Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:13 AM EST

PDB ID	:	3JB2
EMDB ID	:	EMD-6376
Title	:	Atomic model of cytoplasmic polyhedrosis virus with SAM and GTP
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:

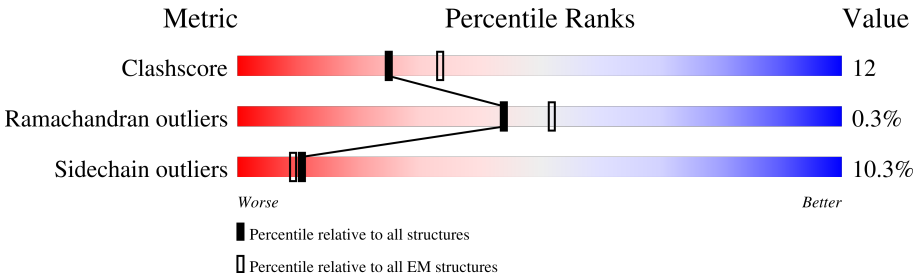
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	17% 68% 29%
2	B	1333	59% 26% 11%
2	C	1333	63% 27% 6%
3	D	448	45% 17% 35%
3	E	448	45% 18% 35%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32369 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Structural protein VP3.

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

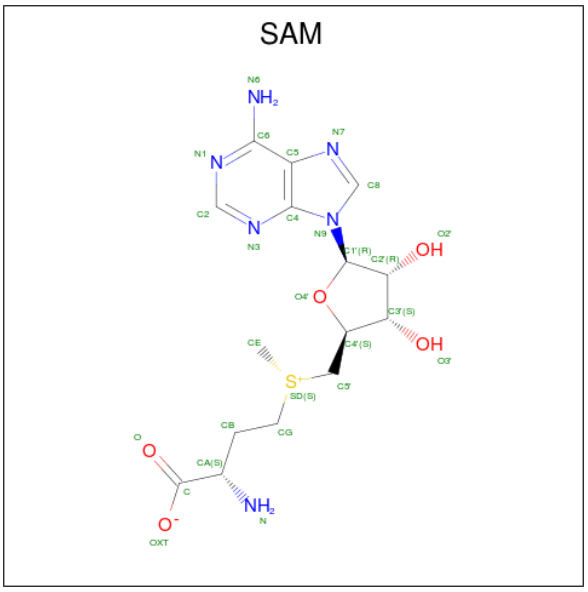
- Molecule 2 is a protein called Capsid protein VP1.

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

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

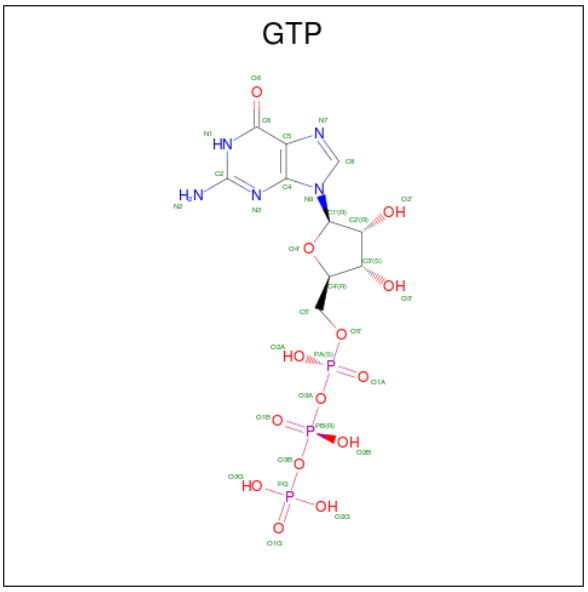
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

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



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

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



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			64	20	10	28	6	

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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			64	20	10	28	6	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

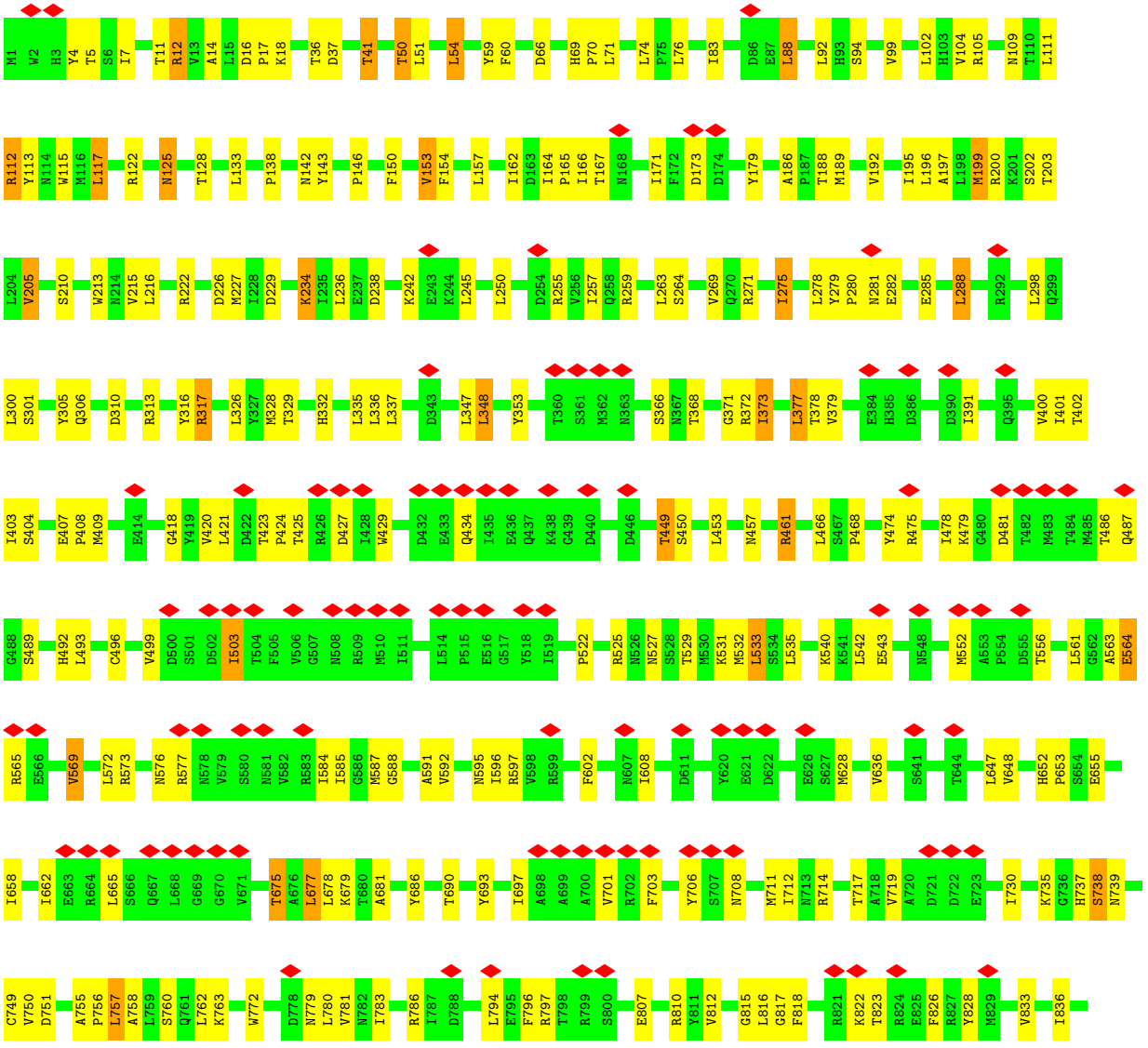
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

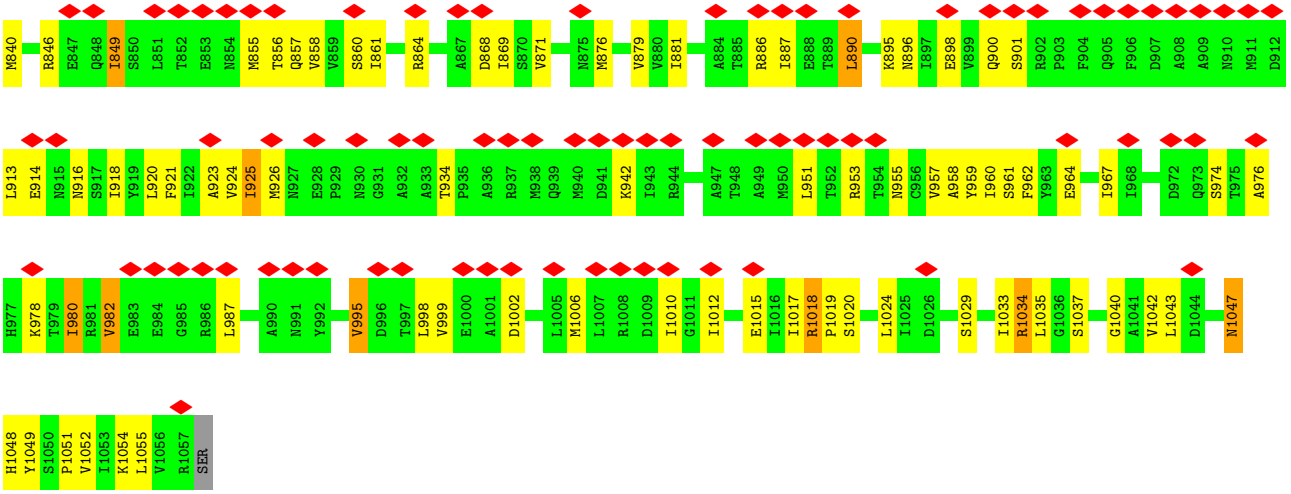
3 Residue-property plots (i)

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

- Molecule 1: Structural protein VP3

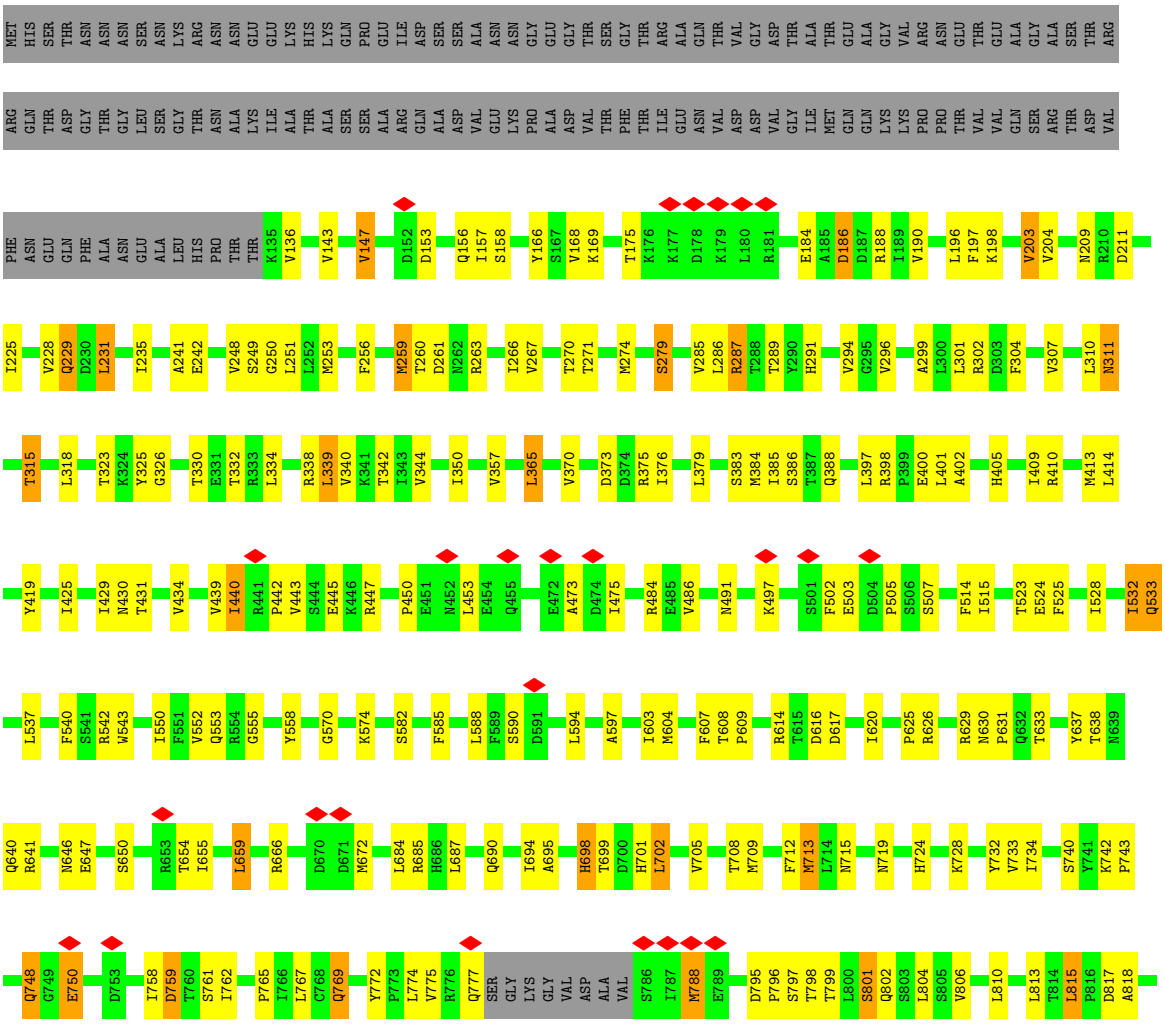
Chain A:

