD11	1.98	0.45
1:A:238:ASP:OD2	1:A:259:ARG:NE	2.36	0.45
1:A:741:TYR:CZ	1:A:746:PHE:HZ	2.35	0.45
2:C:307:VAL:HA	2:C:1247:ASN:ND2	2.32	0.45
2:C:833:ARG:HD2	2:C:941:TYR:CD2	2.52	0.45
1:A:473:VAL:HG11	1:A:494:THR:HG23	1.98	0.45
1:A:677:LEU:HG	1:A:706:TYR:CE2	2.52	0.45
1:A:772:TRP:HH2	1:A:784:ILE:HD11	1.82	0.45
2:C:626:ARG:HG2	2:C:631:PRO:HB3	1.99	0.45
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.99	0.45
1:A:890:LEU:HD13	1:A:891:THR:N	2.32	0.45
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.17	0.45
2:B:543:TRP:CH2	2:B:666:ARG:HG2	2.52	0.45
2:B:547:GLU:HG2	2:B:599:THR:OG1	2.17	0.45
2:B:616:ASP:O	2:B:620:ILE:HG13	2.16	0.45
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.52	0.45
3:E:159:GLU:O	3:E:225:ARG:HG2	2.17	0.45
1:A:42:PHE:CZ	1:A:44:SER:HA	2.51	0.44
1:A:93:HIS:NE2	1:A:97:ARG:HD2	2.33	0.44
2:B:332:THR:HA	2:B:344:VAL:HG12	1.99	0.44
2:B:1139:MET:HB3	2:B:1166:VAL:HG12	1.99	0.44
2:B:1214:GLU:HG2	2:B:1215:PRO:HD2	1.98	0.44
2:B:1233:LEU:HD13	2:B:1233:LEU:HA	1.66	0.44
1:A:114:ASN:HD22	1:A:149:ALA:HB1	1.81	0.44
1:A:869:ILE:O	1:A:872:VAL:HG12	2.17	0.44
2:B:169:LYS:O	2:B:202:ALA:N	2.46	0.44
2:B:447:ARG:HH22	2:B:770:CYS:N	2.15	0.44
2:C:289:THR:O	2:C:328:GLY:HA3	2.16	0.44
2:C:515:ILE:HD12	2:C:659:LEU:HD11	1.99	0.44
2:C:1076:ILE:HB	2:C:1166:VAL:HG22	2.00	0.44
2:C:1212:ARG:HA	2:C:1213:PRO:HD2	1.82	0.44
2:B:774:LEU:HD23	2:B:774:LEU:HA	1.78	0.44
2:C:1031:TYR:HH	2:C:1038:GLU:HA	1.81	0.44
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:LEU:HB2	2:B:528:ILE:HD12	1.98	0.44
2:B:921:ASP:O	2:B:928:ARG:NH1	2.51	0.44
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.34	0.44
2:C:615:THR:H	2:C:1333:ALA:HA	1.82	0.44
2:C:646:ASN:HD21	2:C:699:THR:HG21	1.81	0.44
1:A:256:VAL:HG22	1:A:335:LEU:HD13	2.00	0.44
1:A:679:LYS:HE3	1:A:714:ARG:HH21	1.81	0.44
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	2.00	0.44
2:C:196:LEU:HD12	2:C:196:LEU:HA	1.87	0.44
2:C:227:LEU:HD22	2:C:246:GLU:HB2	1.99	0.44
2:C:775:VAL:HA	2:C:776:ARG:HA	1.62	0.44
2:C:850:THR:HG22	2:C:916:LEU:HD11	1.99	0.44
3:D:68:ILE:HD12	3:D:68:ILE:HA	1.74	0.44
2:B:176:LYS:HB2	2:B:176:LYS:HE2	1.60	0.44
2:B:362:LEU:HD22	2:B:1303:SER:OG	2.18	0.44
2:C:699:THR:OG1	2:C:700:ASP:OD2	2.33	0.44
3:D:102:SER:O	3:D:114:SER:HA	2.18	0.44
1:A:278:LEU:HD21	1:A:315:LEU:HD11	2.00	0.44
1:A:849:ILE:HD12	1:A:871:VAL:HG12	2.00	0.44
2:B:267:VAL:HG13	2:B:291:HIS:HE1	1.82	0.44
2:B:843:LEU:HG	2:B:942:HIS:CG	2.52	0.44
2:B:846:GLY:O	2:B:911:ARG:HG3	2.17	0.44
2:B:1305:MET:HE2	2:B:1309:ILE:HG21	2.00	0.44
2:C:303:ASP:N	2:C:311:ASN:OD1	2.48	0.44
2:C:674:LYS:HD2	2:C:674:LYS:HA	1.64	0.44
2:C:736:SER:HB3	2:C:1017:ALA:HA	2.00	0.44
1:A:308:ALA:HB1	1:A:312:LEU:HB3	1.99	0.44
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.99	0.44
2:C:150:LEU:HD21	2:C:399:PRO:HD2	2.00	0.44
2:C:633:THR:HG21	2:C:710:SER:HB2	1.99	0.44
3:D:239:VAL:CG1	3:D:250:ARG:HD2	2.47	0.44
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.51	0.44
1:A:936:ALA:HA	1:A:939:GLN:HG3	1.99	0.44
2:B:762:ILE:HD12	2:B:762:ILE:HA	1.88	0.44
2:B:1170:ASP:OD1	2:B:1198:LYS:HE2	2.18	0.43
2:C:163:TYR:O	2:C:209:ASN:N	2.40	0.43
2:C:446:LYS:HB3	2:C:448:TYR:CD2	2.52	0.43
2:C:873:TYR:HA	2:C:896:LEU:O	2.18	0.43
3:D:19:ILE:H	3:D:19:ILE:HG13	1.73	0.43
1:A:388:VAL:HG23	1:A:736:GLY:HA3	2.01	0.43
2:B:204:VAL:HG12	2:B:1241:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:ILE:HG23	2:B:766:ILE:HD11	2.00	0.43
2:B:629:ARG:HH11	2:B:1037:ILE:HA	1.83	0.43
1:A:114:ASN:OD1	1:A:117:LEU:HB2	2.18	0.43
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.53	0.43
1:A:812:VAL:HA	1:A:813:PRO:HA	1.79	0.43
2:B:223:LYS:HB3	2:B:1174:THR:HG21	2.00	0.43
2:C:478:ILE:HG12	2:C:762:ILE:HD11	2.01	0.43
2:C:816:PRO:HB3	2:C:986:ILE:HG22	2.00	0.43
2:B:462:LEU:HD12	2:B:506:SER:HB3	1.99	0.43
2:B:1270:LEU:HA	2:B:1270:LEU:HD23	1.66	0.43
2:C:600:ILE:O	2:C:604:MET:HG2	2.18	0.43
2:B:147:VAL:HG22	2:B:379:LEU:HD11	2.00	0.43
2:B:385:ILE:H	2:B:385:ILE:HG12	1.59	0.43
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.34	0.43
2:B:765:PRO:HA	2:B:769:GLN:HG2	2.01	0.43
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.46	0.43
2:C:931:ASN:HD21	2:C:936:MET:HB3	1.84	0.43
2:C:1075:ARG:NH1	2:C:1090:PRO:O	2.52	0.43
3:E:53:GLU:CD	3:E:53:GLU:H	2.21	0.43
1:A:62:PHE:HB2	1:A:67:ARG:HD3	1.99	0.43
1:A:828:TYR:HA	1:A:1032:GLY:O	2.18	0.43
2:B:707:ALA:O	2:B:710:SER:HB3	2.19	0.43
2:C:714:LEU:HD23	2:C:714:LEU:HA	1.87	0.43
1:A:864:ARG:HD3	4:A:1101:SAM:HG2	2.01	0.43
2:B:1159:VAL:HA	2:B:1164:TRP:HB2	2.01	0.43
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.52	0.43
2:C:352:HIS:O	2:C:356:SER:OG	2.22	0.43
3:D:229:PHE:O	3:D:233:THR:HG23	2.19	0.43
3:E:70:ASP:O	3:E:74:GLN:HB2	2.19	0.43
2:B:557:THR:OG1	2:B:558:TYR:N	2.50	0.43
2:C:154:PHE:CE2	2:C:365:LEU:HB2	2.54	0.43
2:C:325:TYR:HA	2:C:1267:THR:CG2	2.48	0.43
2:C:862:ARG:NH1	2:C:948:ILE:HG12	2.34	0.43
3:D:4:GLN:HA	3:D:5:PRO:HD3	1.90	0.43
1:A:462:ILE:HG12	1:A:682:SER:O	2.19	0.43
2:B:948:ILE:HA	2:B:948:ILE:HD12	1.74	0.43
2:C:528:ILE:HA	2:C:577:GLN:NE2	2.33	0.43
3:E:137:LEU:HD21	3:E:282:PHE:HB2	2.01	0.43
1:A:184:TRP:HB3	1:A:195:ILE:HD13	2.00	0.43
1:A:207:THR:CG2	1:A:218:THR:HG22	2.48	0.43
1:A:886:ARG:H	1:A:886:ARG:HG3	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:ILE:H	2:B:515:ILE:HG12	1.53	0.43
2:B:546:VAL:O	2:B:550:ILE:HG13	2.19	0.43
2:C:1050:LEU:HD12	2:C:1050:LEU:HA	1.84	0.43
2:C:1097:VAL:HG11	2:C:1123:PRO:HG2	2.00	0.43
2:B:419:TYR:CG	2:B:1005:LEU:HD13	2.54	0.42
2:C:152:ASP:OD1	2:C:152:ASP:N	2.46	0.42
2:C:1175:ALA:HA	2:C:1204:LEU:O	2.19	0.42
1:A:204:LEU:HB3	1:A:221:TYR:HB2	2.01	0.42
2:B:414:LEU:HD12	2:B:414:LEU:HA	1.70	0.42
2:B:511:VAL:O	2:B:515:ILE:HG12	2.19	0.42
2:C:251:LEU:HD23	2:C:251:LEU:HA	1.76	0.42
1:A:537:VAL:HG13	1:A:550:TYR:CE2	2.53	0.42
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.19	0.42
2:C:157:ILE:HG12	2:C:263:ARG:HB3	2.00	0.42
1:A:565:ARG:HA	1:A:565:ARG:HD3	1.74	0.42
1:A:841:MET:HA	1:A:1019:PRO:HG3	2.02	0.42
2:B:886:SER:O	2:B:890:THR:HG23	2.20	0.42
2:C:502:PHE:O	2:C:542:ARG:HG2	2.19	0.42
2:C:890:THR:OG1	2:C:892:VAL:HG12	2.19	0.42
2:C:1022:ILE:HG22	2:C:1028:VAL:HA	2.01	0.42
3:D:7:GLY:HA3	3:D:11:THR:HG21	2.01	0.42
3:D:133:THR:OG1	3:D:134:TYR:N	2.51	0.42
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.54	0.42
1:A:456:PHE:HD1	1:A:456:PHE:HA	1.67	0.42
2:C:637:TYR:OH	2:C:702:LEU:HD23	2.19	0.42
3:D:187:ILE:HD13	3:D:187:ILE:HA	1.92	0.42
1:A:681:ALA:HA	1:A:1041:ALA:HB2	2.00	0.42
1:A:977:HIS:O	1:A:981:ARG:HB3	2.19	0.42
2:B:255:LEU:HD23	2:B:819:PHE:CZ	2.54	0.42
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	2.01	0.42
3:E:105:LEU:HD13	3:E:111:ILE:HG12	2.02	0.42
3:E:240:VAL:O	3:E:250:ARG:HD3	2.20	0.42
2:B:147:VAL:HG11	2:B:375:ARG:HB3	2.02	0.42
2:B:537:LEU:HD23	2:B:537:LEU:HA	1.73	0.42
2:B:793:TYR:HA	2:B:794:PRO:HD3	1.88	0.42
2:B:931:ASN:OD1	2:B:931:ASN:N	2.40	0.42