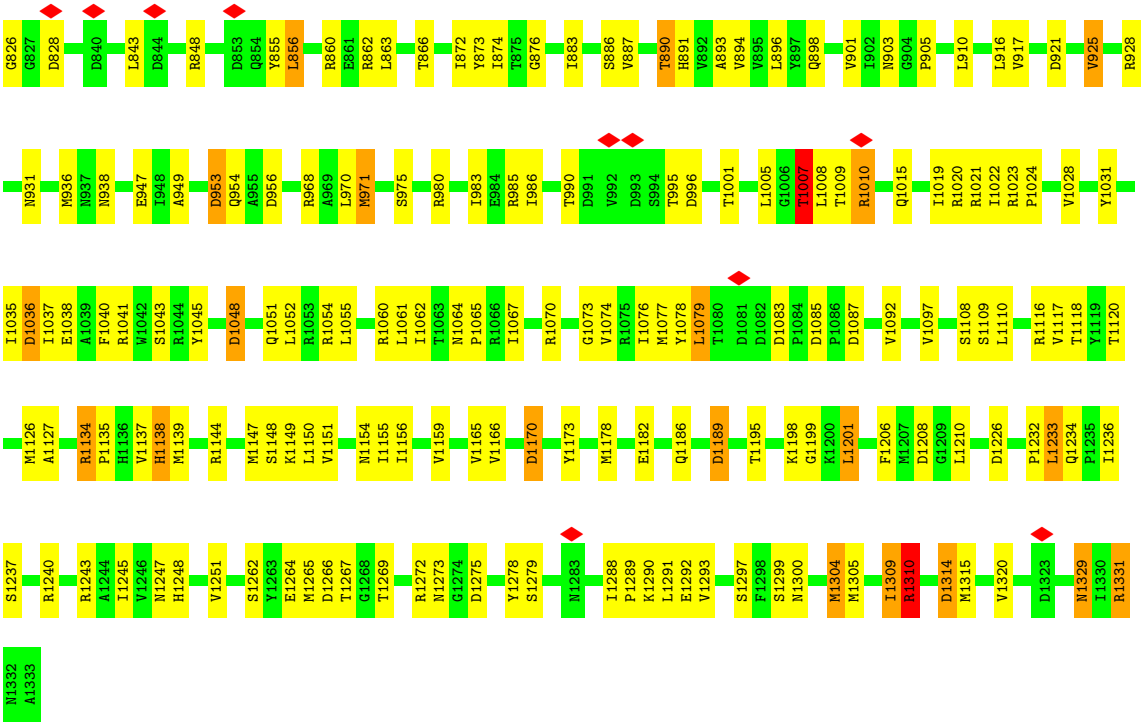




• Molecule 2: Capsid protein VP1

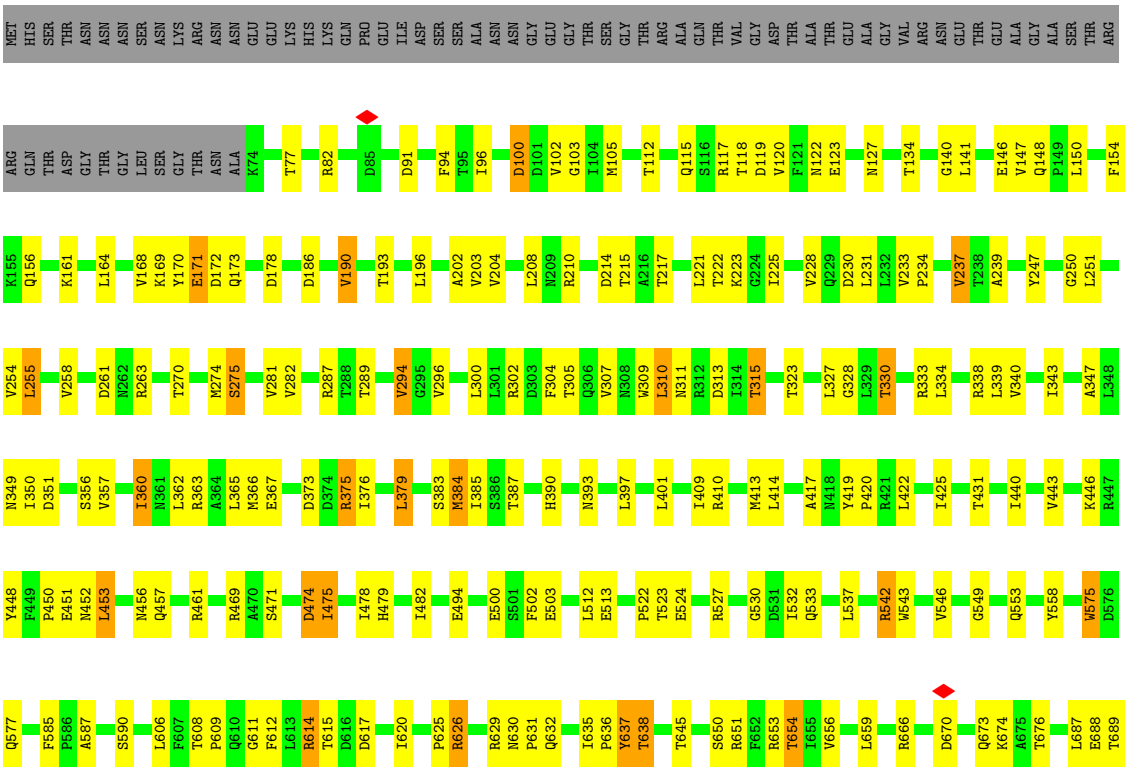
Chain B: 59% 26% 11%

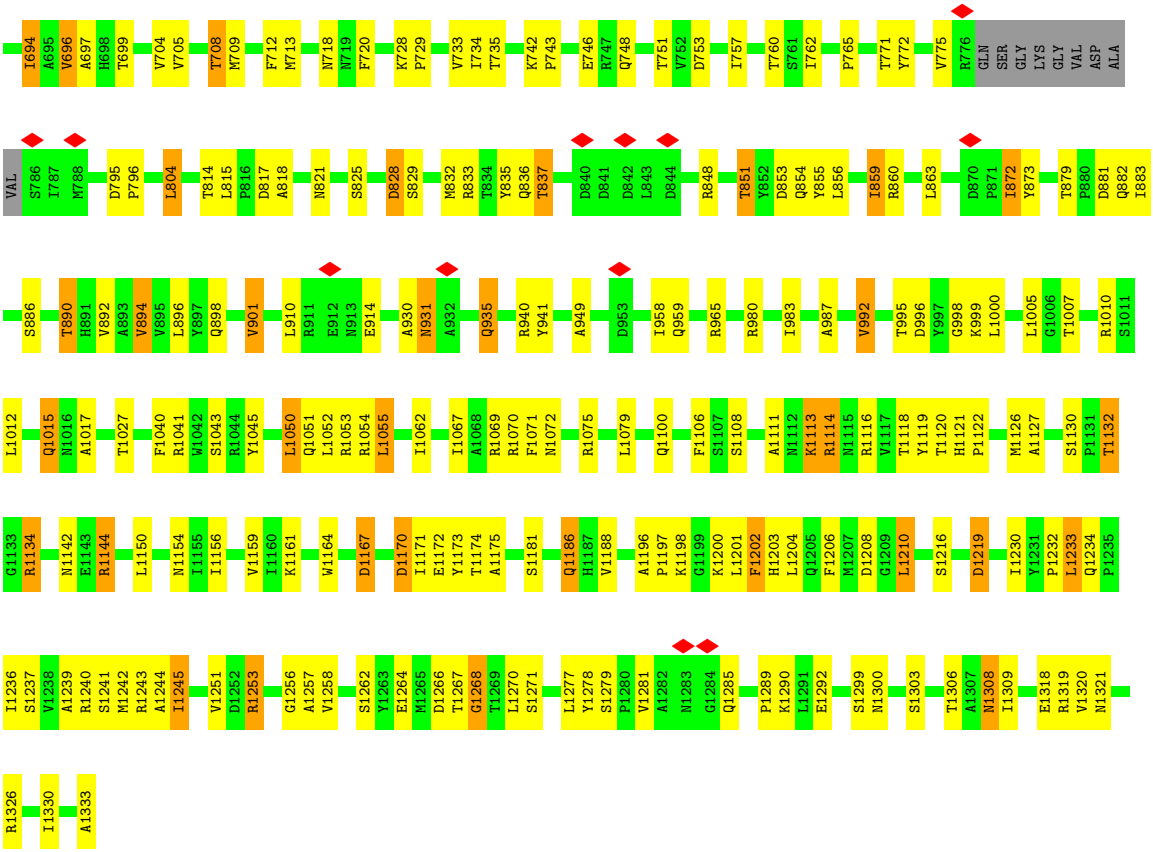




• Molecule 2: Capsid protein VP1

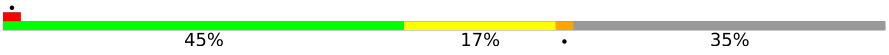
Chain C:

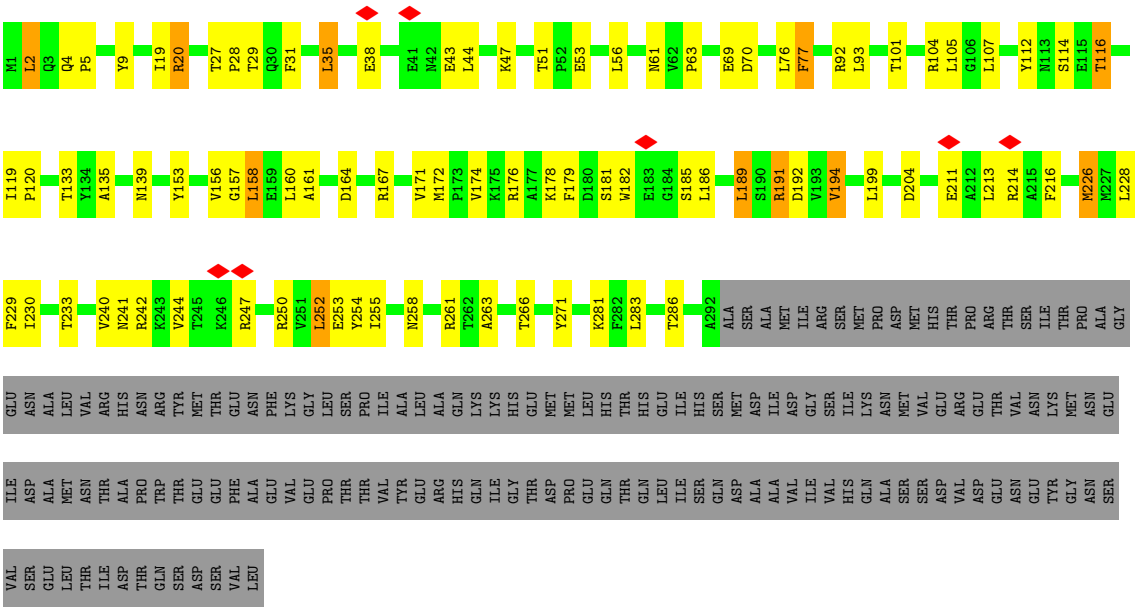




• Molecule 3: Viral structural protein 5

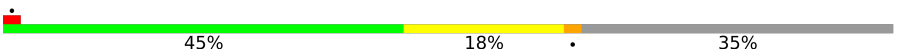
Chain D:

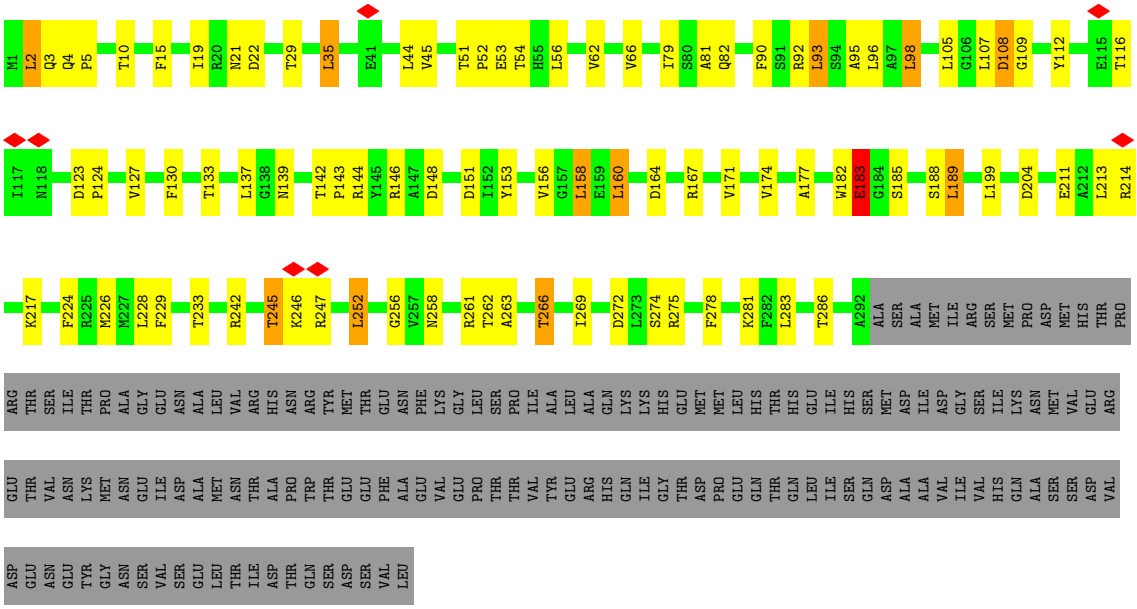




• Molecule 3: Viral structural protein 5

Chain E:




M1 L2 Q3 Q4 P5 T10 F15 I19 R20 N21 D22 T29 L35 E41 L44 V45 T51 P52 E53 T54 H55 L56 V62 V66 I79 S80 A81 Q82 F90 S91 R92 L93 S94 A95 L96 A97 L98 L105 G106 L107 D108 G109 Y112 E115 T116
I117 N118 D123 P124 V127 F130 T133 L137 G138 N139 T142 P143 R144 Y145 R146 A147 D148 D151 I152 Y153 V156 G157 L158 E159 L160 D164 R167 V171 V174 A177 W182 E183 G184 S185 S188 L189 L199 D204 E211 A212 L213 R214
K217 F224 R225 M226 M227 L228 F229 T233 R242 T245 K246 R247 L252 G256 Y257 N258 R261 T262 A263 T266 I269 D272 L273 S274 R275 F278 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 LYS 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	46147	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	27.933	Depositor
Minimum map value	-16.676	Depositor
Average map value	0.086	Depositor
Map value standard deviation	1.602	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	772.8, 772.8, 772.8	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SAM, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/8619	0.49	0/11737
2	B	0.33	0/9590	0.55	0/13056
2	C	0.34	0/10058	0.56	0/13695
3	D	0.31	0/2327	0.54	0/3163
3	E	0.31	0/2327	0.53	0/3163
All	All	0.32	0/32921	0.54	0/44814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8399	192	0
2	B	9397	0	9315	244	0
2	C	9857	0	9767	235	0
3	D	2281	0	2282	57	0
3	E	2281	0	2282	52	0
4	A	54	0	44	4	0
5	A	64	0	24	2	0
6	A	1	0	0	0	0
All	All	32369	0	32113	749	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 (749) 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:383:SER:HB3	2:C:796:PRO:HG3	1.51	0.93
1:A:857:GLN:NE2	1:A:914:GLU:OE1	2.03	0.91
2:C:360:ILE:HD11	2:C:1054:ARG:HG2	1.54	0.89
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.58	0.84
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.57	0.84
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.63	0.80
2:B:339:LEU:HD11	3:D:63:PRO:HB2	1.61	0.79
3:D:77:PHE:HB2	3:D:194:VAL:HG23	1.63	0.78
2:B:1144:ARG:NH1	2:B:1170:ASP:OD2	2.16	0.78
1:A:305:TYR:O	1:A:317:ARG:NH1	2.17	0.77
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.68	0.76
2:B:694:ILE:HD12	2:B:775:VAL:HG21	1.69	0.75
2:B:1060:ARG:NH1	2:B:1291:LEU:O	2.19	0.75
1:A:288:LEU:HD21	1:A:300:LEU:HD22	1.68	0.74
2:C:233:VAL:HG23	2:C:239:ALA:HB2	1.69	0.74
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.69	0.74
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.17	0.73
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.21	0.73
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.71	0.72
2:C:384:MET:HA	2:C:708:THR:HG21	1.72	0.72
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.23	0.72
2:B:975:SER:HB2	2:C:696:VAL:HG21	1.72	0.72
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.71	0.71
3:E:81:ALA:HB3	3:E:275:ARG:HD3	1.72	0.71
2:C:1144:ARG:NH1	2:C:1170:ASP:OD1	2.23	0.71
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.23	0.71
2:C:1289:PRO:HG2	2:C:1292:GLU:HB2	1.71	0.70
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.72	0.70
1:A:12:ARG:NH2	1:A:16:ASP:OD1	2.24	0.70
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.73	0.70
2:B:1048:ASP:HB2	2:B:1051:GLN:HG3	1.73	0.70
1:A:213:TRP:HB2	1:A:215:VAL:HG12	1.74	0.69
1:A:797:ARG:NH2	1:A:876:MET:O	2.25	0.69
1:A:41:THR:HG23	1:A:50:THR:HG23	1.74	0.69
1:A:202:SER:O	1:A:264:SER:OG	2.06	0.69
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.21	0.69
3:E:53:GLU:OE2	3:E:281:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:HD11	1:A:701:VAL:HG22	1.75	0.69
2:C:478:ILE:HG12	2:C:762:ILE:HD11	1.74	0.68
2:B:156:GLN:HB3	2:B:266:ILE:HD11	1.76	0.68
2:B:484:ARG:NH1	2:B:524:GLU:OE2	2.27	0.68
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.76	0.68
1:A:662:ILE:HD12	1:A:675:THR:HG21	1.74	0.67
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.28	0.67
2:C:1069:ARG:HD2	2:C:1239:ALA:HB2	1.76	0.67
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.76	0.67
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.18	0.67
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.13	0.66
2:C:614:ARG:NH1	2:C:617:ASP:OD1	2.28	0.66
2:C:836:GLN:NE2	2:C:940:ARG:O	2.29	0.66
1:A:573:ARG:NH2	1:A:584:ILE:O	2.29	0.66
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.22	0.66
2:B:231:LEU:HB3	2:B:249:SER:HB2	1.78	0.66
2:C:817:ASP:O	2:C:821:ASN:ND2	2.26	0.65
2:B:169:LYS:HB2	2:B:203:VAL:HG23	1.78	0.65
2:B:419:TYR:HH	2:B:1009:THR:HG1	1.43	0.65
2:B:828:ASP:OD2	2:B:862:ARG:NH2	2.29	0.65
3:D:176:ARG:HG3	3:D:253:GLU:HB3	1.78	0.65
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.79	0.65
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.30	0.65
2:B:186:ASP:OD2	2:B:279:SER:OG	2.14	0.65
2:B:614:ARG:NH1	2:B:617:ASP:OD1	2.30	0.65
2:B:891:HIS:HB3	3:D:242:ARG:HG2	1.78	0.64
1:A:923:ALA:H	1:A:961:SER:HB3	1.61	0.64
2:B:196:LEU:HD23	2:B:296:VAL:HG11	1.79	0.64
2:B:505:PRO:HG2	2:B:672:MET:SD	2.38	0.64
1:A:372:ARG:HD3	1:A:823:THR:HG21	1.80	0.63
1:A:420:VAL:HA	1:A:974:SER:HB2	1.80	0.63
2:B:473:ALA:HB2	2:B:765:PRO:HB3	1.80	0.63
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	1.80	0.63
2:B:287:ARG:HE	2:B:330:THR:HG22	1.62	0.63
1:A:373:ILE:HD13	1:A:817:GLY:HA2	1.82	0.62
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.80	0.62
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.33	0.62
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.81	0.62
2:C:171:GLU:OE2	2:C:173:GLN:NE2	2.32	0.62
1:A:474:TYR:HD1	1:A:499:VAL:HG12	1.64	0.61
2:C:1236:ILE:HG22	2:C:1237:SER:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.82	0.61
3:E:245:THR:OG1	3:E:246:LYS:N	2.33	0.61
2:B:491:ASN:ND2	2:B:750:GLU:O	2.33	0.61
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.83	0.61
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.83	0.61
2:B:887:VAL:HG22	2:B:893:ALA:HA	1.83	0.61
1:A:192:VAL:HG21	1:A:347:LEU:HD13	1.82	0.61
1:A:563:ALA:HB3	1:A:588:GLY:H	1.65	0.61
2:B:709:MET:O	2:B:715:ASN:ND2	2.34	0.61
2:C:670:ASP:HB2	2:C:673:GLN:HG3	1.82	0.61
1:A:561:LEU:HD11	1:A:602:PHE:HZ	1.66	0.60
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.83	0.60
2:C:1308:ASN:HD22	2:C:1309:ILE:N	1.98	0.60
2:C:347:ALA:HB1	2:C:1267:THR:HG21	1.83	0.60
2:B:248:VAL:HG22	2:B:970:LEU:HB3	1.83	0.60
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.37	0.60
2:B:1305:MET:HE2	2:B:1309:ILE:HG21	1.83	0.59
2:C:996:ASP:HA	2:C:999:LYS:HD2	1.83	0.59
2:C:474:ASP:OD1	2:C:474:ASP:N	2.33	0.59
2:C:746:GLU:OE2	2:C:1010:ARG:NH2	2.35	0.59
1:A:409:MET:HE1	1:A:1037:SER:HB3	1.84	0.59
2:C:251:LEU:HD22	2:C:1062:ILE:HD12	1.85	0.59
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.83	0.59
3:D:211:GLU:OE2	3:D:214:ARG:NH2	2.35	0.59
2:C:653:ARG:HG3	2:C:688:GLU:CD	2.22	0.59
1:A:540:LYS:NZ	1:A:543:GLU:OE2	2.36	0.59
1:A:479:LYS:NZ	1:A:481:ASP:OD2	2.35	0.59
1:A:828:TYR:HB3	1:A:1034:ARG:HB3	1.84	0.59
2:C:856:LEU:HD12	2:C:860:ARG:HD3	1.84	0.59
1:A:166:ILE:HG21	1:A:179:TYR:CE1	2.38	0.59
2:C:289:THR:O	2:C:328:GLY:HA3	2.03	0.59
1:A:60:PHE:H	1:A:167:THR:HG21	1.68	0.58
2:C:146:GLU:OE2	2:C:1319:ARG:NE	2.28	0.58
2:B:267:VAL:HG22	2:B:1304:MET:HG3	1.84	0.58
2:B:1007:THR:OG1	2:B:1008:LEU:N	2.36	0.58
2:B:810:LEU:HA	2:B:813:LEU:HB2	1.84	0.58
2:C:100:ASP:OD1	2:C:338:ARG:NH2	2.37	0.58
2:C:339:LEU:HD21	2:C:365:LEU:HG	1.85	0.58
2:C:148:GLN:OE1	2:C:375:ARG:NH1	2.37	0.58
3:D:2:LEU:HD12	3:D:107:LEU:HD21	1.85	0.58
2:B:1292:GLU:OE2	3:D:20:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:SER:O	2:B:728:LYS:HE3	2.04	0.57
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.28	0.57
2:C:373:ASP:HA	2:C:376:ILE:HG12	1.85	0.57
3:E:79:ILE:HG13	3:E:269:ILE:HG22	1.86	0.57
1:A:278:LEU:HD11	1:A:316:TYR:HB2	1.86	0.57
1:A:913:LEU:O	1:A:953:ARG:NE	2.38	0.57
2:B:409:ILE:HD13	2:B:625:PRO:HB2	1.87	0.57
1:A:125:ASN:ND2	2:B:647:GLU:OE2	2.37	0.57
1:A:128:THR:HG22	2:B:1331:ARG:HD3	1.84	0.57
2:B:229:GLN:HB2	2:B:985:ARG:HH21	1.69	0.57
2:C:987:ALA:HB1	2:C:992:VAL:HG22	1.86	0.57
1:A:189:MET:HE1	1:A:348:LEU:H	1.68	0.57
1:A:677:LEU:HB3	1:A:711:MET:HG3	1.87	0.57
2:B:1232:PRO:HB3	2:B:1236:ILE:HD11	1.87	0.57
2:C:1232:PRO:HB3	2:C:1236:ILE:HD11	1.87	0.57
2:B:863:LEU:HA	2:B:866:THR:HG22	1.87	0.57
2:C:385:ILE:HG12	2:C:708:THR:HG22	1.86	0.57
1:A:424:PRO:HG3	1:A:706:TYR:CZ	2.40	0.57
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.86	0.57
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.85	0.57
2:B:705:VAL:HA	2:B:708:THR:HG22	1.85	0.57
2:B:921:ASP:O	2:B:928:ARG:NH1	2.33	0.56
1:A:918:ILE:HG23	1:A:957:VAL:HG13	1.87	0.56
2:B:883:ILE:HD13	2:B:910:LEU:HD21	1.88	0.56
2:B:1206:PHE:CE2	2:B:1232:PRO:HD3	2.39	0.56
2:C:379:LEU:HD12	2:C:796:PRO:HB2	1.87	0.56
1:A:275:ILE:HG12	1:A:301:SER:HB3	1.87	0.56
2:C:1268:GLY:HA3	2:C:1277:LEU:O	2.06	0.56
3:D:77:PHE:HB3	3:D:230:ILE:HG21	1.87	0.56
1:A:400:VAL:HG12	1:A:401:ILE:HG13	1.87	0.56
2:B:157:ILE:HG12	2:B:263:ARG:HB3	1.86	0.56
2:B:184:GLU:O	2:B:188:ARG:HG3	2.06	0.56
3:E:283:LEU:HA	3:E:286:THR:HG22	1.87	0.56
2:C:366:MET:HE3	2:C:367:GLU:HG3	1.88	0.56
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.30	0.56
1:A:282:GLU:HG3	1:A:300:LEU:HD11	1.87	0.56
2:C:611:GLY:HA3	2:C:635:ILE:O	2.06	0.56
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.05	0.55
3:E:182:TRP:NE1	3:E:185:SER:HA	2.21	0.55
1:A:427:ASP:HA	1:A:703:PHE:HA	1.88	0.55
2:B:307:VAL:HG21	2:B:1245:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.36	0.55
2:B:1020:ARG:NH1	2:B:1040:PHE:O	2.38	0.55
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.37	0.55
3:D:38:GLU:OE1	3:D:242:ARG:NH1	2.25	0.55
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.88	0.55
2:B:1031:TYR:CD2	2:B:1041:ARG:HG3	2.41	0.55
2:C:422:LEU:HA	2:C:425:ILE:HD12	1.89	0.55
1:A:210:SER:O	1:A:255:ARG:NH1	2.40	0.55
1:A:238:ASP:OD2	1:A:279:TYR:OH	2.21	0.55
2:B:1022:ILE:HG22	2:B:1028:VAL:HA	1.88	0.55
3:D:101:THR:O	3:D:104:ARG:NH1	2.33	0.55
1:A:104:VAL:HG23	1:A:138:PRO:HB2	1.89	0.55
1:A:203:THR:HG22	2:B:1035:ILE:HA	1.89	0.55
2:C:294:VAL:O	2:C:349:ASN:ND2	2.40	0.55
1:A:202:SER:HB2	2:B:630:ASN:HB3	1.89	0.54
2:B:894:VAL:HG22	2:B:916:LEU:HB3	1.90	0.54
1:A:234:LYS:HB3	1:A:259:ARG:HA	1.89	0.54
2:B:1289:PRO:HG2	2:B:1292:GLU:HB2	1.89	0.54
2:B:168:VAL:HG22	2:B:204:VAL:HG22	1.89	0.54
2:B:1077:MET:HG3	2:B:1165:VAL:HG22	1.88	0.54
2:B:1118:THR:HG21	2:B:1127:ALA:HB1	1.90	0.54
2:B:1272:ARG:NH2	3:D:69:GLU:OE2	2.41	0.54
2:C:196:LEU:HD23	2:C:296:VAL:HG11	1.90	0.54
1:A:329:THR:HG22	1:A:332:HIS:ND1	2.22	0.54
2:B:620:ILE:HD11	2:B:631:PRO:HG2	1.89	0.54
1:A:461:ARG:HB3	1:A:527:ASN:HD21	1.73	0.53
2:B:410:ARG:HD3	2:B:1043:SER:HA	1.90	0.53
2:B:1267:THR:HG22	2:B:1299:SER:HB3	1.88	0.53
1:A:921:PHE:HB2	1:A:960:ILE:HA	1.89	0.53
2:B:310:LEU:HD22	2:B:1245:ILE:HG23	1.88	0.53
2:C:156:GLN:OE1	2:C:1308:ASN:ND2	2.41	0.53
2:C:214:ASP:OD1	2:C:215:THR:N	2.41	0.53
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	1.91	0.53
2:B:1076:ILE:HG22	2:B:1159:VAL:HG11	1.90	0.53
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.31	0.53
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.91	0.53
2:B:153:ASP:OD1	2:B:153:ASP:N	2.36	0.53
2:C:305:THR:HG21	2:C:310:LEU:HD12	1.91	0.53
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.90	0.53
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.90	0.53
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:THR:HB	1:A:1020:SER:HB2	1.91	0.53
1:A:797:ARG:HH12	1:A:896:ASN:HB3	1.72	0.53
3:E:153:TYR:CD2	3:E:258:ASN:HB2	2.44	0.53
2:B:231:LEU:HD21	2:B:986:ILE:HG12	1.91	0.52
2:C:356:SER:O	2:C:360:ILE:HG23	2.09	0.52
2:C:851:THR:OG1	2:C:853:ASP:OD2	2.21	0.52
1:A:860:SER:OG	1:A:868:ASP:OD2	2.27	0.52
2:B:302:ARG:HD2	2:B:318:LEU:HD12	1.91	0.52
2:B:594:LEU:HB3	2:B:597:ALA:HB3	1.92	0.52
2:C:512:LEU:HD21	2:C:687:LEU:HD12	1.91	0.52
2:B:503:GLU:HG2	2:B:542:ARG:HH12	1.74	0.52
3:E:229:PHE:O	3:E:233:THR:HG23	2.09	0.52
2:B:261:ASP:CG	2:B:263:ARG:HE	2.13	0.52
2:C:1118:THR:HG21	2:C:1127:ALA:HB1	1.90	0.52
2:C:186:ASP:OD1	2:C:282:VAL:HG21	2.10	0.52
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.91	0.52
1:A:964:GLU:HB3	1:A:1049:TYR:HD2	1.75	0.52
2:B:439:VAL:HG21	2:B:702:LEU:HD13	1.91	0.52
3:D:213:LEU:O	3:D:216:PHE:HB3	2.10	0.52
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.92	0.52
2:B:968:ARG:HA	2:B:971:MET:SD	2.49	0.52
2:C:1188:VAL:HG11	2:C:1202:PHE:HE1	1.75	0.52
1:A:916:ASN:N	1:A:955:ASN:O	2.43	0.52
2:B:370:VAL:HG11	2:B:402:ALA:HB2	1.92	0.52