3:D:69:GLU:O	3:D:73:THR:OG1	2.30	0.42
1:A:324:ARG:O	1:A:349:TYR:OH	2.28	0.42
1:A:398:GLU:HA	1:A:401:ILE:O	2.19	0.42
1:A:406:VAL:HG13	1:A:1034:ARG:HD2	2.02	0.42
1:A:453:LEU:HA	1:A:1025:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:THR:O	1:A:696:PRO:HD2	2.19	0.42
2:B:924:ASP:O	2:B:927:SER:OG	2.29	0.42
2:C:348:LEU:HD12	2:C:1302:VAL:HG21	2.00	0.42
2:C:664:ASN:HB2	2:C:681:LYS:NZ	2.34	0.42
1:A:417:TYR:CD1	1:A:537:VAL:HG21	2.55	0.42
2:B:336:TYR:HD2	3:D:89:TYR:CE2	2.37	0.42
2:B:379:LEU:HD23	2:B:379:LEU:HA	1.89	0.42
2:B:659:LEU:HD23	2:B:659:LEU:HA	1.84	0.42
2:C:168:VAL:HG11	2:C:196:LEU:HG	2.02	0.42
3:D:35:LEU:HA	3:D:35:LEU:HD12	1.79	0.42
3:D:188:SER:O	3:D:191:ARG:HG3	2.19	0.42
1:A:114:ASN:HA	1:A:143:TYR:HE2	1.85	0.42
1:A:894:LYS:HD3	1:A:894:LYS:HA	1.73	0.42
1:A:1007:LEU:HD12	1:A:1007:LEU:HA	1.79	0.42
2:B:685:ARG:O	2:B:689:THR:HG23	2.19	0.42
2:B:1193:ILE:HD13	2:B:1193:ILE:HA	1.74	0.42
1:A:36:THR:O	1:A:54:LEU:HB2	2.20	0.41
1:A:183:ILE:H	1:A:183:ILE:HG12	1.56	0.41
1:A:415:ASP:HB3	1:A:1038:THR:HG21	2.01	0.41
1:A:728:PRO:HG3	1:A:828:TYR:CE2	2.54	0.41
2:B:806:VAL:O	2:B:810:LEU:HG	2.20	0.41
2:B:885:ALA:HA	2:B:888:GLN:HE21	1.85	0.41
2:C:307:VAL:HA	2:C:1247:ASN:HD21	1.85	0.41
2:C:450:PRO:HG3	2:C:686:HIS:CB	2.49	0.41
2:C:537:LEU:HA	2:C:537:LEU:HD23	1.74	0.41
2:C:852:TYR:CZ	2:C:856:LEU:HD21	2.54	0.41
2:C:1211:LEU:HD23	2:C:1211:LEU:HA	1.68	0.41
3:E:153:TYR:O	3:E:156:VAL:HB	2.20	0.41
1:A:714:ARG:NE	1:A:1044:ASP:OD2	2.53	0.41
1:A:765:TYR:HA	1:A:792:ILE:HG13	2.01	0.41
2:B:1176:GLU:HB2	2:B:1203:HIS:CE1	2.55	0.41
2:C:636:PRO:HG2	2:C:706:TYR:CE2	2.54	0.41
2:C:1193:ILE:HD12	2:C:1202:PHE:CE1	2.55	0.41
1:A:561:LEU:HD23	1:A:561:LEU:N	2.36	0.41
1:A:788:ASP:HA	1:A:789:PRO:HD3	1.88	0.41
2:B:392:PRO:HD2	2:B:1315:MET:HE2	2.02	0.41
2:B:425:ILE:HG13	2:B:1004:PHE:HD2	1.85	0.41
2:C:1025:ASP:OD1	2:C:1027:THR:HG23	2.20	0.41
2:C:1230:ILE:H	2:C:1230:ILE:HG12	1.74	0.41
3:D:123:ASP:O	3:D:127:VAL:HG23	2.20	0.41
3:E:253:GLU:HA	3:E:254:TYR:HA	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:HE1	1:A:47:ARG:HA	1.84	0.41
2:C:414:LEU:HD12	2:C:414:LEU:HA	1.92	0.41
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.44	0.41
2:C:838:GLU:HB2	2:C:911:ARG:HH21	1.84	0.41
2:C:1116:ARG:HH11	2:C:1116:ARG:HB3	1.84	0.41
1:A:528:SER:O	1:A:532:MET:HG2	2.20	0.41
1:A:710:ALA:HB2	1:A:1048:HIS:HB3	2.02	0.41
2:B:278:LEU:HD22	2:B:282:VAL:HG11	2.03	0.41
2:B:482:ILE:HG23	2:B:706:TYR:CZ	2.55	0.41
2:B:529:LYS:HB2	2:B:589:PHE:CE2	2.56	0.41
2:B:1278:TYR:CD2	2:B:1290:LYS:HE2	2.56	0.41
2:C:1049:GLU:O	2:C:1053:ARG:HG2	2.20	0.41
1:A:828:TYR:O	1:A:1034:ARG:HG2	2.21	0.41
2:B:810:LEU:HD23	2:B:810:LEU:HA	1.83	0.41
2:C:1267:THR:HB	2:C:1299:SER:CB	2.50	0.41
2:B:769:GLN:HE21	2:B:769:GLN:HB2	1.74	0.41
2:C:1233:LEU:HD12	2:C:1233:LEU:HA	1.67	0.41
3:E:156:VAL:HG22	3:E:228:LEU:HD22	2.02	0.41
1:A:764:SER:HB2	1:A:765:TYR:CE2	2.55	0.41
2:B:227:LEU:HA	2:B:246:GLU:O	2.21	0.41
2:B:271:THR:O	2:B:289:THR:HA	2.21	0.41
2:B:343:ILE:HD12	2:B:362:LEU:HD11	2.02	0.41
2:B:382:HIS:HA	2:B:712:PHE:CE1	2.56	0.41
2:B:639:ASN:OD1	2:B:639:ASN:N	2.54	0.41
2:B:659:LEU:O	2:B:663:VAL:HG23	2.21	0.41
2:B:714:LEU:HA	2:B:714:LEU:HD23	1.61	0.41
2:C:223:LYS:HZ2	2:C:1203:HIS:HB2	1.86	0.41
2:C:251:LEU:HD22	2:C:1062:ILE:HG13	2.02	0.41
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.20	0.41
3:E:35:LEU:HD21	3:E:229:PHE:CE2	2.55	0.41
1:A:46:ARG:HD2	1:A:46:ARG:N	2.36	0.41
1:A:419:TYR:HB2	1:A:678:LEU:HG	2.03	0.41
1:A:773:ARG:O	1:A:818:PHE:HA	2.21	0.41
1:A:912:ASP:OD1	1:A:912:ASP:N	2.52	0.41
4:A:1101:SAM:HE1	4:A:1101:SAM:HB2	1.85	0.41
2:B:135:LYS:HB3	2:B:136:VAL:H	1.67	0.41
2:B:243:GLN:O	2:B:246:GLU:HB2	2.20	0.41
2:B:347:ALA:HB1	2:B:1267:THR:OG1	2.21	0.41
2:B:492:VAL:HB	2:B:747:ARG:HG2	2.03	0.41
2:B:709:MET:HG2	2:B:712:PHE:CE2	2.56	0.41
2:B:728:LYS:HD3	2:B:728:LYS:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:THR:O	2:B:802:GLN:HG2	2.21	0.41
2:B:1220:PRO:HA	2:B:1221:PRO:HD3	1.90	0.41
2:C:102:VAL:H	2:C:102:VAL:HG23	1.66	0.41
2:C:244:SER:HB2	2:C:1201:LEU:HD13	2.03	0.41
2:C:366:MET:HG2	3:E:266:THR:HG21	2.02	0.41
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	2.02	0.41
2:C:1064:ASN:HA	2:C:1065:PRO:HD3	1.91	0.41
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.92	0.41
3:D:28:PRO:HG3	3:D:223:VAL:HG22	2.02	0.41
3:E:19:ILE:HG23	3:E:196:TRP:CZ2	2.56	0.41
1:A:289:ASP:OD1	1:A:291:SER:OG	2.37	0.41
1:A:658:ILE:O	1:A:662:ILE:HG12	2.20	0.41
2:B:338:ARG:HD2	2:B:338:ARG:N	2.35	0.41
2:B:514:PHE:CD2	2:B:532:ILE:HG23	2.56	0.41
2:B:809:VAL:O	2:B:813:LEU:HB2	2.21	0.41
2:B:820:ILE:HD13	2:B:820:ILE:HA	1.92	0.41
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.56	0.41
2:B:836:GLN:OE1	2:B:836:GLN:N	2.55	0.41
2:C:375:ARG:HE	2:C:375:ARG:HB2	1.60	0.41
2:C:1267:THR:HB	2:C:1299:SER:HB3	2.03	0.41
3:E:185:SER:O	3:E:189:LEU:HB2	2.21	0.41
2:B:875:THR:HG23	2:B:877:ALA:H	1.86	0.40
2:B:1219:ASP:HA	2:B:1220:PRO:HD3	1.83	0.40
2:C:171:GLU:HG3	2:C:1211:LEU:HB3	2.02	0.40
2:C:213:PHE:CE1	2:C:254:VAL:HG13	2.56	0.40
2:C:244:SER:HB3	2:C:1199:GLY:O	2.20	0.40
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.91	0.40
2:C:1080:THR:HG22	2:C:1227:MET:SD	2.61	0.40
3:E:44:LEU:HD13	3:E:154:ALA:HA	2.03	0.40
1:A:967:ILE:HD12	1:A:987:LEU:HD12	2.03	0.40
2:B:354:ALA:O	2:B:358:LEU:HG	2.21	0.40
2:B:541:SER:HA	2:B:548:TYR:CG	2.56	0.40
3:D:14:GLN:HE22	3:D:107:LEU:HD23	1.87	0.40
3:E:123:ASP:HA	3:E:124:PRO:HD3	1.88	0.40
1:A:166:ILE:HD11	1:A:178:PRO:HD2	2.04	0.40
1:A:427:ASP:HB3	1:A:703:PHE:CD1	2.57	0.40
2:B:330:THR:HG23	2:B:331:GLU:H	1.86	0.40
2:C:248:VAL:HG13	2:C:970:LEU:HB3	2.03	0.40
2:C:301:LEU:HB3	2:C:305:THR:HG22	2.04	0.40
2:C:1013:LYS:HE2	2:C:1015:GLN:HE21	1.85	0.40
3:D:75:ALA:O	3:D:275:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:HB1	1:A:187:PRO:HA	2.02	0.40
1:A:460:VAL:HG12	1:A:465:LEU:HD11	2.03	0.40
1:A:928:GLU:HG2	1:A:934:THR:HG22	2.04	0.40
2:B:193:THR:HA	2:B:296:VAL:HG12	2.04	0.40
2:B:267:VAL:HG22	2:B:1304:MET:HG3	2.03	0.40
2:B:489:MET:HE3	2:B:580:TYR:HE2	1.86	0.40
2:C:603:ILE:HD11	2:C:662:VAL:HG21	2.03	0.40
1:A:40:TYR:OH	1:A:83:ILE:HG13	2.22	0.40
1:A:161:TYR:HB2	1:A:183:ILE:O	2.22	0.40
1:A:236:LEU:HD21	1:A:240:ARG:HH21	1.87	0.40
1:A:711:MET:H	1:A:711:MET:HG2	1.69	0.40
1:A:797:ARG:HD2	1:A:869:ILE:HD11	2.03	0.40
2:B:493:HIS:O	2:B:577:GLN:NE2	2.54	0.40
2:B:926:VAL:HG22	2:B:936:MET:HG2	2.03	0.40
2:C:253:MET:N	2:C:253:MET:SD	2.93	0.40
2:C:650:SER:HA	2:C:653:ARG:CZ	2.52	0.40
2:C:795:ASP:O	2:C:798:THR:HG22	2.22	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%)	1004 (95%)	45 (4%)	6 (1%)	25	59
2	B	1187/1333 (89%)	1135 (96%)	49 (4%)	3 (0%)	41	73
2	C	1246/1333 (94%)	1181 (95%)	60 (5%)	5 (0%)	34	69
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	41	73
3	E	290/448 (65%)	281 (97%)	9 (3%)	0	100	100
All	All	4068/4620 (88%)	3882 (95%)	171 (4%)	15 (0%)	38	69