1:A:686:TYR:HA	1:A:714:ARG:HH21	1.75	0.51
2:B:558:TYR:CZ	2:B:585:PHE:HB2	2.45	0.51
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.92	0.51
1:A:751:ASP:OD1	1:A:779:ASN:ND2	2.43	0.51
2:B:1008:LEU:HD11	2:B:1010:ARG:HB2	1.92	0.51
2:C:606:LEU:HA	2:C:651:ARG:HH21	1.76	0.51
2:B:1147:MET:HE3	2:B:1155:ILE:HD12	1.91	0.51
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.93	0.51
2:C:1210:LEU:HD12	2:C:1244:ALA:HB2	1.92	0.51
2:B:931:ASN:ND2	2:B:936:MET:O	2.43	0.51
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.11	0.51
1:A:353:TYR:OH	3:D:43:GLU:OE1	2.26	0.51
2:B:326:GLY:H	2:B:1267:THR:HG21	1.74	0.51
2:B:1036:ASP:N	2:B:1036:ASP:OD1	2.43	0.51
2:B:806:VAL:O	2:B:810:LEU:HG	2.11	0.51
2:B:925:VAL:HA	2:B:928:ARG:HD2	1.93	0.51
2:C:164:LEU:HD21	2:C:1067:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:VAL:HG13	2:C:1054:ARG:HD3	1.91	0.51
2:B:285:VAL:HG22	2:B:325:TYR:HD2	1.76	0.51
2:B:1001:THR:O	2:B:1005:LEU:HG	2.10	0.51
2:C:494:GLU:HB2	2:C:757:ILE:HD13	1.92	0.51
2:C:851:THR:HG23	2:C:854:GLN:HB2	1.92	0.51
2:C:1216:SER:OG	2:C:1219:ASP:OD2	2.18	0.51
3:E:79:ILE:HD12	3:E:79:ILE:H	1.76	0.51
2:B:235:ILE:HG13	2:C:1326:ARG:HD2	1.92	0.51
2:B:425:ILE:HD12	2:B:1001:THR:HG22	1.93	0.51
2:B:1248:HIS:ND1	2:B:1251:VAL:HG12	2.26	0.51
2:B:186:ASP:OD1	2:B:186:ASP:N	2.41	0.51
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.93	0.51
2:B:1148:SER:HB2	2:C:390:HIS:CG	2.46	0.50
2:C:469:ARG:HH21	2:C:513:GLU:CD	2.15	0.50
1:A:924:VAL:HG12	4:A:1102:SAM:H5'2	1.92	0.50
2:B:443:VAL:O	2:B:769:GLN:NE2	2.45	0.50
2:C:1075:ARG:NH1	2:C:1167:ASP:OD1	2.44	0.50
1:A:379:VAL:HG11	1:A:794:LEU:HG	1.92	0.50
1:A:655:GLU:HG2	1:A:712:ILE:HG21	1.94	0.50
2:B:886:SER:O	2:B:890:THR:HG23	2.11	0.50
2:B:772:TYR:HB2	2:B:775:VAL:HB	1.93	0.50
3:E:261:ARG:NH1	3:E:263:ALA:O	2.45	0.50
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.41	0.50
2:B:419:TYR:OH	2:B:1009:THR:OG1	2.21	0.50
1:A:564:GLU:OE1	4:A:1101:SAM:O3'	2.30	0.50
1:A:890:LEU:HD23	1:A:890:LEU:H	1.76	0.50
2:B:523:THR:HG21	2:B:719:ASN:HB2	1.93	0.50
2:C:287:ARG:HH11	2:C:330:THR:HB	1.77	0.50
2:C:471:SER:O	2:C:765:PRO:HG3	2.11	0.50
3:D:229:PHE:O	3:D:233:THR:HG23	2.12	0.50
1:A:391:ILE:HD11	1:A:757:LEU:HD22	1.94	0.49
2:B:251:LEU:HD22	2:B:1062:ILE:HD12	1.94	0.49
2:C:879:THR:HG22	2:C:881:ASP:H	1.77	0.49
1:A:525:ARG:HG2	1:A:529:THR:HG21	1.94	0.49
1:A:552:MET:H	1:A:576:ASN:ND2	2.10	0.49
2:C:339:LEU:HD22	2:C:366:MET:HA	1.94	0.49
2:C:414:LEU:HD23	2:C:814:THR:HB	1.95	0.49
2:C:1159:VAL:HA	2:C:1164:TRP:HB2	1.94	0.49
3:E:148:ASP:OD1	3:E:151:ASP:N	2.36	0.49
1:A:658:ILE:O	1:A:662:ILE:HG12	2.12	0.49
2:B:638:THR:HG23	2:B:1331:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:LYS:O	2:C:202:ALA:N	2.44	0.49
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.95	0.49
2:C:431:THR:HG23	2:C:479:HIS:HB3	1.94	0.49
2:C:1243:ARG:HB3	2:C:1258:VAL:HG22	1.94	0.49
1:A:926:MET:HB2	1:A:995:VAL:HG21	1.94	0.49
2:C:746:GLU:OE1	2:C:748:GLN:NE2	2.33	0.49
2:C:1271:SER:HB3	2:C:1277:LEU:HD21	1.93	0.49
3:D:157:GLY:HA2	3:D:255:ILE:HG22	1.94	0.49
1:A:449:THR:HG22	1:A:450:SER:H	1.78	0.49
1:A:681:ALA:O	1:A:1037:SER:HB2	2.12	0.49
2:C:366:MET:HG2	3:E:266:THR:HG21	1.94	0.49
3:D:31:PHE:CZ	3:D:189:LEU:HD21	2.48	0.49
1:A:328:MET:HE2	1:A:332:HIS:HB3	1.94	0.49
1:A:628:MET:HE1	1:A:652:HIS:HB2	1.93	0.49
2:B:806:VAL:HG22	2:B:1001:THR:HG21	1.92	0.49
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.48	0.49
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.13	0.49
2:B:370:VAL:HG22	2:B:400:GLU:O	2.12	0.49
2:B:528:ILE:HG13	2:B:532:ILE:HD12	1.94	0.49
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.95	0.49
2:B:209:ASN:ND2	2:B:211:ASP:OD1	2.45	0.49
2:B:890:THR:O	2:B:890:THR:OG1	2.27	0.49
2:B:1031:TYR:CE2	2:B:1041:ARG:HG3	2.48	0.49
2:C:795:ASP:OD1	2:C:1319:ARG:NH2	2.46	0.49
1:A:5:THR:O	1:A:250:LEU:HA	2.12	0.48
2:B:525:PHE:HD2	2:B:724:HIS:CE1	2.31	0.48
2:C:543:TRP:CD2	2:C:666:ARG:HD3	2.48	0.48
2:B:270:THR:HG22	2:B:291:HIS:HA	1.95	0.48
2:B:558:TYR:CE2	2:B:590:SER:HB3	2.48	0.48
2:C:261:ASP:OD2	2:C:263:ARG:NE	2.40	0.48
1:A:66:ASP:CG	1:A:122:ARG:HH22	2.14	0.48
1:A:587:MET:HA	1:A:596:ILE:O	2.13	0.48
1:A:849:ILE:HD11	1:A:918:ILE:HG21	1.96	0.48
2:B:777:GLN:HG2	2:B:788:MET:HA	1.95	0.48
3:E:95:ALA:HA	3:E:98:LEU:HD22	1.96	0.48
2:B:261:ASP:HB3	2:B:357:VAL:HG11	1.95	0.48
2:B:695:ALA:HA	2:B:698:HIS:HB2	1.94	0.48
2:C:855:TYR:CD1	2:C:859:ILE:HG12	2.47	0.48
1:A:735:LYS:HB2	1:A:738:SER:HB2	1.95	0.48
2:B:1085:ASP:OD1	2:B:1085:ASP:N	2.47	0.48
2:C:1072:ASN:OD1	2:C:1172:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:HIS:NE2	1:A:94:SER:OG	2.45	0.48
1:A:285:GLU:O	1:A:366:SER:HB3	2.14	0.48
1:A:531:LYS:O	1:A:535:LEU:HG	2.13	0.48
1:A:925:ILE:HG12	1:A:942:LYS:HD2	1.95	0.48
2:C:1243:ARG:CB	2:C:1258:VAL:HG22	2.44	0.48
3:D:153:TYR:HA	3:D:156:VAL:HG23	1.95	0.48
1:A:879:VAL:HG22	1:A:898:GLU:HB3	1.96	0.48
1:A:958:ALA:HB3	1:A:1055:LEU:HB2	1.96	0.48
2:B:379:LEU:HD22	2:B:796:PRO:HB2	1.95	0.48
1:A:51:LEU:HD23	1:A:171:ILE:HD11	1.96	0.48
1:A:154:PHE:CE1	1:A:162:ILE:HG23	2.48	0.48
2:C:234:PRO:HB2	2:C:237:VAL:HG23	1.94	0.48
1:A:192:VAL:HG13	1:A:216:LEU:HD22	1.95	0.48
2:B:540:PHE:HE1	2:B:603:ILE:HD12	1.79	0.48
2:C:901:VAL:HG13	2:C:930:ALA:HB2	1.96	0.48
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.96	0.48
2:B:641:ARG:HH22	2:B:1329:ASN:HB3	1.79	0.47
2:B:903:ASN:HD22	2:B:905:PRO:HG2	1.79	0.47
2:C:558:TYR:CE1	2:C:590:SER:HB3	2.48	0.47
2:C:848:ARG:HE	2:C:914:GLU:HB3	1.79	0.47
2:C:1267:THR:HA	2:C:1299:SER:O	2.14	0.47
1:A:807:GLU:OE2	1:A:810:ARG:NH1	2.47	0.47
1:A:1043:LEU:O	1:A:1047:ASN:HB3	2.14	0.47
2:C:451:GLU:HA	2:C:452:ASN:HA	1.57	0.47
1:A:797:ARG:NH1	1:A:895:LYS:O	2.45	0.47
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.79	0.47
2:B:626:ARG:NH2	2:B:712:PHE:O	2.46	0.47
2:C:210:ARG:HA	2:C:221:LEU:HD12	1.96	0.47
1:A:59:TYR:HB3	5:A:1104:GTP:C6	2.50	0.47
1:A:797:ARG:HD2	1:A:869:ILE:HD11	1.95	0.47
2:B:585:PHE:CZ	2:B:728:LYS:HD2	2.48	0.47
2:C:656:VAL:HG21	2:C:688:GLU:HB2	1.96	0.47
3:D:253:GLU:HA	3:D:254:TYR:HA	1.48	0.47
1:A:203:THR:HG23	2:B:629:ARG:HB3	1.95	0.47
2:C:524:GLU:HA	2:C:527:ARG:HD2	1.96	0.47
2:C:1308:ASN:HD22	2:C:1309:ILE:H	1.61	0.47
2:B:616:ASP:HB2	2:B:631:PRO:HB2	1.96	0.47
2:C:1106:PHE:CE1	2:C:1119:TYR:HB2	2.50	0.47
3:E:93:LEU:HD23	3:E:96:LEU:HD12	1.96	0.47
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.96	0.47
1:A:758:ALA:O	1:A:762:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:VAL:HG13	1:A:1002:ASP:HB2	1.95	0.47
2:B:439:VAL:HG13	2:B:440:ILE:HG13	1.97	0.47
2:B:713:MET:HB2	2:B:713:MET:HE2	1.63	0.47
2:B:891:HIS:CD2	3:D:240:VAL:HG21	2.50	0.47
2:C:154:PHE:CE2	2:C:401:LEU:HD13	2.49	0.47
2:C:713:MET:HE1	2:C:804:LEU:HD13	1.96	0.47
1:A:280:PRO:HG3	1:A:300:LEU:HD21	1.96	0.47
1:A:487:GLN:O	1:A:492:HIS:ND1	2.46	0.47
1:A:856:THR:HG23	1:A:857:GLN:HG2	1.97	0.47
1:A:1012:ILE:HD13	1:A:1055:LEU:HD22	1.97	0.47
2:B:1077:MET:SD	2:B:1079:LEU:HD21	2.54	0.47
1:A:14:ALA:HA	1:A:112:ARG:NH2	2.30	0.47
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.49	0.47
2:B:259:MET:O	2:B:1054:ARG:NH1	2.44	0.47
2:B:762:ILE:HD12	2:B:762:ILE:HA	1.75	0.47
3:D:114:SER:O	3:D:116:THR:HG22	2.15	0.47
3:E:4:GLN:NE2	3:E:204:ASP:OD1	2.41	0.47
2:B:1314:ASP:OD1	2:B:1314:ASP:N	2.47	0.47
2:C:837:THR:O	2:C:935:GLN:HB3	2.15	0.47
2:C:1050:LEU:HD23	2:C:1050:LEU:HA	1.68	0.47
2:C:1206:PHE:CE1	2:C:1232:PRO:HD3	2.49	0.47
1:A:402:THR:HG23	1:A:822:LYS:HD2	1.97	0.46
1:A:71:LEU:HD22	1:A:92:LEU:HA	1.97	0.46
2:B:338:ARG:HB3	2:B:340:VAL:HG13	1.97	0.46
2:B:515:ILE:HD12	2:B:659:LEU:HD21	1.97	0.46
3:D:153:TYR:CD2	3:D:258:ASN:HB2	2.51	0.46
2:B:443:VAL:HG22	2:B:445:GLU:H	1.81	0.46
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.96	0.46
2:B:903:ASN:ND2	2:B:905:PRO:HG2	2.31	0.46
2:B:956:ASP:CG	3:D:266:THR:H	2.19	0.46
2:C:833:ARG:HB3	2:C:941:TYR:HB2	1.97	0.46
2:C:1114:ARG:HE	2:C:1114:ARG:HB2	1.36	0.46
2:B:430:ASN:O	2:B:434:VAL:HG23	2.15	0.46
2:B:1278:TYR:CE2	2:B:1290:LYS:HA	2.51	0.46
2:C:450:PRO:HG2	2:C:453:LEU:HB3	1.98	0.46
1:A:1035:LEU:HD21	1:A:1040:GLY:HA2	1.96	0.46
2:B:409:ILE:O	2:B:413:MET:HG2	2.16	0.46
2:B:528:ILE:HG21	2:B:758:ILE:HG13	1.98	0.46
2:C:705:VAL:O	2:C:709:MET:HB2	2.16	0.46
2:C:859:ILE:HD11	2:C:894:VAL:HG11	1.98	0.46
2:C:1266:ASP:OD2	2:C:1279:SER:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.68	0.46
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.50	0.46
2:B:447:ARG:HD2	2:B:690:GLN:OE1	2.16	0.46
2:C:379:LEU:HD12	2:C:379:LEU:HA	1.75	0.46
2:C:863:LEU:HD23	2:C:863:LEU:HA	1.75	0.46
2:B:701:HIS:HB2	2:B:774:LEU:HD12	1.97	0.46
2:B:828:ASP:HA	2:C:645:THR:HG23	1.97	0.46
2:B:1289:PRO:HG3	3:D:191:ARG:NH2	2.31	0.46
2:C:171:GLU:HG2	2:C:1181:SER:OG	2.16	0.46
2:C:615:THR:H	2:C:1333:ALA:HB1	1.81	0.46
2:C:935:GLN:HG2	2:C:940:ARG:HH12	1.80	0.46
2:C:1241:SER:OG	2:C:1264:GLU:OE2	2.30	0.46
1:A:4:TYR:HB3	1:A:245:LEU:HD22	1.96	0.46
1:A:154:PHE:HE1	1:A:162:ILE:HG23	1.81	0.46
1:A:496:CYS:SG	1:A:503:ILE:HD11	2.56	0.46
2:B:555:GLY:HA3	2:B:570:GLY:H	1.81	0.46
1:A:404:SER:HB3	1:A:826:PHE:CD1	2.51	0.46
1:A:591:ALA:HB3	1:A:597:ARG:HA	1.97	0.46
1:A:1019:PRO:HG2	1:A:1047:ASN:OD1	2.15	0.46
2:C:872:ILE:HD12	2:C:886:SER:CB	2.46	0.46
2:C:1119:TYR:CE2	2:C:1121:HIS:HB2	2.51	0.46
2:C:443:VAL:HG11	2:C:771:THR:HG23	1.96	0.45
2:C:446:LYS:HB3	2:C:448:TYR:CD2	2.50	0.45
2:C:608:THR:HA	2:C:609:PRO:HD3	1.69	0.45
2:C:751:THR:OG1	2:C:753:ASP:OD1	2.31	0.45
1:A:403:ILE:HG21	1:A:730:ILE:HD11	1.98	0.45
1:A:197:ALA:O	1:A:200:ARG:HG2	2.16	0.45
2:B:617:ASP:OD1	2:B:617:ASP:N	2.49	0.45
2:C:503:GLU:HG3	2:C:542:ARG:HH11	1.81	0.45
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.25	0.45
2:B:1267:THR:HG22	2:B:1299:SER:CB	2.47	0.45
2:C:409:ILE:HD13	2:C:625:PRO:HB2	1.97	0.45
1:A:60:PHE:N	1:A:167:THR:HG21	2.29	0.45
2:B:241:ALA:O	2:B:1199:GLY:HA3	2.16	0.45
2:B:1278:TYR:HE1	2:B:1297:SER:HB2	1.82	0.45
3:D:44:LEU:HG	3:D:174:VAL:HG22	1.99	0.45
3:E:35:LEU:HD13	3:E:35:LEU:HA	1.83	0.45
1:A:226:ASP:HA	1:A:229:ASP:OD2	2.17	0.45
1:A:281:ASN:O	1:A:285:GLU:HG2	2.17	0.45
1:A:409:MET:HE1	1:A:1037:SER:CB	2.45	0.45
1:A:757:LEU:O	1:A:760:SER:OG	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:LEU:HD23	2:B:397:LEU:HA	1.77	0.45
2:B:701:HIS:HB2	2:B:774:LEU:CD1	2.46	0.45
2:B:759:ASP:OD2	2:B:761:SER:OG	2.31	0.45
3:D:4:GLN:HA	3:D:5:PRO:HD3	1.86	0.45
3:D:253:GLU:HB2	3:D:254:TYR:CD2	2.51	0.45
1:A:113:TYR:O	1:A:115:TRP:N	2.49	0.45
1:A:653:PRO:O	1:A:712:ILE:HG23	2.17	0.45
1:A:959:TYR:CE1	1:A:1054:LYS:HG3	2.52	0.45
2:B:550:ILE:O	2:B:553:GLN:HG3	2.17	0.45
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.52	0.45
2:C:549:GLY:O	2:C:553:GLN:HB2	2.17	0.45
2:C:704:VAL:O	2:C:708:THR:HG23	2.16	0.45
3:E:143:PRO:HA	3:E:146:ARG:HD3	1.97	0.45
1:A:371:GLY:N	1:A:818:PHE:O	2.47	0.45
1:A:840:MET:HG2	1:A:1024:LEU:HA	1.98	0.45
2:B:256:PHE:CE1	2:B:815:LEU:HD22	2.52	0.45
2:C:1000:LEU:O	2:C:1007:THR:HA	2.17	0.45
2:C:1278:TYR:CE1	2:C:1290:LYS:HG2	2.52	0.45
1:A:143:TYR:CE2	1:A:146:PRO:HA	2.51	0.45
1:A:271:ARG:O	1:A:275:ILE:HG13	2.17	0.45
2:C:456:ASN:OD1	2:C:457:GLN:N	2.50	0.45
2:C:1266:ASP:OD1	2:C:1279:SER:OG	2.29	0.45
2:B:409:ILE:HD12	2:B:409:ILE:HA	1.74	0.44
2:B:638:THR:O	2:B:699:THR:HB	2.17	0.44
2:B:640:GLN:HG3	2:B:646:ASN:ND2	2.32	0.44
2:C:225:ILE:HB	2:C:247:TYR:HD1	1.82	0.44
1:A:166:ILE:HD13	1:A:179:TYR:CZ	2.52	0.44
1:A:887:ILE:HD11	1:A:901:SER:HB2	1.99	0.44
2:B:225:ILE:HD13	2:B:1070:ARG:HB2	1.99	0.44
3:D:9:TYR:H	3:D:204:ASP:CG	2.19	0.44
3:E:142:THR:HA	3:E:143:PRO:HD3	1.87	0.44
3:E:213:LEU:HD11	3:E:217:LYS:HE3	1.99	0.44
1:A:88:LEU:HD22	1:A:88:LEU:HA	1.86	0.44
1:A:310:ASP:OD1	1:A:313:ARG:NH2	2.50	0.44
1:A:486:THR:HB	1:A:489:SER:HB3	1.99	0.44
2:B:325:TYR:HA	2:B:1267:THR:HG23	1.99	0.44
2:B:980:ARG:HG3	2:B:1010:ARG:HG2	2.00	0.44
3:D:35:LEU:HD12	3:D:179:PHE:HB3	1.98	0.44
1:A:772:TRP:HA	1:A:817:GLY:HA3	1.99	0.44
1:A:836:ILE:HD11	1:A:1033:ILE:HG21	2.00	0.44
2:B:633:THR:HA	2:B:719:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:828:ASP:OD1	2:C:828:ASP:N	2.50	0.44
3:D:186:LEU:HD23	3:D:186:LEU:HA	1.82	0.44
2:B:515:ILE:HG21	2:B:655:ILE:HG21	1.99	0.44
2:B:828:ASP:OD2	2:B:1015:GLN:HG2	2.18	0.44
3:D:158:LEU:HD13	3:D:158:LEU:HA	1.78	0.44
2:C:835:TYR:HA	2:C:941:TYR:HA	2.00	0.44
3:D:161:ALA:HB3	3:D:172:MET:HE1	1.99	0.44
3:E:44:LEU:HD11	3:E:256:GLY:HA3	1.98	0.44
1:A:257:ILE:HG21	1:A:326:LEU:HD11	2.00	0.44