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	C	1145	ALA
2	C	1251	VAL
2	B	1123	PRO
3	D	244	VAL
1	A	483	MET
1	A	979	THR
2	C	1267	THR
1	A	728	PRO
2	B	288	THR
2	B	1068	ALA
1	A	854	ASN
1	A	884	ALA
2	C	775	VAL
2	C	1093	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	942/943 (100%)	829 (88%)	113 (12%)	5 20
2	B	1038/1153 (90%)	963 (93%)	75 (7%)	14 44
2	C	1089/1153 (94%)	980 (90%)	109 (10%)	7 28
3	D	240/379 (63%)	215 (90%)	25 (10%)	7 27
3	E	240/379 (63%)	222 (92%)	18 (8%)	13 42
All	All	3549/4007 (89%)	3209 (90%)	340 (10%)	12 31

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	39	LEU
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	52	ARG
1	A	74	LEU
1	A	76	LEU
1	A	83	ILE
1	A	88	LEU
1	A	92	LEU
1	A	110	THR
1	A	117	LEU
1	A	128	THR
1	A	133	LEU
1	A	157	LEU
1	A	166	ILE
1	A	185	HIS
1	A	199	MET
1	A	205	VAL
1	A	222	ARG
1	A	234	LYS
1	A	254	ASP
1	A	260	LEU
1	A	272	LEU
1	A	275	ILE
1	A	284	THR
1	A	293	LEU
1	A	300	LEU
1	A	311	GLN
1	A	312	LEU
1	A	315	LEU
1	A	324	ARG
1	A	335	LEU
1	A	337	LEU
1	A	340	ILE
1	A	346	ILE
1	A	357	THR
1	A	358	ILE
1	A	362	MET
1	A	379	VAL
1	A	388	VAL
1	A	390	ASP
1	A	401	ILE
1	A	402	THR
1	A	405	MET