1:A:708:ASN:O	1:A:1048:HIS:NE2	2.51	0.44
1:A:786:ARG:NH2	1:A:826:PHE:O	2.47	0.44
1:A:967:ILE:HD13	1:A:987:LEU:HD11	2.00	0.44
2:B:873:TYR:HA	2:B:896:LEU:O	2.18	0.44
2:B:876:GLY:HA3	2:B:901:VAL:O	2.16	0.44
2:C:168:VAL:HG13	2:C:204:VAL:HG22	1.99	0.44
2:C:311:ASN:O	2:C:315:THR:HB	2.17	0.44
1:A:675:THR:HA	1:A:693:TYR:O	2.18	0.44
2:C:360:ILE:HD12	2:C:1053:ARG:HB3	1.98	0.44
2:C:417:ALA:HB1	2:C:742:LYS:HB3	1.99	0.44
3:D:283:LEU:HA	3:D:286:THR:HG22	1.99	0.44
3:E:4:GLN:HA	3:E:5:PRO:HD3	1.84	0.44
3:E:109:GLY:HA2	3:E:199:LEU:HD12	2.00	0.44
1:A:111:LEU:HD23	1:A:142:ASN:HB3	2.00	0.44
1:A:199:MET:HB3	1:A:263:LEU:HD13	1.99	0.44
1:A:227:MET:HG2	1:A:269:VAL:HG21	2.00	0.44
2:B:1173:TYR:HA	2:B:1201:LEU:HD23	2.00	0.44
1:A:83:ILE:HG21	1:A:88:LEU:HD23	2.00	0.43
1:A:739:ASN:HB2	1:A:796:PHE:CE1	2.53	0.43
2:B:1139:MET:HB3	2:B:1166:VAL:HG22	1.99	0.43
2:C:1075:ARG:HB2	2:C:1233:LEU:HD13	1.99	0.43
3:E:56:LEU:HD23	3:E:56:LEU:HA	1.82	0.43
2:C:94:PHE:HB3	2:C:105:MET:HG2	2.00	0.43
2:C:1156:ILE:O	2:C:1159:VAL:HB	2.18	0.43
2:C:1240:ARG:HD2	2:C:1243:ARG:HB2	2.00	0.43
1:A:301:SER:HB2	1:A:316:TYR:OH	2.18	0.43
1:A:836:ILE:CD1	1:A:1033:ILE:HG21	2.48	0.43
1:A:849:ILE:HG12	1:A:918:ILE:HD13	1.99	0.43
2:B:166:TYR:OH	2:B:1264:GLU:OE1	2.29	0.43
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.46	0.43
3:D:156:VAL:HG13	3:D:228:LEU:HD22	1.99	0.43
3:E:158:LEU:HD13	3:E:158:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:OG1	1:A:37:ASP:N	2.51	0.43
2:B:818:ALA:HB1	2:B:1045:TYR:O	2.19	0.43
2:B:1052:LEU:HD13	2:B:1052:LEU:HA	1.88	0.43
2:C:612:PHE:CE2	2:C:614:ARG:HB2	2.53	0.43
1:A:166:ILE:HD13	1:A:179:TYR:CE1	2.53	0.43
1:A:864:ARG:NH1	4:A:1102:SAM:O3'	2.51	0.43
2:B:398:ARG:NH2	2:B:1310:ARG:HG3	2.33	0.43
2:C:363:ARG:HH22	2:C:1270:LEU:HD13	1.82	0.43
2:C:390:HIS:HB2	2:C:1318:GLU:HB3	2.00	0.43
1:A:858:VAL:HG22	1:A:918:ILE:HD12	2.01	0.43
2:C:704:VAL:HA	2:C:1330:ILE:HG21	2.00	0.43
1:A:864:ARG:HD2	1:A:864:ARG:HA	1.78	0.43
2:B:197:PHE:HB2	2:B:301:LEU:HD11	2.00	0.43
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.72	0.43
2:C:475:ILE:H	2:C:475:ILE:HG13	1.60	0.43
2:C:585:PHE:CZ	2:C:728:LYS:HD3	2.54	0.43
2:C:817:ASP:HA	2:C:983:ILE:HG12	1.99	0.43
2:C:1071:PHE:HB2	2:C:1173:TYR:CE1	2.53	0.43
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	1.99	0.43
1:A:980:ILE:H	1:A:980:ILE:HG12	1.56	0.43
2:C:351:ASP:OD1	2:C:351:ASP:N	2.51	0.43
2:C:615:THR:HG23	2:C:1333:ALA:HB1	2.00	0.43
2:C:1050:LEU:HD13	2:C:1054:ARG:NH2	2.34	0.43
2:C:1100:GLN:OE1	2:C:1142:ASN:ND2	2.52	0.43
2:C:1114:ARG:HG3	2:C:1116:ARG:HD3	1.99	0.43
3:D:76:LEU:O	3:D:271:TYR:OH	2.27	0.43
2:B:379:LEU:CD2	2:B:796:PRO:HB2	2.49	0.43
2:C:530:GLY:HA3	2:C:575:TRP:CE3	2.54	0.43
3:D:178:LYS:HA	3:D:250:ARG:O	2.19	0.43
3:D:261:ARG:NH1	3:D:263:ALA:O	2.51	0.43
1:A:74:LEU:HB3	1:A:83:ILE:HD13	2.01	0.43
2:B:385:ILE:O	2:B:386:SER:OG	2.35	0.43
2:B:1043:SER:O	2:B:1045:TYR:N	2.50	0.43
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.48	0.43
2:C:100:ASP:HA	3:E:82:GLN:NE2	2.33	0.43
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.87	0.43
2:B:1118:THR:CG2	2:B:1127:ALA:HB1	2.48	0.42
2:C:883:ILE:HD13	2:C:910:LEU:HD21	2.00	0.42
2:C:1005:LEU:HA	2:C:1005:LEU:HD13	1.84	0.42
1:A:602:PHE:CG	1:A:608:ILE:HD13	2.54	0.42
4:A:1102:SAM:HE2	4:A:1102:SAM:HB1	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LEU:O	2:B:383:SER:OG	2.29	0.42
2:B:856:LEU:HD22	2:B:860:ARG:HD2	2.01	0.42
2:B:1048:ASP:OD1	2:B:1048:ASP:N	2.52	0.42
1:A:408:PRO:HB2	1:A:468:PRO:HG2	2.01	0.42
1:A:962:PHE:HB2	1:A:998:LEU:HD23	2.02	0.42
1:A:1006:MET:O	1:A:1010:ILE:HG12	2.19	0.42
2:B:514:PHE:HB3	2:B:607:PHE:HE2	1.84	0.42
2:B:874:ILE:HD11	2:B:917:VAL:HG13	2.00	0.42
2:B:1208:ASP:OD1	2:B:1243:ARG:NH1	2.52	0.42
2:C:193:THR:HA	2:C:296:VAL:HG22	2.01	0.42
2:C:1171:ILE:HG22	2:C:1173:TYR:HD2	1.84	0.42
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.86	0.42
2:B:650:SER:O	2:B:654:THR:HG23	2.20	0.42
2:B:795:ASP:HA	2:B:796:PRO:HD3	1.88	0.42
2:C:694:ILE:HD12	2:C:775:VAL:HG21	2.01	0.42
2:C:1201:LEU:HD23	2:C:1201:LEU:HA	1.86	0.42
3:D:28:PRO:CB	3:D:226:MET:HG3	2.49	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.83	0.42
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.88	0.42
1:A:457:ASN:HA	1:A:686:TYR:HB2	2.01	0.42
1:A:474:TYR:CD1	1:A:499:VAL:HG12	2.48	0.42
2:B:872:ILE:HD11	2:B:883:ILE:HA	2.01	0.42
2:C:452:ASN:OD1	2:C:452:ASN:N	2.50	0.42
2:C:638:THR:O	2:C:699:THR:HB	2.19	0.42
2:C:1132:THR:HG22	2:C:1161:LYS:HB3	2.02	0.42
1:A:18:LYS:NZ	1:A:109:ASN:O	2.45	0.42
2:B:311:ASN:O	2:B:315:THR:HB	2.19	0.42
2:B:373:ASP:O	2:B:376:ILE:HG12	2.20	0.42
2:B:687:LEU:HD23	2:B:687:LEU:HA	1.91	0.42
2:B:798:THR:O	2:B:802:GLN:HG3	2.20	0.42
2:C:637:TYR:HB2	2:C:699:THR:HG22	2.01	0.42
2:C:1243:ARG:NH1	2:C:1256:GLY:O	2.53	0.42
3:D:19:ILE:H	3:D:19:ILE:HG13	1.70	0.42
3:E:15:PHE:HZ	3:E:107:LEU:HD22	1.83	0.42
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.71	0.42
1:A:1015:GLU:HG2	1:A:1017:ILE:HG23	2.02	0.42
2:C:1121:HIS:HA	2:C:1122:PRO:HD3	1.83	0.42
3:E:153:TYR:HA	3:E:156:VAL:HG23	2.02	0.42
2:B:608:THR:HA	2:B:609:PRO:HD3	1.85	0.42
2:C:190:VAL:HG23	2:C:300:LEU:HB3	2.02	0.42
2:C:190:VAL:HG11	2:C:304:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:GLU:HG2	2:C:577:GLN:HG3	2.01	0.42
2:C:522:PRO:HB3	2:C:609:PRO:HB3	2.01	0.42
2:C:829:SER:O	2:C:965:ARG:NH2	2.51	0.42
2:C:1055:LEU:HD22	2:C:1055:LEU:HA	1.89	0.42
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.83	0.42
3:D:283:LEU:HA	3:D:283:LEU:HD23	1.79	0.42
3:E:51:THR:HA	3:E:52:PRO:HD3	1.86	0.42
1:A:366:SER:HA	1:A:815:GLY:HA2	2.02	0.42
1:A:678:LEU:HD23	1:A:679:LYS:N	2.35	0.42
2:B:1092:VAL:HG21	2:B:1138:HIS:CD2	2.55	0.42
2:C:728:LYS:HG3	2:C:729:PRO:HD2	2.01	0.42
2:B:1309:ILE:HD12	2:B:1309:ILE:HG23	1.86	0.41
2:C:413:MET:HG3	2:C:1040:PHE:CZ	2.55	0.41
3:D:105:LEU:HD21	3:D:199:LEU:HD13	2.01	0.41
1:A:164:ILE:HG22	1:A:165:PRO:O	2.19	0.41
1:A:421:LEU:HD11	1:A:542:LEU:HD21	2.02	0.41
2:B:748:GLN:H	2:B:748:GLN:HG2	1.46	0.41
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.85	0.41
2:C:478:ILE:O	2:C:482:ILE:HG12	2.20	0.41
2:C:1111:ALA:HB3	2:C:1116:ARG:HG3	2.03	0.41
2:C:1277:LEU:HA	2:C:1289:PRO:HA	2.01	0.41
3:E:137:LEU:HD22	3:E:278:PHE:CE1	2.55	0.41
1:A:418:GLY:C	1:A:976:ALA:HB2	2.40	0.41
2:B:365:LEU:HD23	2:B:365:LEU:HA	1.84	0.41
2:B:388:GLN:HB2	2:B:1320:VAL:HB	2.03	0.41
2:B:767:LEU:HD12	2:B:767:LEU:HA	1.87	0.41
2:C:161:LYS:HE3	2:C:161:LYS:HB2	1.76	0.41
2:C:334:LEU:HD23	2:C:334:LEU:HA	1.74	0.41
2:C:804:LEU:HD13	2:C:804:LEU:HA	1.82	0.41
3:E:10:THR:HG23	3:E:204:ASP:OD2	2.21	0.41
3:E:90:PHE:HA	3:E:93:LEU:HB2	2.02	0.41
3:E:185:SER:O	3:E:189:LEU:HD22	2.20	0.41
1:A:860:SER:HA	1:A:920:LEU:HB2	2.03	0.41
2:B:604:MET:HE1	2:B:607:PHE:CE1	2.55	0.41
2:C:383:SER:HB2	2:C:387:THR:HG21	2.02	0.41
1:A:377:LEU:H	1:A:377:LEU:HD22	1.84	0.41
2:B:574:LYS:NZ	2:B:574:LYS:HB3	2.35	0.41
3:D:19:ILE:HG22	3:D:192:ASP:HB2	2.02	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.21	0.41
1:A:425:THR:O	1:A:703:PHE:HB3	2.21	0.41
2:B:147:VAL:HG22	2:B:379:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:PRO:O	2:B:1137:VAL:HG23	2.20	0.41
2:B:1156:ILE:HD13	2:B:1156:ILE:HA	1.86	0.41
2:C:636:PRO:HB2	2:C:637:TYR:CD2	2.56	0.41
2:C:650:SER:O	2:C:654:THR:HG23	2.21	0.41
3:E:53:GLU:CD	3:E:53:GLU:H	2.24	0.41
2:B:537:LEU:HD23	2:B:537:LEU:HA	1.82	0.41
2:B:1064:ASN:HA	2:B:1065:PRO:HD3	1.80	0.41
2:B:1288:ILE:HG12	3:D:20:ARG:CZ	2.51	0.41
2:C:343:ILE:HD13	2:C:362:LEU:HD21	2.03	0.41
2:C:620:ILE:HD11	2:C:631:PRO:HG2	2.02	0.41
2:C:1175:ALA:HA	2:C:1204:LEU:O	2.21	0.41
1:A:54:LEU:HD13	1:A:54:LEU:HA	1.82	0.41
2:B:228:VAL:HG21	2:B:253:MET:CG	2.51	0.41
2:B:375:ARG:HE	2:B:400:GLU:CD	2.23	0.41
2:C:119:ASP:OD1	2:C:119:ASP:N	2.53	0.41
2:C:558:TYR:CE1	2:C:587:ALA:HA	2.56	0.41
2:C:636:PRO:HB2	2:C:637:TYR:CE2	2.56	0.41
2:C:931:ASN:O	2:C:931:ASN:ND2	2.43	0.41
3:D:182:TRP:NE1	3:D:185:SER:HA	2.35	0.41
3:E:108:ASP:OD2	3:E:112:TYR:OH	2.27	0.41
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.75	0.41
1:A:255:ARG:NH2	5:A:1104:GTP:O1A	2.53	0.41
1:A:474:TYR:CZ	1:A:522:PRO:HD3	2.56	0.41
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.87	0.41
1:A:561:LEU:HD11	1:A:602:PHE:CZ	2.53	0.41
1:A:677:LEU:HG	1:A:690:THR:HG21	2.03	0.41
2:B:299:ALA:HB2	2:B:1265:MET:HB3	2.02	0.41
2:B:342:THR:HB	2:B:1309:ILE:HD11	2.03	0.41
2:B:450:PRO:HG2	2:B:453:LEU:CB	2.51	0.41
2:B:502:PHE:HA	2:B:507:SER:CB	2.51	0.41
2:B:1189:ASP:HA	2:C:118:THR:HA	2.03	0.41
2:C:154:PHE:CE2	2:C:365:LEU:HB2	2.56	0.41
2:C:223:LYS:NZ	2:C:1203:HIS:HB2	2.35	0.41
2:C:254:VAL:O	2:C:258:VAL:HG12	2.21	0.41
2:C:523:THR:HG23	2:C:720:PHE:HB2	2.02	0.41
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.32	0.41
1:A:372:ARG:HD2	1:A:772:TRP:CE3	2.56	0.41
1:A:1018:ARG:NH1	1:A:1051:PRO:HG3	2.36	0.41
2:B:1126:MET:HE2	3:E:146:ARG:HH21	1.86	0.41
2:B:1233:LEU:HD12	2:B:1233:LEU:HA	1.84	0.41
2:C:96:ILE:HD13	2:C:103:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:LEU:HD13	2:C:397:LEU:HD21	2.03	0.41
2:C:401:LEU:HD12	2:C:401:LEU:HA	1.72	0.41
2:C:626:ARG:NH2	2:C:712:PHE:O	2.34	0.41
2:C:694:ILE:HG13	2:C:772:TYR:CE1	2.56	0.41
2:C:825:SER:HA	2:C:1015:GLN:HB3	2.02	0.41
2:C:1186:GLN:NE2	2:C:1203:HIS:O	2.54	0.41
3:E:2:LEU:HD22	3:E:3:GLN:O	2.21	0.41
3:E:44:LEU:HG	3:E:174:VAL:HG22	2.02	0.41
1:A:423:THR:HA	1:A:424:PRO:HD3	1.93	0.40
2:B:147:VAL:HG11	2:B:375:ARG:HB3	2.03	0.40
2:B:379:LEU:HD23	2:B:379:LEU:HA	1.74	0.40
2:C:818:ALA:HB1	2:C:1045:TYR:O	2.21	0.40
2:C:890:THR:HB	2:C:892:VAL:HG22	2.02	0.40
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.57	0.40
1:A:755:ALA:N	1:A:756:PRO:HD2	2.36	0.40
2:B:442:PRO:HD3	2:B:475:ILE:HD12	2.03	0.40
2:B:450:PRO:HG2	2:B:453:LEU:HB2	2.03	0.40
2:B:719:ASN:OD1	2:B:719:ASN:N	2.54	0.40
2:B:1236:ILE:HG22	2:B:1237:SER:H	1.85	0.40
2:C:694:ILE:HD12	2:C:694:ILE:HA	1.82	0.40
2:C:1119:TYR:OH	2:C:1121:HIS:HD2	2.04	0.40
3:E:123:ASP:HA	3:E:124:PRO:HD3	1.92	0.40
1:A:186:ALA:HB2	1:A:195:ILE:HD12	2.02	0.40
2:B:659:LEU:HD12	2:B:659:LEU:HA	1.77	0.40
2:B:817:ASP:HA	2:B:983:ILE:HG12	2.02	0.40
2:B:910:LEU:HD13	2:B:917:VAL:HG22	2.04	0.40
2:C:697:ALA:HB2	2:C:775:VAL:HG23	2.02	0.40
2:C:879:THR:HB	2:C:882:GLN:HG3	2.03	0.40
3:E:19:ILE:H	3:E:19:ILE:HG13	1.71	0.40
1:A:173:ASP:OD1	1:A:173:ASP:N	2.49	0.40
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.93	0.40
1:A:602:PHE:CD2	1:A:608:ILE:HD13	2.56	0.40
1:A:686:TYR:HA	1:A:714:ARG:NH2	2.35	0.40
2:B:797:SER:O	2:B:801:SER:HB3	2.22	0.40
2:B:1109:SER:HA	2:C:393:ASN:HD22	1.86	0.40
2:C:309:TRP:CZ2	2:C:1257:ALA:HB1	2.56	0.40
2:C:327:LEU:HD12	2:C:327:LEU:HA	1.91	0.40
2:C:500:GLU:HG3	2:C:502:PHE:H	1.86	0.40
2:C:855:TYR:CE1	2:C:859:ILE:HG12	2.57	0.40
2:C:1113:LYS:HE2	2:C:1113:LYS:HB2	1.92	0.40
3:E:160:LEU:HD11	3:E:229:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HB3	1:A:143:TYR:CZ	2.57	0.40
1:A:143:TYR:CD2	1:A:146:PRO:HA	2.56	0.40
1:A:150:PHE:O	1:A:153:VAL:HG22	2.22	0.40
1:A:849:ILE:HD12	1:A:871:VAL:CG1	2.51	0.40
1:A:959:TYR:HE1	1:A:1054:LYS:HG3	1.86	0.40
2:B:332:THR:HG23	2:B:344:VAL:HG12	2.04	0.40
2:B:429:ILE:HG23	2:B:799:THR:HG22	2.04	0.40
2:B:543:TRP:CD1	2:B:666:ARG:NH1	2.89	0.40
2:B:769:GLN:HE21	2:B:769:GLN:HB2	1.50	0.40
2:B:1073:GLY:O	2:B:1173:TYR:HE1	2.02	0.40
2:C:170:TYR:HB2	2:C:172:ASP:OD1	2.22	0.40
2:C:255:LEU:HD23	2:C:255:LEU:HA	1.86	0.40
2:C:537:LEU:HD23	2:C:537:LEU:HA	1.74	0.40
2:C:632:GLN:HG2	2:C:718:ASN:ND2	2.36	0.40
3:E:211:GLU:HG3	3:E:214:ARG:HH21	1.85	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%)	1006 (95%)	48 (4%)	1 (0%)	51	83
2	B	1187/1333 (89%)	1128 (95%)	55 (5%)	4 (0%)	41	73
2	C	1247/1333 (94%)	1183 (95%)	58 (5%)	6 (0%)	29	64
3	D	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	41	73
3	E	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	22	57
All	All	4069/4620 (88%)	3882 (95%)	173 (4%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	GLN
2	B	1007	THR
2	B	1310	ARG
2	C	275	SER
3	E	183	GLU
1	A	982	VAL
3	D	61	ASN
3	E	116	THR
2	C	901	VAL
2	C	1245	ILE
2	C	1268	GLY
2	C	140	GLY
2	C	340	VAL
2	B	1309	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	942/943 (100%)	850 (90%)	92 (10%)	8 29
2	B	1038/1153 (90%)	933 (90%)	105 (10%)	7 28
2	C	1090/1153 (94%)	973 (89%)	117 (11%)	6 26
3	D	240/379 (63%)	218 (91%)	22 (9%)	9 33
3	E	240/379 (63%)	212 (88%)	28 (12%)	5 22
All	All	3550/4007 (89%)	3186 (90%)	364 (10%)	11 27

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	11	THR
1	A	12	ARG
1	A	41	THR
1	A	50	THR
1	A	54	LEU

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	88	LEU
1	A	99	VAL
1	A	102	LEU
1	A	105	ARG
1	A	112	ARG
1	A	117	LEU
1	A	125	ASN
1	A	133	LEU
1	A	153	VAL
1	A	157	LEU
1	A	188	THR
1	A	196	LEU
1	A	199	MET
1	A	205	VAL
1	A	222	ARG
1	A	234	LYS
1	A	236	LEU
1	A	242	LYS
1	A	275	ILE
1	A	288	LEU
1	A	298	LEU
1	A	306	GLN
1	A	317	ARG
1	A	336	LEU
1	A	348	LEU
1	A	368	THR
1	A	373	ILE
1	A	377	LEU
1	A	378	THR
1	A	449	THR
1	A	453	LEU
1	A	461	ARG
1	A	466	LEU
1	A	475	ARG
1	A	478	ILE
1	A	493	LEU
1	A	503	ILE
1	A	532	MET
1	A	533	LEU
1	A	556	THR
1	A	564	GLU

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Mol	Chain	Res	Type
1	A	565	ARG
1	A	569	VAL
1	A	572	LEU
1	A	577	ARG
1	A	585	ILE
1	A	592	VAL
1	A	595	ASN
1	A	647	LEU
1	A	665	LEU
1	A	675	THR
1	A	677	LEU
1	A	719	VAL
1	A	737	HIS
1	A	738	SER
1	A	749	CYS
1	A	750	VAL
1	A	757	LEU
1	A	763	LYS
1	A	780	LEU
1	A	781	VAL
1	A	783	ILE
1	A	812	VAL
1	A	816	LEU
1	A	833	VAL
1	A	849	ILE
1	A	855	MET
1	A	861	ILE
1	A	881	ILE
1	A	886	ARG
1	A	890	LEU
1	A	900	GLN
1	A	925	ILE
1	A	934	THR
1	A	951	LEU
1	A	978	LYS
1	A	980	ILE
1	A	982	VAL
1	A	995	VAL
1	A	1018	ARG
1	A	1029	SER
1	A	1034	ARG
1	A	1042	VAL

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Mol	Chain	Res	Type
1	A	1047	ASN
1	A	1052	VAL
2	B	136	VAL
2	B	143	VAL
2	B	147	VAL
2	B	158	SER
2	B	175	THR
2	B	186	ASP
2	B	190	VAL
2	B	198	LYS
2	B	203	VAL
2	B	231	LEU
2	B	242	GLU
2	B	259	MET
2	B	260	THR
2	B	271	THR
2	B	274	MET
2	B	279	SER
2	B	286	LEU
2	B	287	ARG
2	B	289	THR
2	B	294	VAL
2	B	304	PHE
2	B	311	ASN
2	B	315	THR
2	B	323	THR
2	B	334	LEU
2	B	339	LEU
2	B	365	LEU
2	B	384	MET
2	B	405	HIS
2	B	414	LEU
2	B	431	THR
2	B	440	ILE
2	B	486	VAL
2	B	497	LYS
2	B	532	ILE
2	B	533	GLN
2	B	552	VAL
2	B	637	TYR
2	B	659	LEU
2	B	684	LEU

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Mol	Chain	Res	Type
2	B	685	ARG
2	B	698	HIS
2	B	702	LEU
2	B	713	MET
2	B	740	SER
2	B	742	LYS
2	B	748	GLN
2	B	750	GLU
2	B	759	ASP
2	B	769	GLN
2	B	788	MET
2	B	801	SER
2	B	804	LEU
2	B	815	LEU
2	B	843	LEU
2	B	848	ARG
2	B	855	TYR
2	B	856	LEU
2	B	890	THR
2	B	925	VAL
2	B	938	ASN
2	B	953	ASP
2	B	971	MET
2	B	995	THR
2	B	996	ASP
2	B	1007	THR
2	B	1010	ARG
2	B	1036	ASP
2	B	1048	ASP
2	B	1061	LEU
2	B	1067	ILE
2	B	1074	VAL
2	B	1079	LEU
2	B	1083	ASP
2	B	1087	ASP
2	B	1097	VAL
2	B	1108	SER
2	B	1110	LEU
2	B	1116	ARG
2	B	1117	VAL
2	B	1120	THR
2	B	1134	ARG

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Mol	Chain	Res	Type
2	B	1138	HIS
2	B	1150	LEU
2	B	1170	ASP
2	B	1178	MET
2	B	1182	GLU
2	B	1186	GLN
2	B	1189	ASP
2	B	1198	LYS
2	B	1201	LEU
2	B	1210	LEU
2	B	1233	LEU
2	B	1234	GLN
2	B	1240	ARG
2	B	1247	ASN
2	B	1262	SER
2	B	1269	THR
2	B	1293	VAL
2	B	1304	MET
2	B	1310	ARG
2	B	1314	ASP
2	B	1315	MET
2	B	1329	ASN
2	B	1331	ARG
2	C	77	THR
2	C	82	ARG
2	C	91	ASP
2	C	100	ASP
2	C	102	VAL
2	C	112	THR
2	C	115	GLN
2	C	117	ARG
2	C	120	VAL
2	C	127	ASN
2	C	134	THR
2	C	141	LEU
2	C	147	VAL
2	C	150	LEU
2	C	171	GLU
2	C	178	ASP
2	C	190	VAL
2	C	203	VAL
2	C	208	LEU

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Mol	Chain	Res	Type
2	C	217	THR
2	C	222	THR
2	C	230	ASP
2	C	231	LEU
2	C	237	VAL
2	C	255	LEU
2	C	270	THR
2	C	274	MET
2	C	275	SER
2	C	281	VAL
2	C	294	VAL
2	C	302	ARG
2	C	310	LEU
2	C	315	THR
2	C	323	THR
2	C	330	THR
2	C	360	ILE
2	C	375	ARG
2	C	379	LEU
2	C	384	MET
2	C	440	ILE
2	C	453	LEU
2	C	474	ASP
2	C	475	ILE
2	C	532	ILE
2	C	533	GLN
2	C	542	ARG
2	C	546	VAL
2	C	575	TRP
2	C	614	ARG
2	C	626	ARG
2	C	629	ARG
2	C	630	ASN
2	C	637	TYR
2	C	638	THR
2	C	654	THR
2	C	659	LEU
2	C	674	LYS
2	C	689	THR
2	C	694	ILE
2	C	696	VAL
2	C	708	THR

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Mol	Chain	Res	Type
2	C	735	THR
2	C	760	THR
2	C	804	LEU
2	C	815	LEU
2	C	828	ASP
2	C	832	MET
2	C	837	THR
2	C	851	THR
2	C	859	ILE
2	C	872	ILE
2	C	890	THR
2	C	894	VAL
2	C	896	LEU
2	C	931	ASN
2	C	935	GLN
2	C	959	GLN
2	C	980	ARG
2	C	992	VAL
2	C	995	THR
2	C	1015	GLN
2	C	1027	THR
2	C	1041	ARG
2	C	1050	LEU
2	C	1052	LEU
2	C	1055	LEU
2	C	1070	ARG
2	C	1079	LEU
2	C	1108	SER
2	C	1113	LYS
2	C	1114	ARG
2	C	1120	THR
2	C	1126	MET
2	C	1132	THR
2	C	1134	ARG
2	C	1144	ARG
2	C	1150	LEU
2	C	1167	ASP
2	C	1170	ASP
2	C	1174	THR
2	C	1186	GLN
2	C	1198	LYS
2	C	1202	PHE

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Mol	Chain	Res	Type
2	C	1210	LEU
2	C	1219	ASP
2	C	1230	ILE
2	C	1233	LEU
2	C	1234	GLN
2	C	1251	VAL
2	C	1253	ARG
2	C	1262	SER
2	C	1281	VAL
2	C	1285	GLN
2	C	1306	THR
2	C	1308	ASN
2	C	1320	VAL
2	C	1321	ASN
3	D	2	LEU
3	D	20	ARG
3	D	27	THR
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	51	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	158	LEU
3	D	160	LEU
3	D	171	VAL
3	D	181	SER
3	D	189	LEU
3	D	191	ARG
3	D	194	VAL
3	D	226	MET
3	D	252	LEU
3	E	2	LEU
3	E	21	ASN
3	E	29	THR
3	E	35	LEU
3	E	54	THR
3	E	66	VAL

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Mol	Chain	Res	Type
3	E	93	LEU
3	E	98	LEU
3	E	108	ASP
3	E	127	VAL
3	E	130	PHE
3	E	133	THR
3	E	139	ASN
3	E	144	ARG
3	E	158	LEU
3	E	160	LEU
3	E	183	GLU
3	E	188	SER
3	E	189	LEU
3	E	226	MET
3	E	242	ARG
3	E	245	THR
3	E	247	ARG
3	E	252	LEU
3	E	262	THR
3	E	266	THR
3	E	272	ASP
3	E	274	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	148	GLN
2	B	724	HIS
2	B	935	GLN
2	B	1138	HIS
2	B	1247	ASN
2	C	291	HIS
2	C	1121	HIS
2	C	1308	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SAM	A	1102	-	24,29,29	1.22	3 (12%)	23,42,42	1.62	4 (17%)
5	GTP	A	1103	-	26,34,34	1.10	2 (7%)	32,54,54	1.52	7 (21%)
5	GTP	A	1104	6	26,34,34	1.10	2 (7%)	32,54,54	1.58	7 (21%)
4	SAM	A	1101	-	24,29,29	1.24	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	1102	-	-	4/12/33/33	0/3/3/3
5	GTP	A	1103	-	-	2/18/38/38	0/3/3/3
5	GTP	A	1104	6	-	4/18/38/38	0/3/3/3
4	SAM	A	1101	-	-	6/12/33/33	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N3	4.19	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	SAM	C2-N3	3.95	1.38	1.32
5	A	1103	GTP	C5-C6	-3.95	1.39	1.47
5	A	1104	GTP	C5-C6	-3.62	1.40	1.47
4	A	1101	SAM	C2-N1	2.47	1.38	1.33
4	A	1102	SAM	C2-N1	2.44	1.38	1.33
5	A	1104	GTP	C2-N3	2.38	1.38	1.33
4	A	1102	SAM	OXT-C	-2.17	1.23	1.30
5	A	1103	GTP	C2-N3	2.08	1.38	1.33
4	A	1101	SAM	OXT-C	-2.07	1.23	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	SAM	N3-C2-N1	-5.47	120.13	128.68
4	A	1102	SAM	N3-C2-N1	-5.44	120.18	128.68
5	A	1104	GTP	PA-O3A-PB	-3.81	119.73	132.83
5	A	1103	GTP	PA-O3A-PB	-3.74	119.99	132.83
5	A	1104	GTP	C8-N7-C5	3.42	109.51	102.99
5	A	1104	GTP	C5-C6-N1	3.40	119.96	113.95
5	A	1104	GTP	C2-N1-C6	-3.07	119.45	125.10
5	A	1103	GTP	C5-C6-N1	3.04	119.33	113.95
5	A	1103	GTP	C2-N1-C6	-3.00	119.57	125.10
4	A	1102	SAM	C3'-C2'-C1'	2.99	105.47	100.98
4	A	1101	SAM	C3'-C2'-C1'	2.97	105.45	100.98
5	A	1103	GTP	C3'-C2'-C1'	2.94	105.40	100.98
5	A	1103	GTP	PB-O3B-PG	-2.83	123.10	132.83
5	A	1103	GTP	C8-N7-C5	2.83	108.38	102.99
5	A	1104	GTP	PB-O3B-PG	-2.81	123.20	132.83
4	A	1101	SAM	OXT-C-O	-2.64	118.09	124.09
4	A	1102	SAM	OXT-C-O	-2.46	118.50	124.09
5	A	1104	GTP	O6-C6-C5	-2.35	119.78	124.37
5	A	1104	GTP	C3'-C2'-C1'	2.15	104.22	100.98
4	A	1102	SAM	OXT-C-CA	2.14	120.69	113.38
5	A	1103	GTP	O6-C6-C5	-2.14	120.20	124.37
4	A	1101	SAM	OXT-C-CA	2.04	120.32	113.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	O-C-CA-N
4	A	1102	SAM	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	A	1102	SAM	CB-CG-SD-CE
5	A	1103	GTP	O4'-C4'-C5'-O5'
5	A	1103	GTP	C3'-C4'-C5'-O5'
4	A	1101	SAM	OXT-C-CA-N
5	A	1104	GTP	O4'-C4'-C5'-O5'
5	A	1104	GTP	C3'-C4'-C5'-O5'
4	A	1101	SAM	C-CA-CB-CG
4	A	1102	SAM	O4'-C4'-C5'-SD
4	A	1102	SAM	CA-CB-CG-SD
4	A	1101	SAM	O-C-CA-CB
4	A	1101	SAM	OXT-C-CA-CB
5	A	1104	GTP	PG-O3B-PB-O1B
4	A	1101	SAM	N-CA-CB-CG
5	A	1104	GTP	PB-O3A-PA-O1A

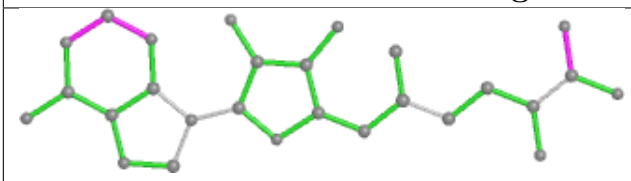
There are no ring outliers.

3 monomers are involved in 6 short contacts:

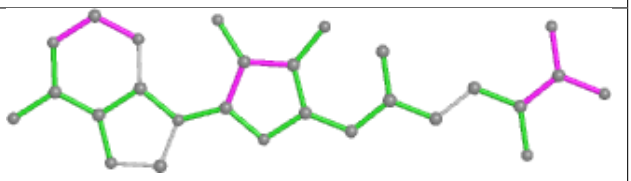
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	SAM	3	0
5	A	1104	GTP	2	0
4	A	1101	SAM	1	0