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Mol	Chain	Res	Type
1	A	420	VAL
1	A	421	LEU
1	A	429	TRP
1	A	444	LEU
1	A	456	PHE
1	A	464	ASP
1	A	466	LEU
1	A	483	MET
1	A	486	THR
1	A	494	THR
1	A	503	ILE
1	A	504	THR
1	A	518	TYR
1	A	523	MET
1	A	545	PHE
1	A	551	LEU
1	A	561	LEU
1	A	583	ARG
1	A	587	MET
1	A	626	GLU
1	A	628	MET
1	A	647	LEU
1	A	648	VAL
1	A	668	LEU
1	A	680	THR
1	A	692	ILE
1	A	719	VAL
1	A	723	GLU
1	A	724	MET
1	A	726	ILE
1	A	731	HIS
1	A	738	SER
1	A	746	PHE
1	A	747	CYS
1	A	763	LYS
1	A	765	TYR
1	A	780	LEU
1	A	782	ASN
1	A	792	ILE
1	A	824	ARG
1	A	832	GLU
1	A	833	VAL

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Mol	Chain	Res	Type
1	A	849	ILE
1	A	866	LEU
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	902	ARG
1	A	910	ASN
1	A	918	ILE
1	A	925	ILE
1	A	926	MET
1	A	941	ASP
1	A	951	LEU
1	A	952	THR
1	A	960	ILE
1	A	967	ILE
1	A	970	ARG
1	A	971	LEU
1	A	981	ARG
1	A	996	ASP
1	A	1007	LEU
1	A	1013	THR
1	A	1018	ARG
1	A	1024	LEU
1	A	1025	ILE
1	A	1034	ARG
1	A	1035	LEU
2	B	144	ASN
2	B	147	VAL
2	B	165	THR
2	B	176	LYS
2	B	190	VAL
2	B	217	THR
2	B	223	LYS
2	B	233	VAL
2	B	235	ILE
2	B	264	LEU
2	B	280	THR
2	B	291	HIS
2	B	293	ASN
2	B	294	VAL
2	B	315	THR
2	B	323	THR

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Mol	Chain	Res	Type
2	B	329	LEU
2	B	330	THR
2	B	335	ASP
2	B	340	VAL
2	B	384	MET
2	B	477	SER
2	B	506	SER
2	B	510	VAL
2	B	515	ILE
2	B	533	GLN
2	B	557	THR
2	B	605	ARG
2	B	633	THR
2	B	637	TYR
2	B	640	GLN
2	B	647	GLU
2	B	661	ASN
2	B	689	THR
2	B	708	THR
2	B	740	SER
2	B	748	GLN
2	B	755	LEU
2	B	767	LEU
2	B	774	LEU
2	B	797	SER
2	B	799	THR
2	B	802	GLN
2	B	811	SER
2	B	815	LEU
2	B	851	THR
2	B	912	GLU
2	B	921	ASP
2	B	931	ASN
2	B	946	LEU
2	B	948	ILE
2	B	966	GLN
2	B	976	THR
2	B	1036	ASP
2	B	1050	LEU
2	B	1052	LEU
2	B	1060	ARG
2	B	1061	LEU

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Mol	Chain	Res	Type
2	B	1062	ILE
2	B	1092	VAL
2	B	1110	LEU
2	B	1120	THR
2	B	1132	THR
2	B	1179	THR
2	B	1193	ILE
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1249	ASN
2	B	1262	SER
2	B	1269	THR
2	B	1270	LEU
2	B	1294	ASP
2	B	1311	THR
2	B	1331	ARG
2	C	74	LYS
2	C	77	THR
2	C	98	ASN
2	C	116	SER
2	C	118	THR
2	C	120	VAL
2	C	133	THR
2	C	142	ASP
2	C	145	THR
2	C	156	GLN
2	C	168	VAL
2	C	180	LEU
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	217	THR
2	C	231	LEU
2	C	243	GLN
2	C	244	SER
2	C	248	VAL
2	C	264	LEU
2	C	281	VAL
2	C	285	VAL
2	C	289	THR
2	C	294	VAL

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Mol	Chain	Res	Type
2	C	296	VAL
2	C	305	THR
2	C	315	THR
2	C	318	LEU
2	C	323	THR
2	C	329	LEU
2	C	330	THR
2	C	339	LEU
2	C	340	VAL
2	C	341	LYS
2	C	342	THR
2	C	363	ARG
2	C	375	ARG
2	C	384	MET
2	C	475	ILE
2	C	484	ARG
2	C	489	MET
2	C	508	ILE
2	C	546	VAL
2	C	552	VAL
2	C	579	LEU
2	C	599	THR
2	C	603	ILE
2	C	626	ARG
2	C	633	THR
2	C	637	TYR
2	C	654	THR
2	C	661	ASN
2	C	663	VAL
2	C	664	ASN
2	C	674	LYS
2	C	678	SER
2	C	684	LEU
2	C	696	VAL
2	C	701	HIS
2	C	708	THR
2	C	710	SER
2	C	713	MET
2	C	760	THR
2	C	767	LEU
2	C	775	VAL
2	C	815	LEU

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Mol	Chain	Res	Type
2	C	820	ILE
2	C	828	ASP
2	C	833	ARG
2	C	851	THR
2	C	865	ILE
2	C	892	VAL
2	C	896	LEU
2	C	911	ARG
2	C	946	LEU
2	C	962	ASP
2	C	980	ARG
2	C	1005	LEU
2	C	1009	THR
2	C	1014	MET
2	C	1016	ASN
2	C	1027	THR
2	C	1029	LEU
2	C	1035	ILE
2	C	1052	LEU
2	C	1055	LEU
2	C	1056	SER
2	C	1060	ARG
2	C	1061	LEU
2	C	1069	ARG
2	C	1070	ARG
2	C	1072	ASN
2	C	1079	LEU
2	C	1092	VAL
2	C	1116	ARG
2	C	1138	HIS
2	C	1163	ASN
2	C	1188	VAL
2	C	1201	LEU
2	C	1202	PHE
2	C	1225	GLU
2	C	1230	ILE
2	C	1233	LEU
2	C	1251	VAL
2	C	1267	THR
2	C	1269	THR
2	C	1320	VAL
2	C	1331	ARG

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Mol	Chain	Res	Type
3	D	2	LEU
3	D	21	ASN
3	D	29	THR
3	D	30	GLN
3	D	47	LYS
3	D	51	THR
3	D	70	ASP
3	D	73	THR
3	D	77	PHE
3	D	92	ARG
3	D	93	LEU
3	D	116	THR
3	D	133	THR
3	D	139	ASN
3	D	142	THR
3	D	149	MET
3	D	158	LEU
3	D	160	LEU
3	D	191	ARG
3	D	226	MET
3	D	240	VAL
3	D	252	LEU
3	D	266	THR
3	D	273	LEU
3	D	281	LYS
3	E	2	LEU
3	E	29	THR
3	E	48	THR
3	E	54	THR
3	E	66	VAL
3	E	92	ARG
3	E	93	LEU
3	E	116	THR
3	E	133	THR
3	E	139	ASN
3	E	160	LEU
3	E	189	LEU
3	E	213	LEU
3	E	226	MET
3	E	252	LEU
3	E	257	VAL
3	E	262	THR

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Mol	Chain	Res	Type
3	E	272	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	HIS
1	A	286	ASN
1	A	595	ASN
1	A	910	ASN
2	B	491	ASN
2	B	526	ASN
2	B	858	HIS
2	B	1138	HIS
2	C	156	GLN
2	C	293	ASN
2	C	430	ASN
2	C	526	ASN
2	C	724	HIS
2	C	981	HIS
2	C	1138	HIS
2	C	1186	GLN
2	C	1203	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

1 ligand is modelled in this entry.