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

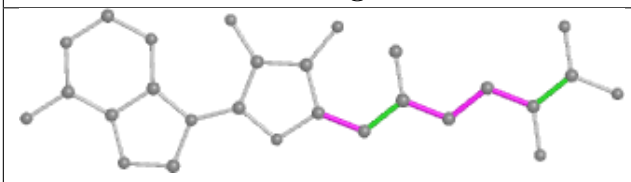
Ligand SAM A 1102



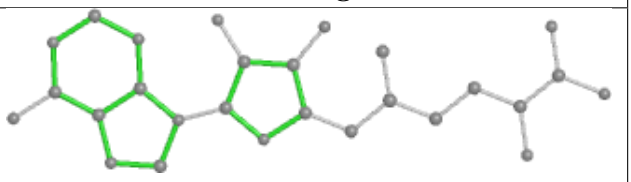
Bond lengths



Bond angles

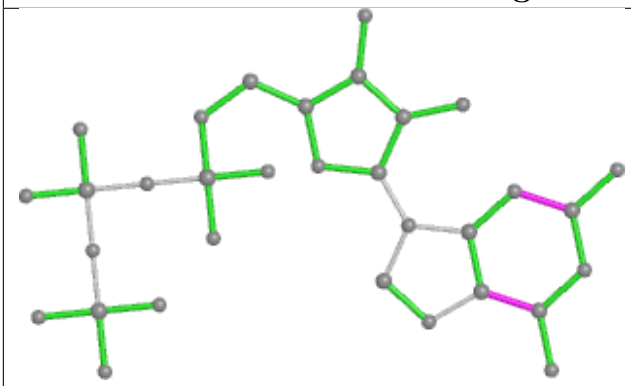


Torsions

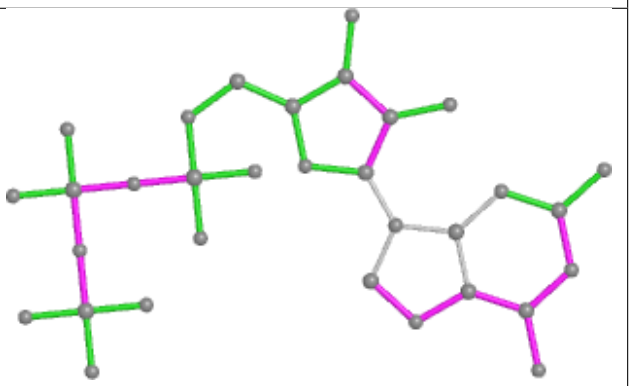


Rings

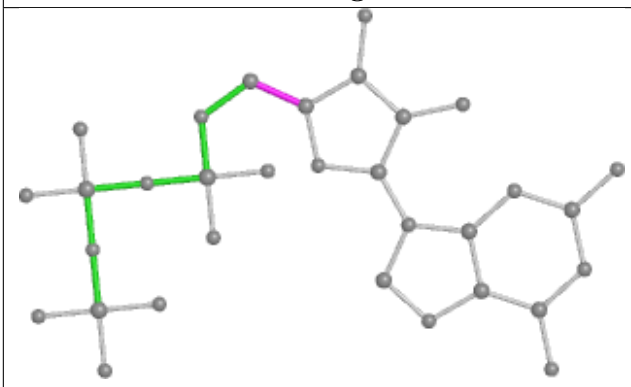
Ligand GTP A 1103



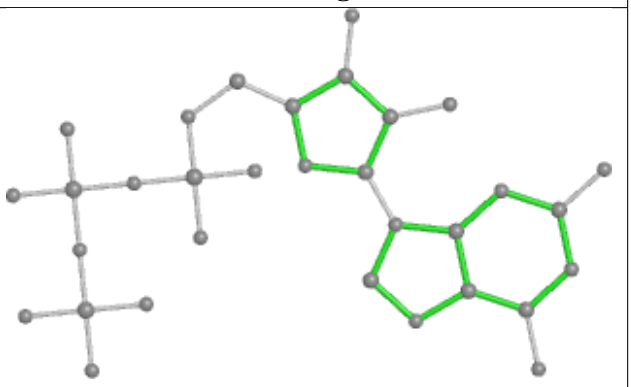
Bond lengths



Bond angles

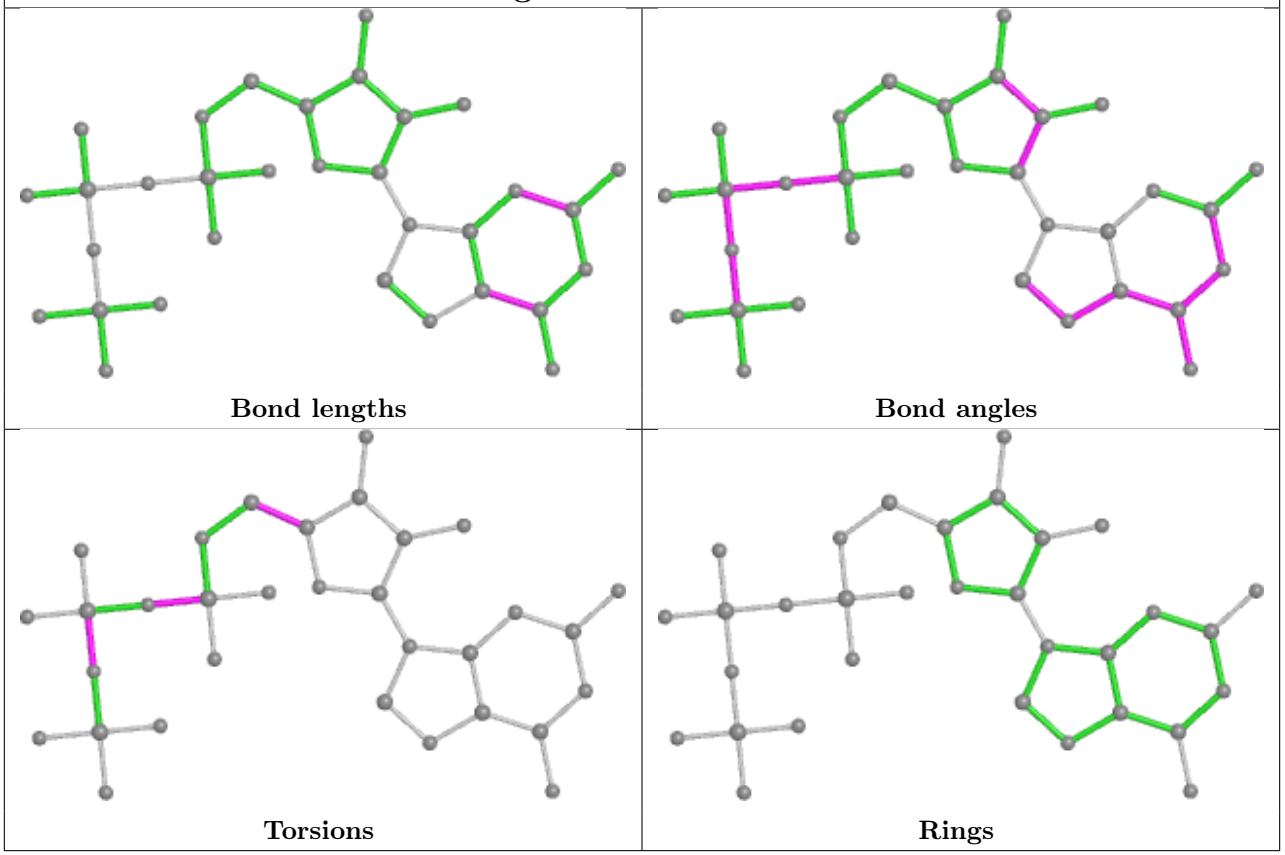


Torsions

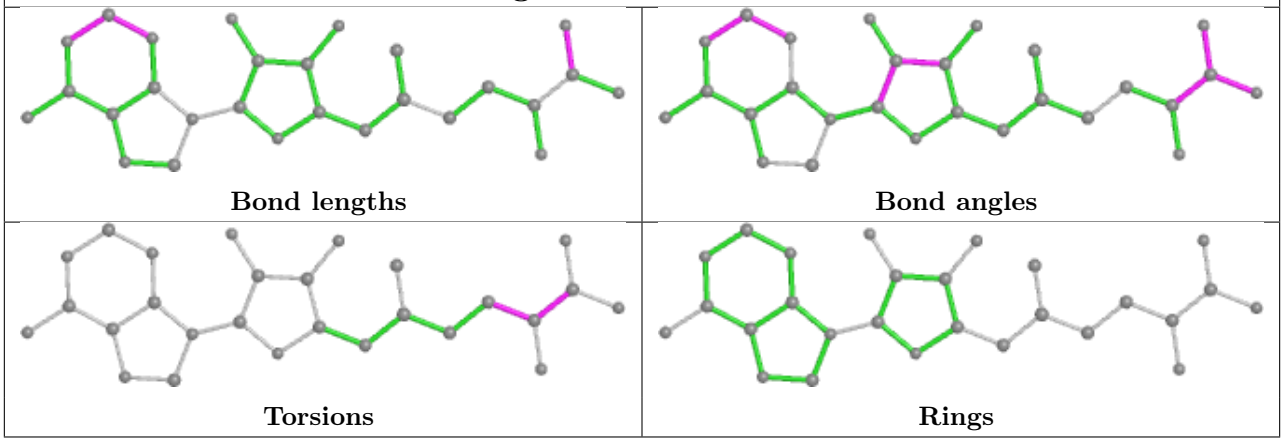


Rings

Ligand GTP A 1104



Ligand SAM A 1101



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.

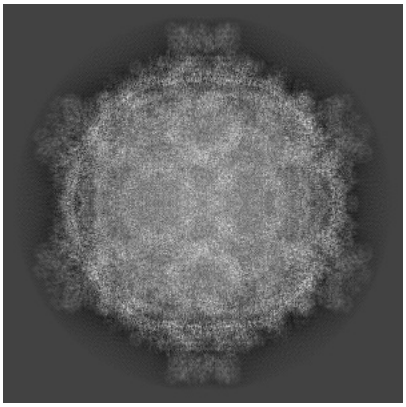
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6376. These allow visual inspection of the internal detail of the map and identification of artifacts.

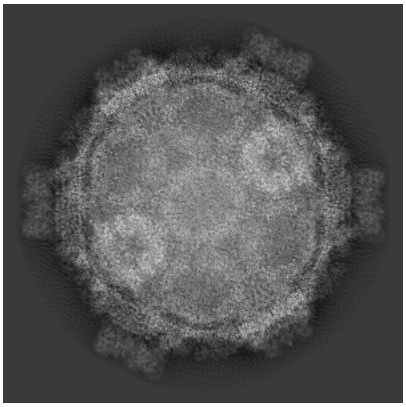
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

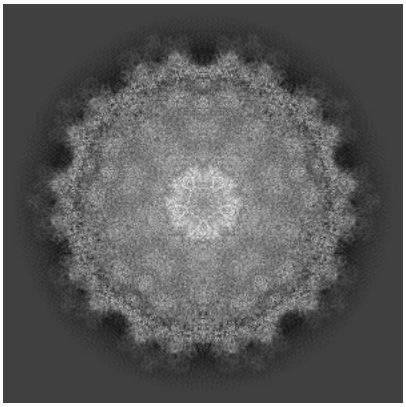
6.1.1 Primary map



X



Y

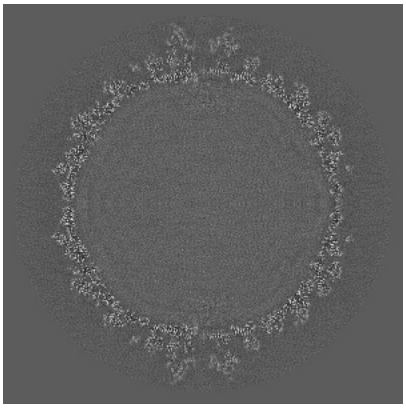


Z

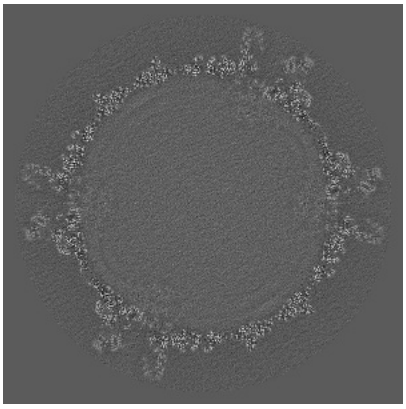
The images above show the map projected in three orthogonal directions.

6.2 Central slices

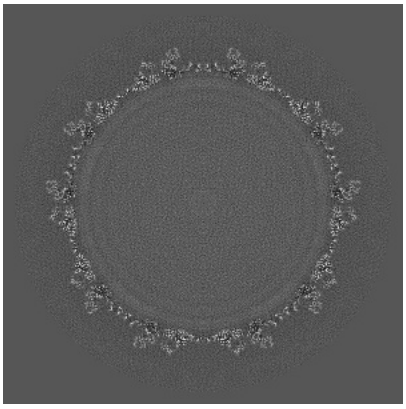
6.2.1 Primary map



X Index: 350



Y Index: 350

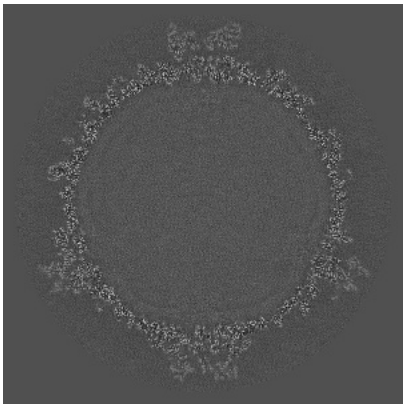


Z Index: 350

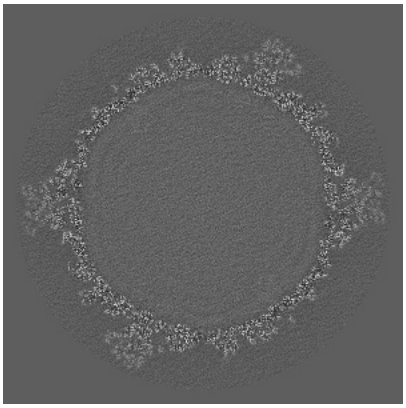
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

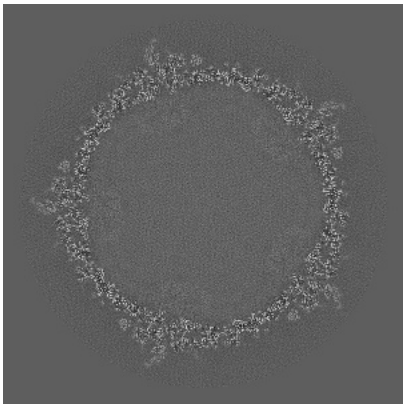
6.3.1 Primary map



X Index: 327



Y Index: 397

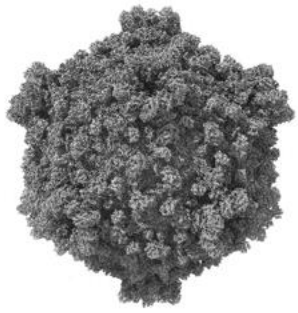


Z Index: 279

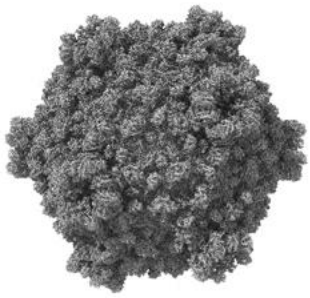
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

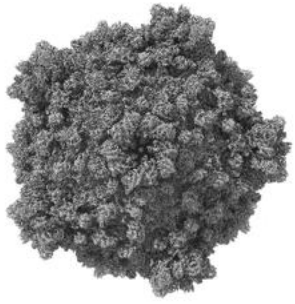
6.4.1 Primary map



X



Y



Z

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

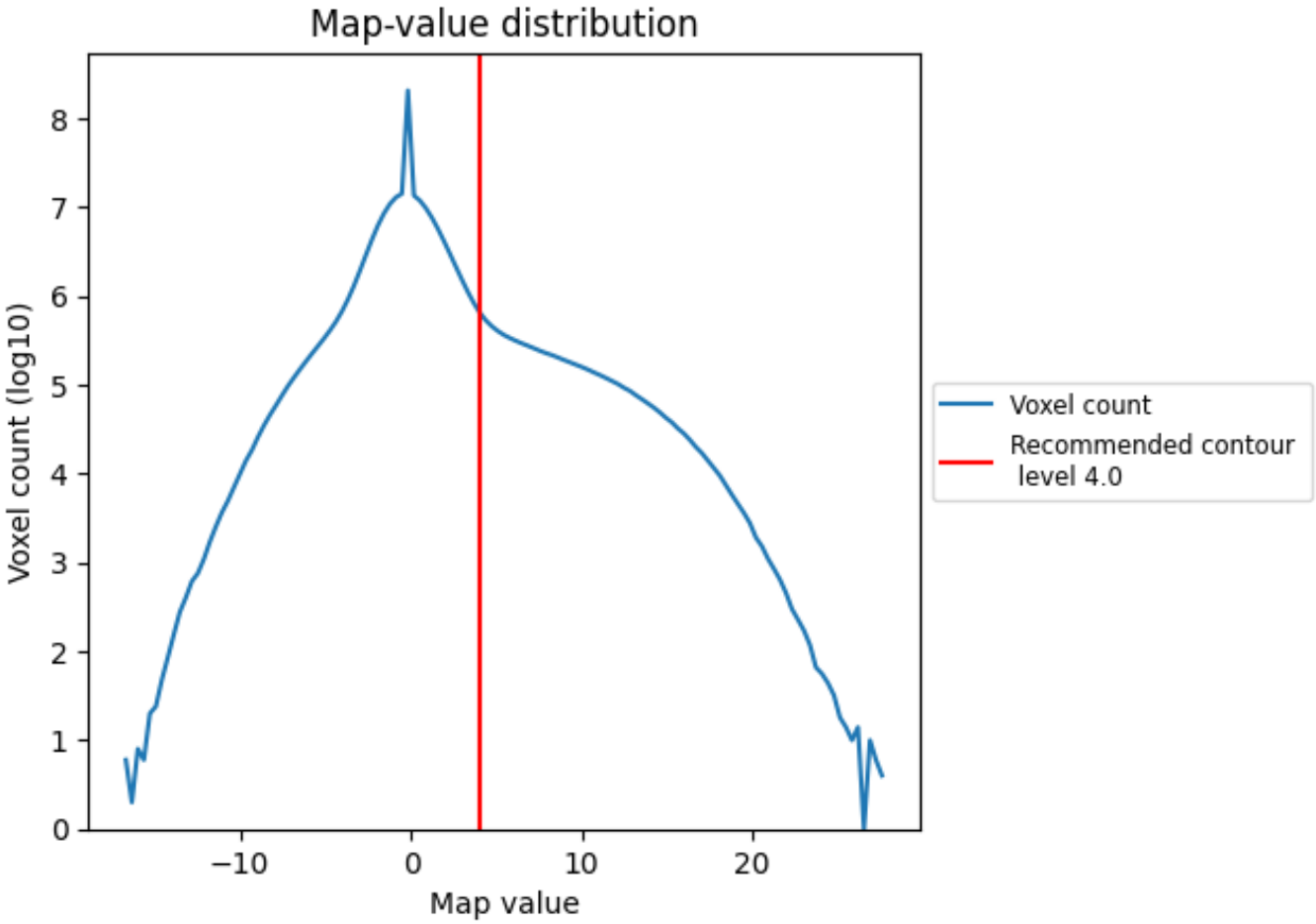
6.5 Mask visualisation (i)