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	1.21	3 (12%)	23,42,42	1.59	4 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	A	1101	-	-	6/12/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N3	3.85	1.38	1.32
4	A	1101	SAM	C2-N1	2.62	1.38	1.33
4	A	1101	SAM	OXT-C	-2.11	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	SAM	N3-C2-N1	-5.23	120.51	128.68
4	A	1101	SAM	C3'-C2'-C1'	3.12	105.67	100.98
4	A	1101	SAM	OXT-C-O	-2.52	118.36	124.09
4	A	1101	SAM	OXT-C-CA	2.22	120.95	113.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	N-CA-CB-CG
4	A	1101	SAM	C-CA-CB-CG
4	A	1101	SAM	CB-CG-SD-CE
4	A	1101	SAM	CB-CG-SD-C5'

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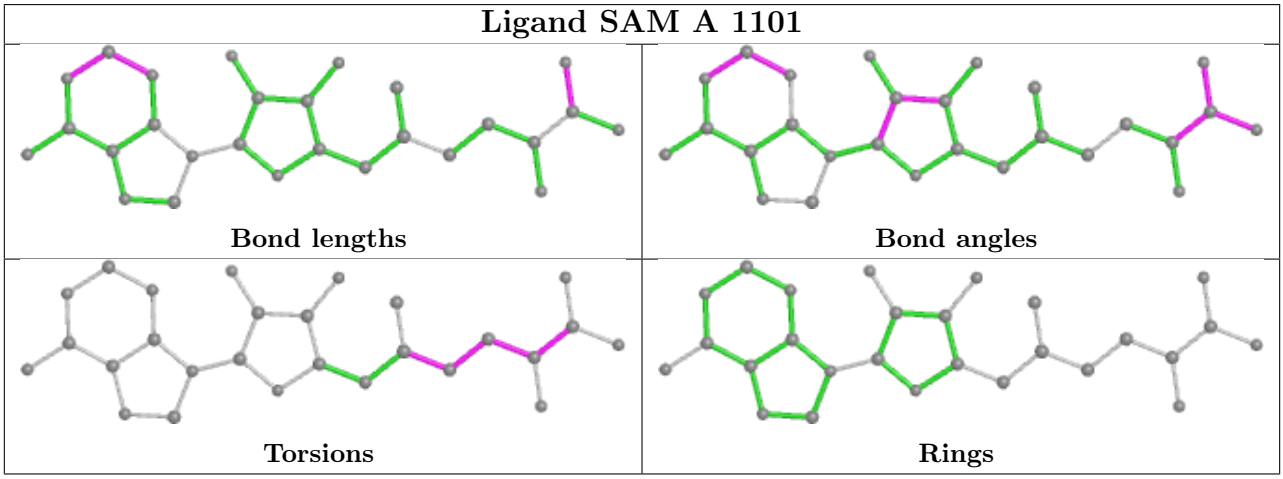
Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	CA-CB-CG-SD
4	A	1101	SAM	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	5	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

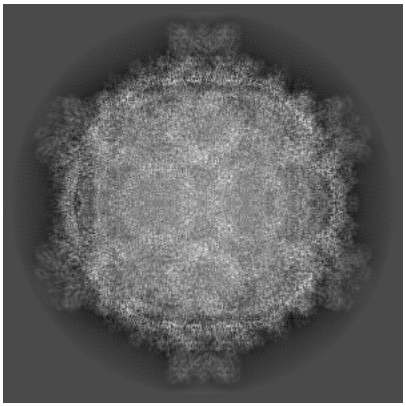
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6375. These allow visual inspection of the internal detail of the map and identification of artifacts.

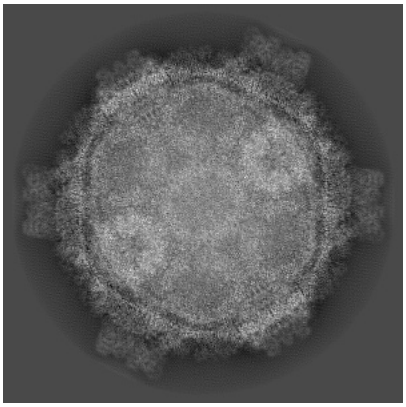
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

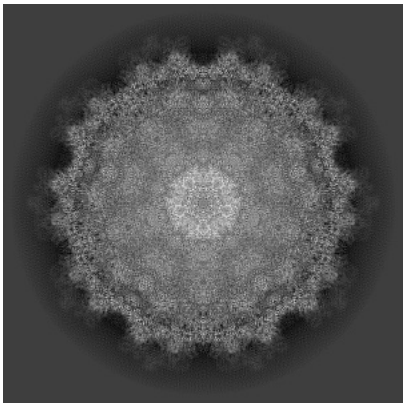
6.1.1 Primary map



X



Y

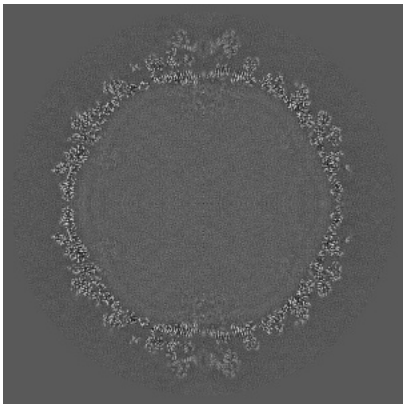


Z

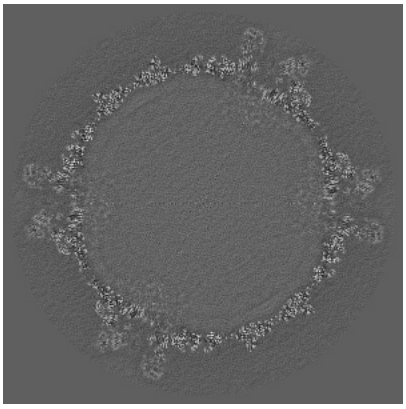
The images above show the map projected in three orthogonal directions.

6.2 Central slices

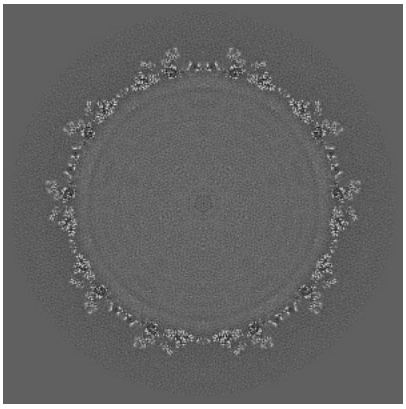
6.2.1 Primary map



X Index: 350



Y Index: 350

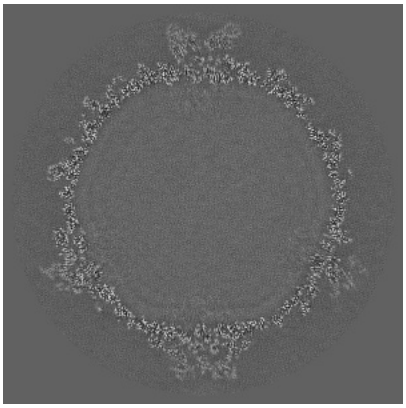


Z Index: 350

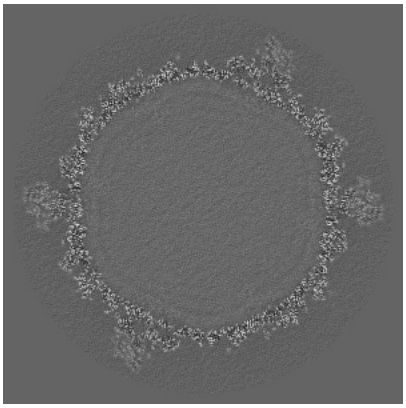
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

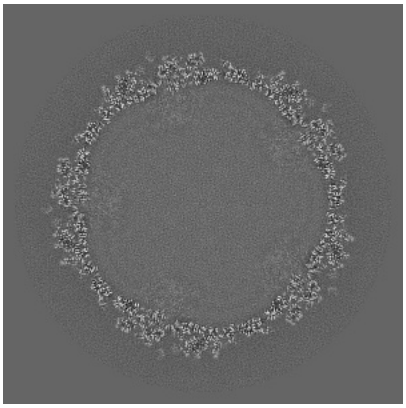
6.3.1 Primary map



X Index: 327



Y Index: 300

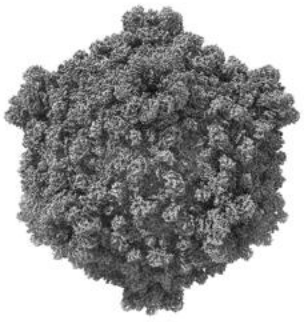


Z Index: 286

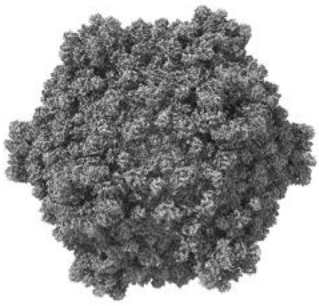
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

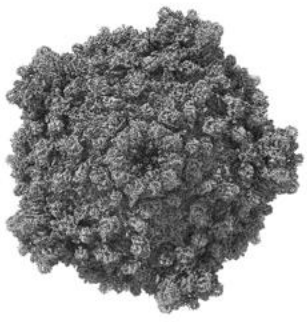
6.4.1 Primary map



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.

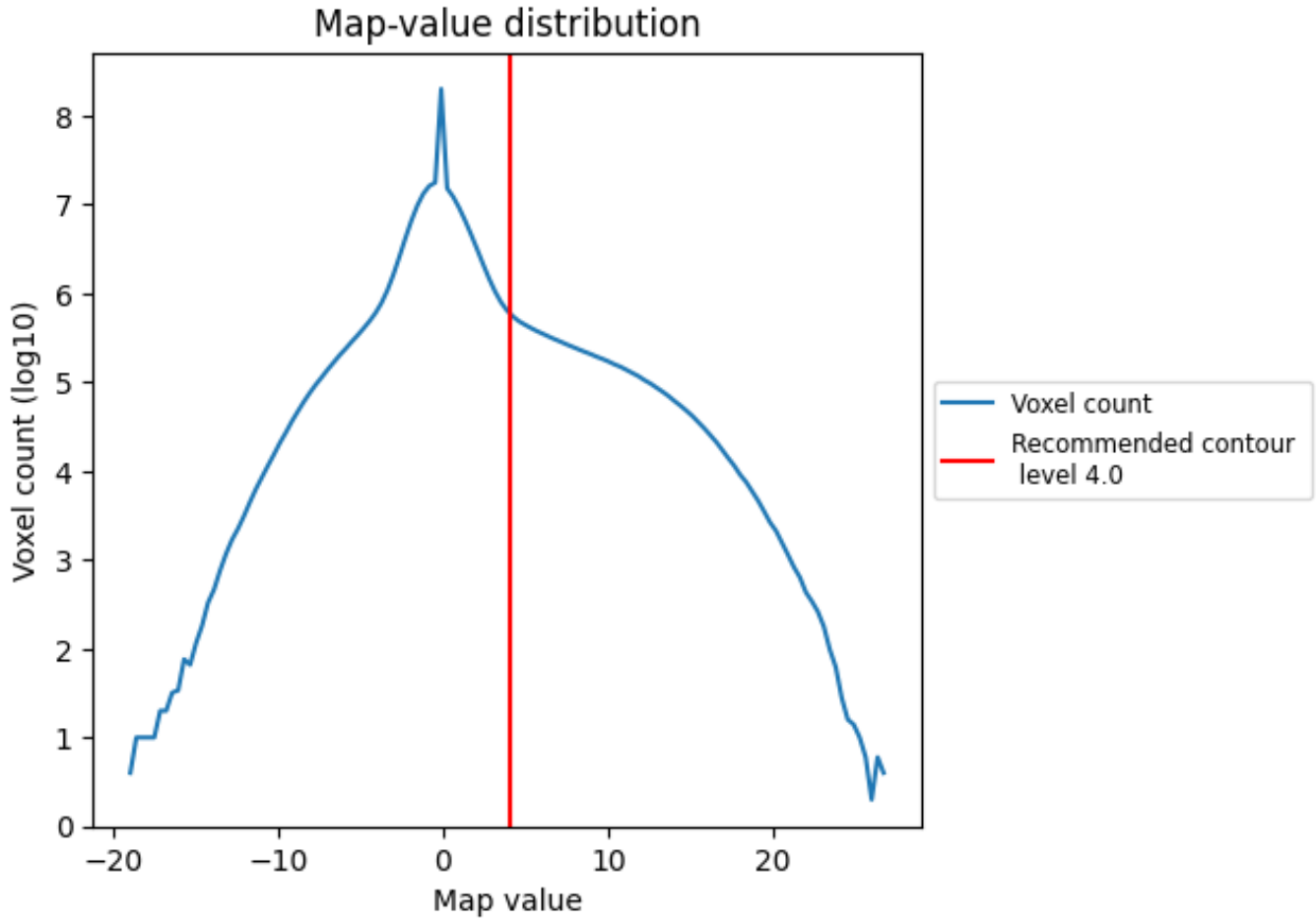
6.5 Mask visualisation (i)

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

7 Map analysis

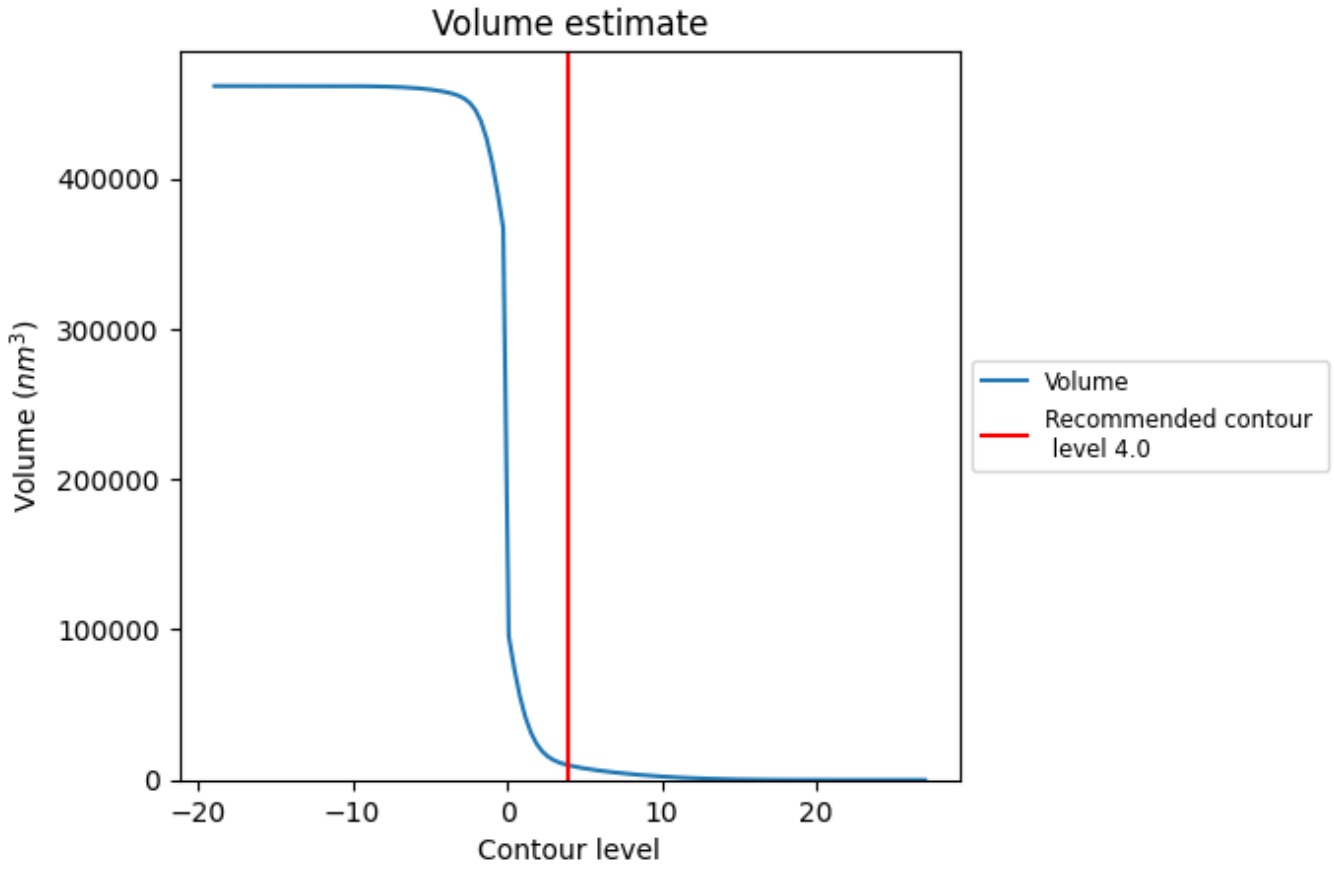
This section contains the results of statistical analysis of the map.