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

7 Map analysis

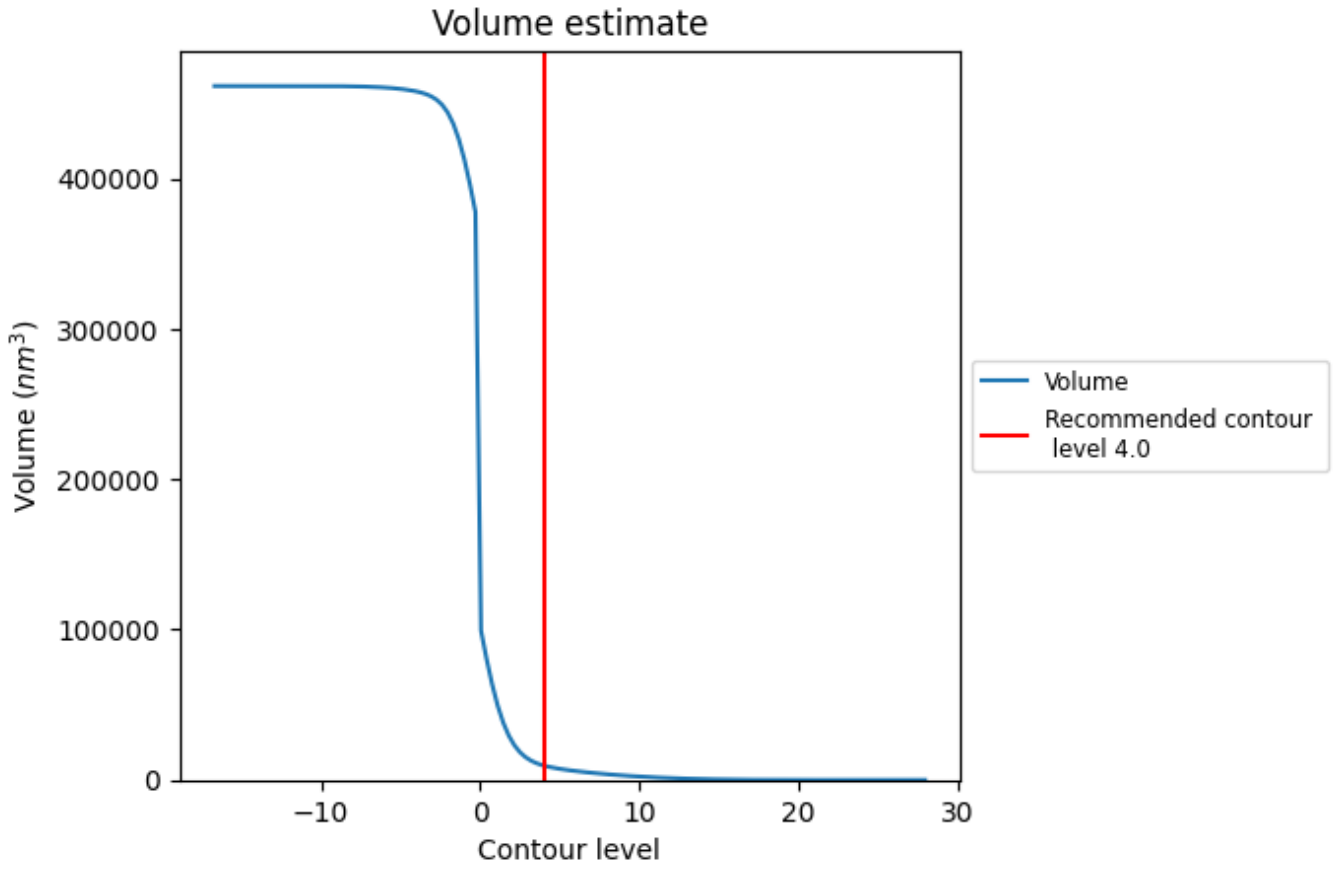
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

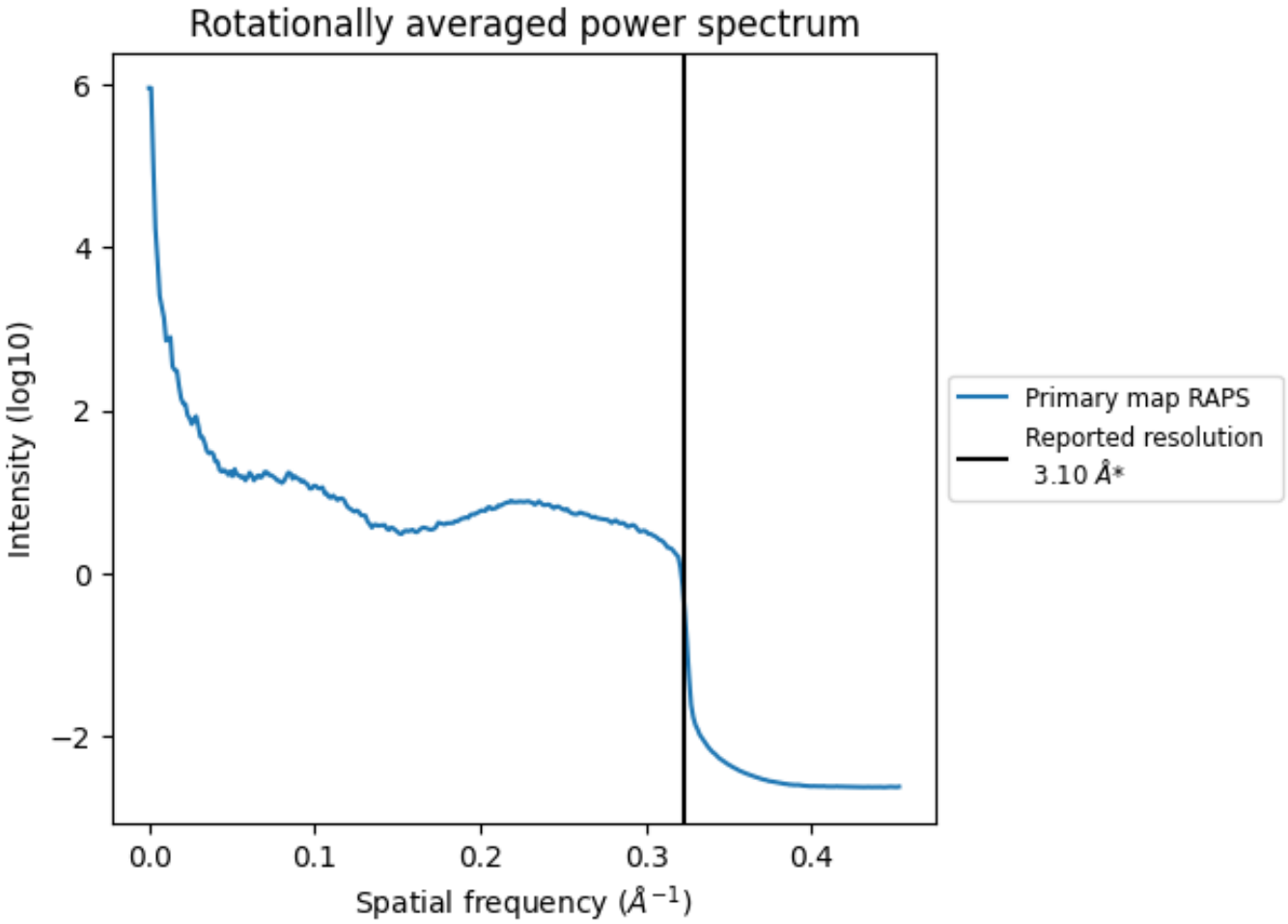
7.2 Volume estimate



The volume at the recommended contour level is 9565 nm^3; this corresponds to an approximate mass of 8641 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)

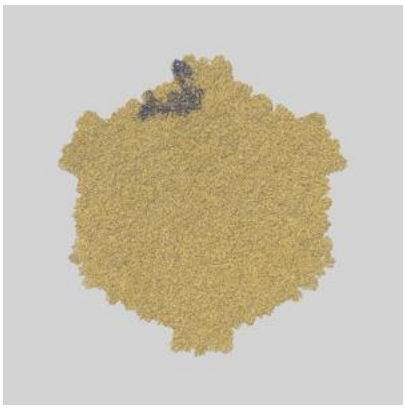
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

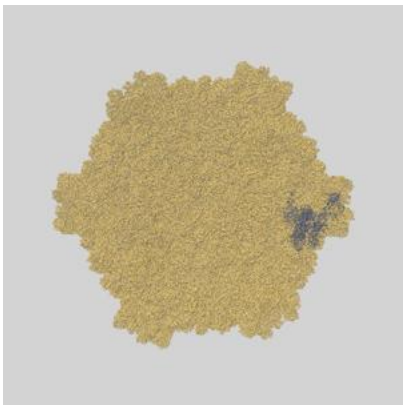
This section contains information regarding the fit between EMDB map EMD-6376 and PDB model 3JB2. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

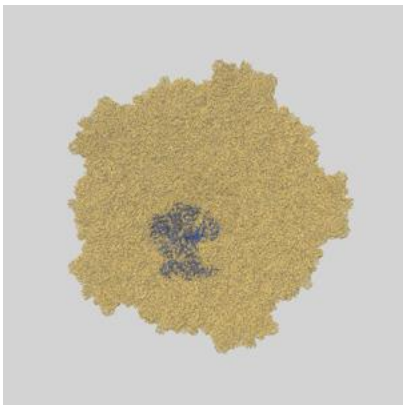
9.1.1 Map-model overlay



X

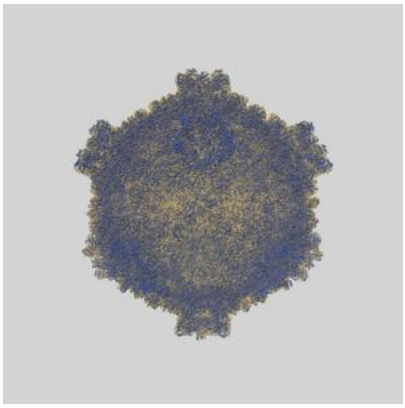


Y

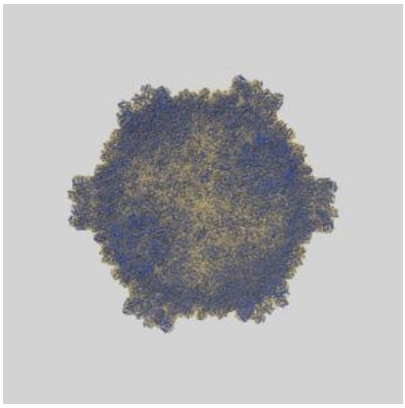


Z

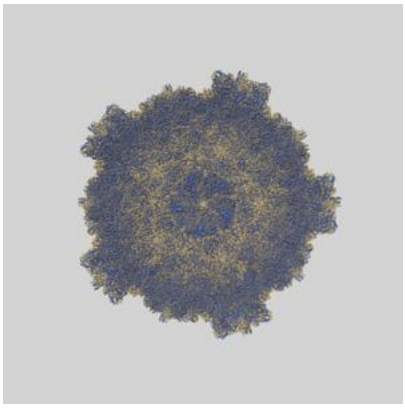
9.1.2 Map-model assembly overlay



X



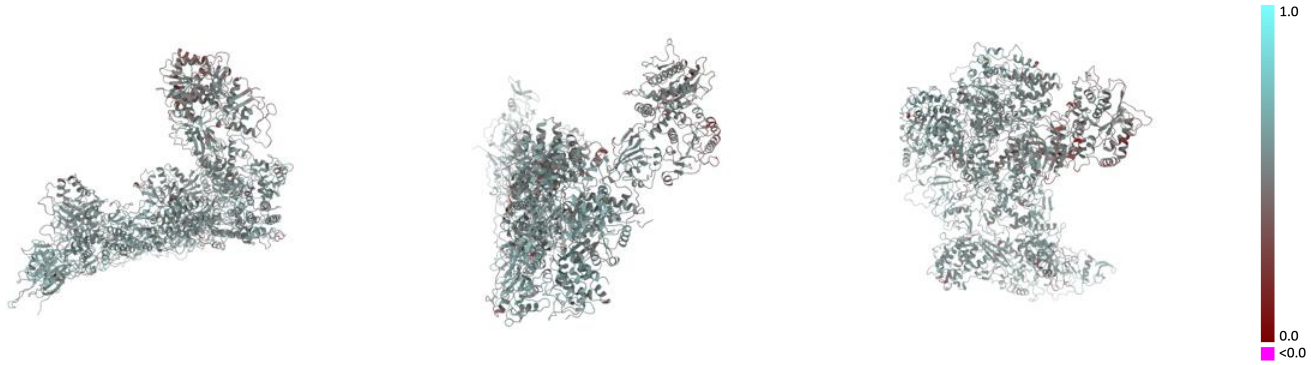
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

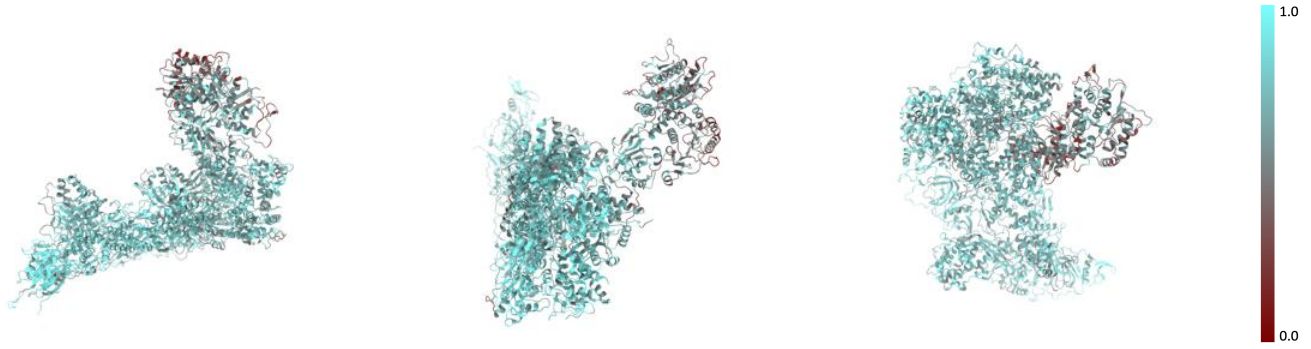
9.2 Q-score mapped to coordinate model



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.

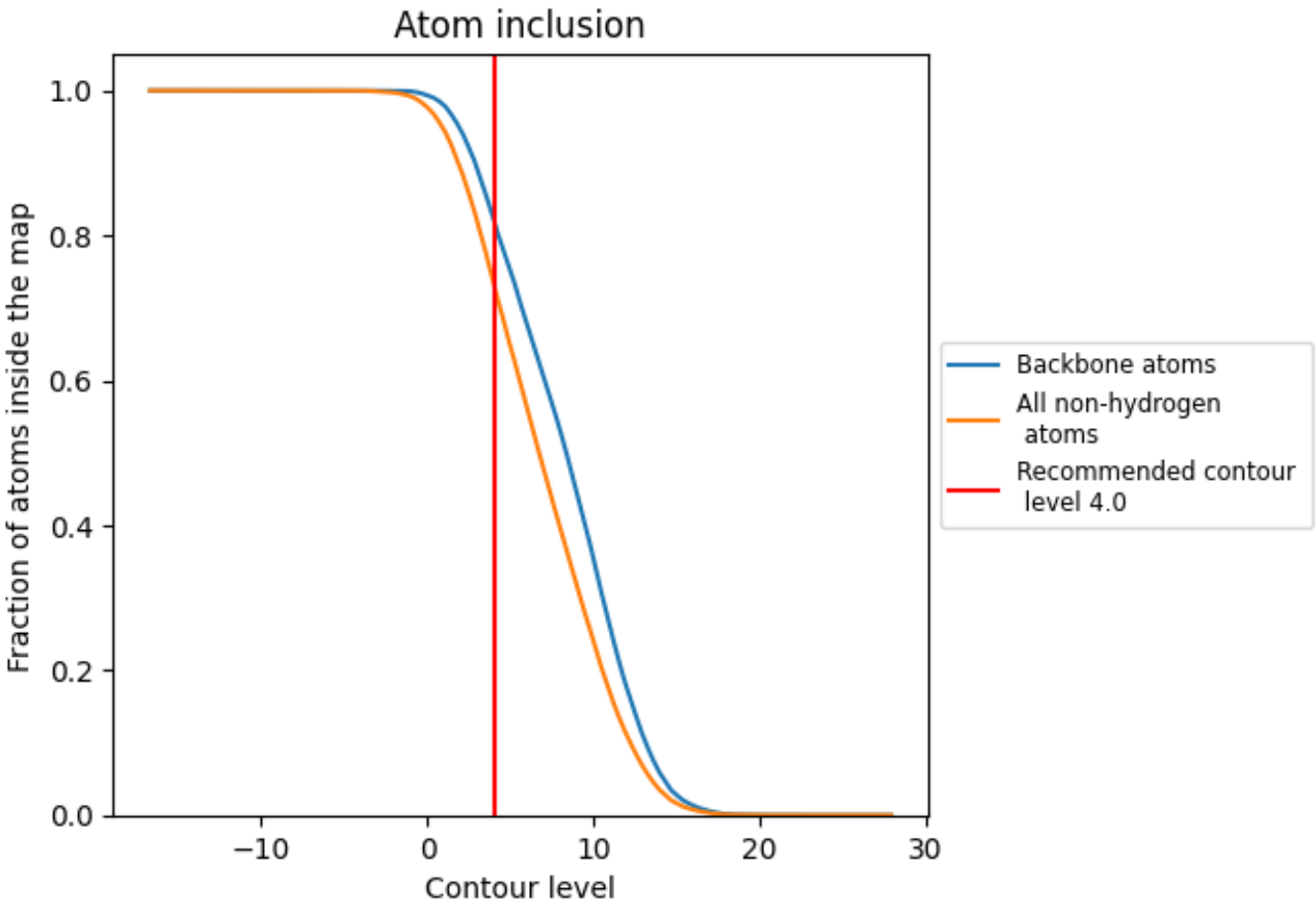
9.3 Atom inclusion mapped to coordinate model



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, 73% 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	0.7347	0.5300
A	0.6130	0.4960
B	0.7657	0.5390
C	0.7897	0.5440
D	0.7854	0.5500
E	0.7746	0.5370