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.

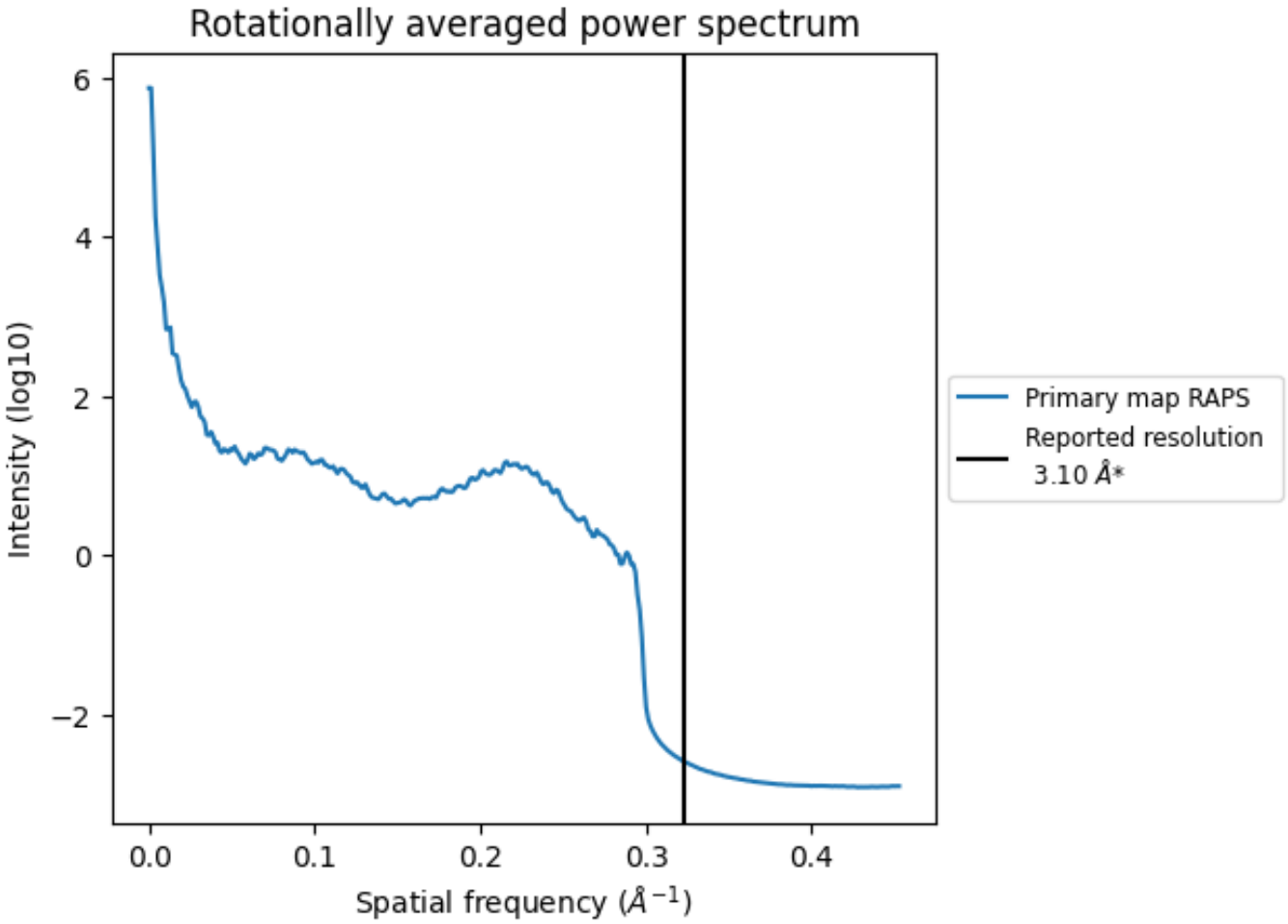
7.2 Volume estimate



The volume at the recommended contour level is 9715 nm^3; this corresponds to an approximate mass of 8776 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

8 Fourier-Shell correlation (i)

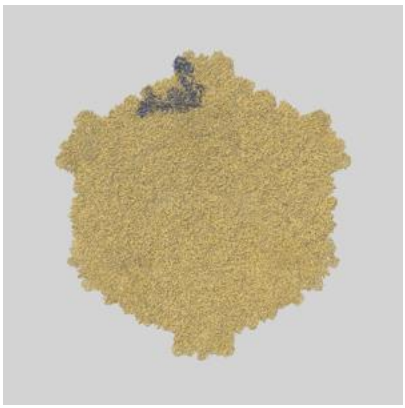
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

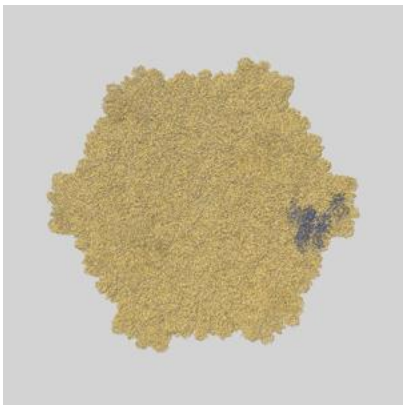
This section contains information regarding the fit between EMDB map EMD-6375 and PDB model 3JB1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

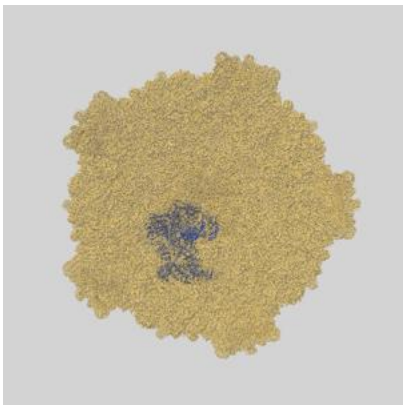
9.1.1 Map-model overlay



X

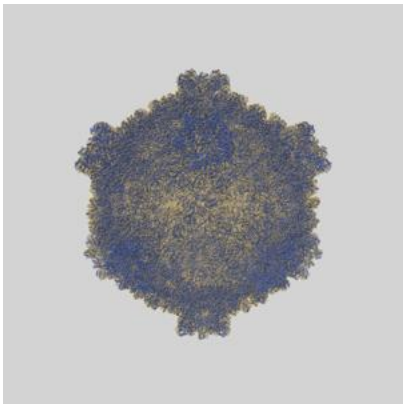


Y

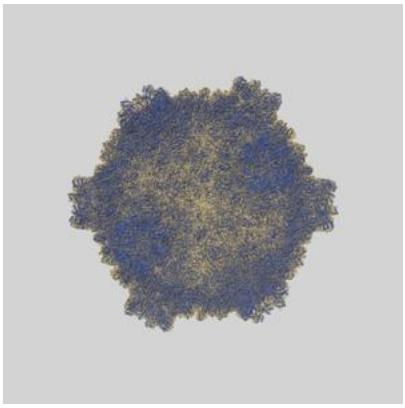


Z

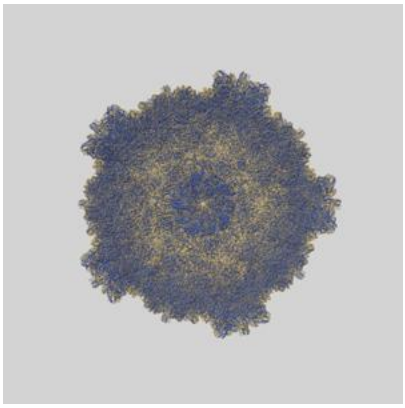
9.1.2 Map-model assembly overlay



X



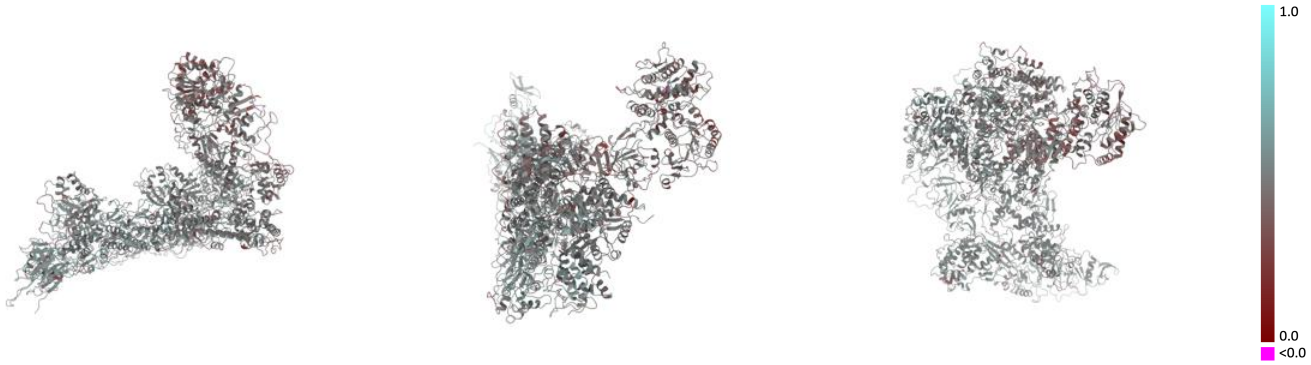
Y



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.

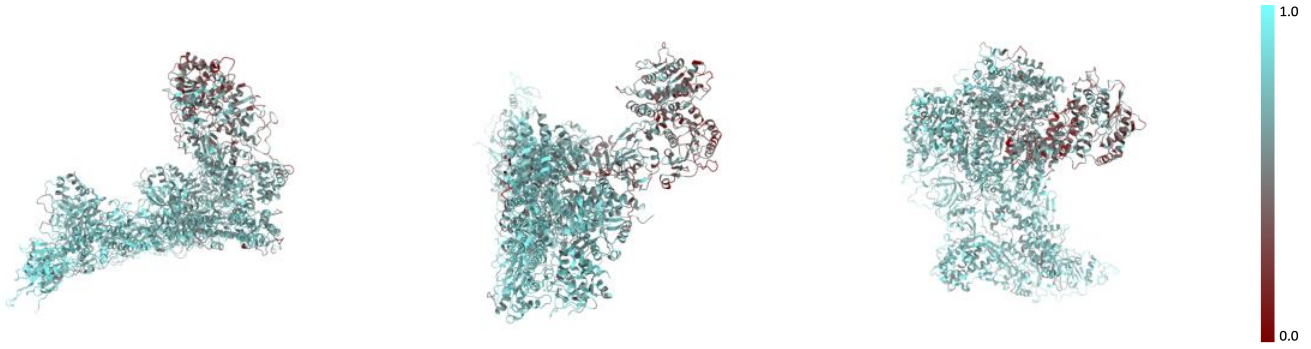
9.2 Q-score mapped to coordinate model (i)



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.

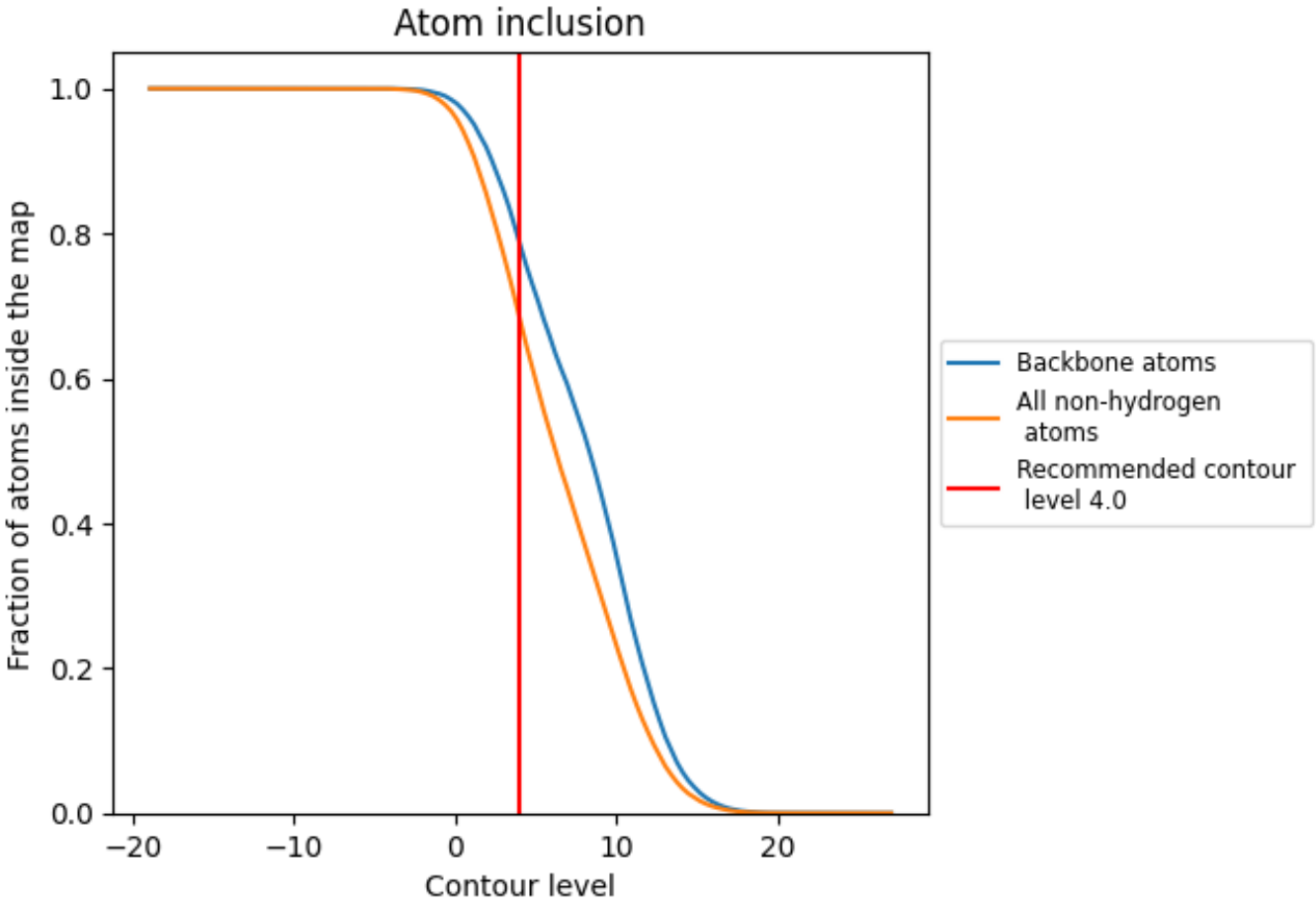
9.3 Atom inclusion mapped to coordinate model (i)



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, 79% of all backbone atoms, 68% 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	0.6821	0.4790
A	0.5307	0.4390
B	0.7221	0.4880
C	0.7447	0.4980
D	0.7409	0.5010
E	0.7481	0.4930