Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 01:45 AM EST

PDB ID	:	3JB0
EMDB ID	:	EMD-6374
Title	:	Atomic model of cytoplasmic polyhedrosis virus with GTP
Authors	:	Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on	:	2015-07-06
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

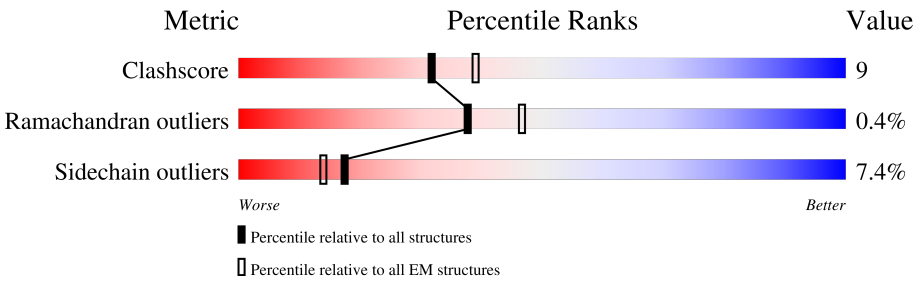
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.90 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%

Mol	Chain	Length	Quality of chain
1	A	1058	69% 28% •
2	B	1333	66% 22% • 11%
2	C	1333	71% 21% • 6%
3	D	448	47% 16% • 35%
3	E	448	48% 16% • 35%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Structural protein VP3.

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

- Molecule 2 is a protein called Capsid protein VP1.

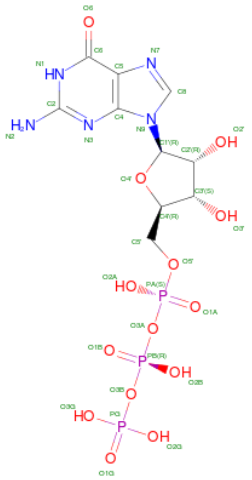
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1191	9397	5937	1634	1789	37	0	0
2	C	1250	9851	6219	1712	1882	38	0	0

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

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



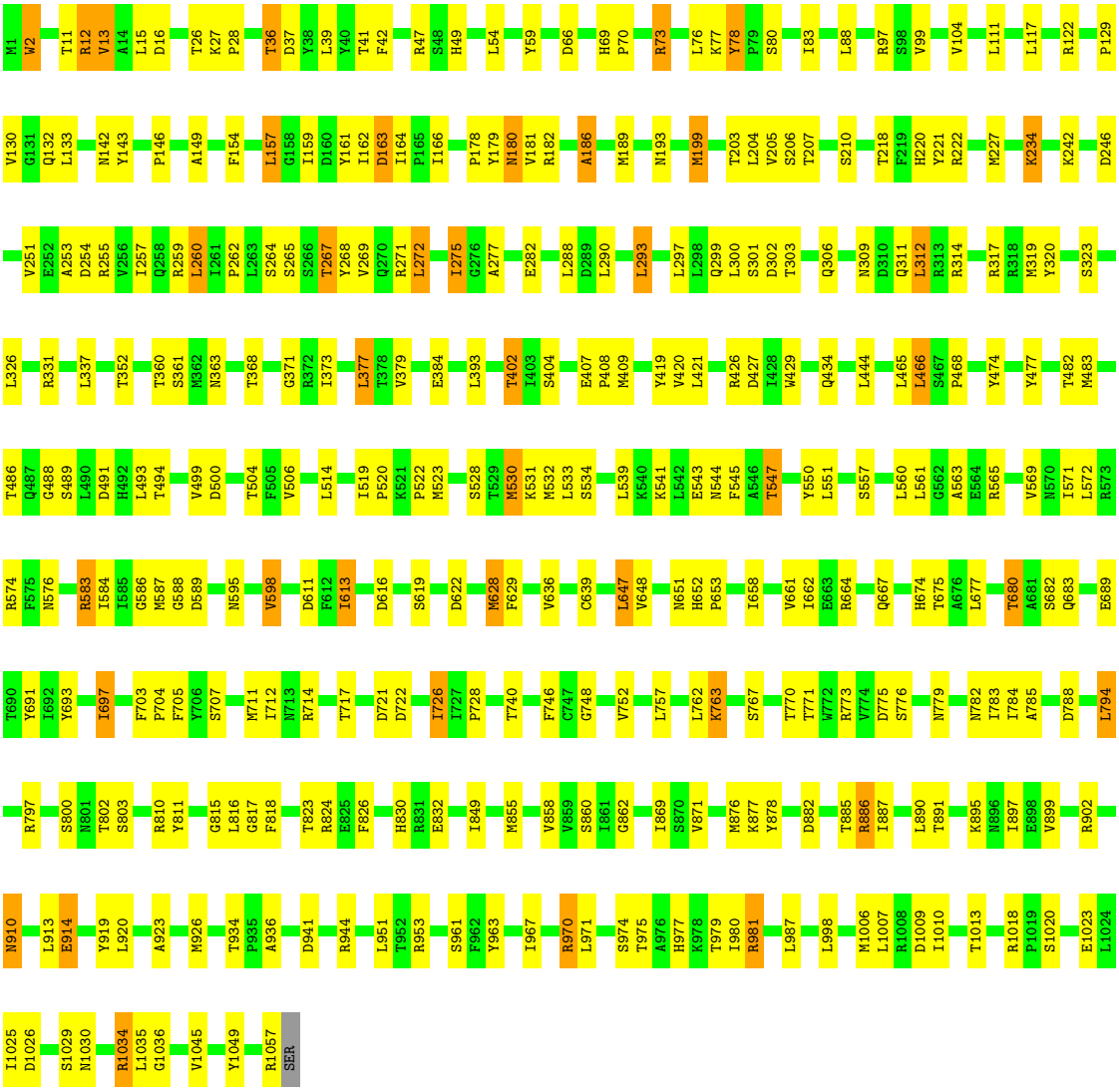
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	32	10	5	14	3	0

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. 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. 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.

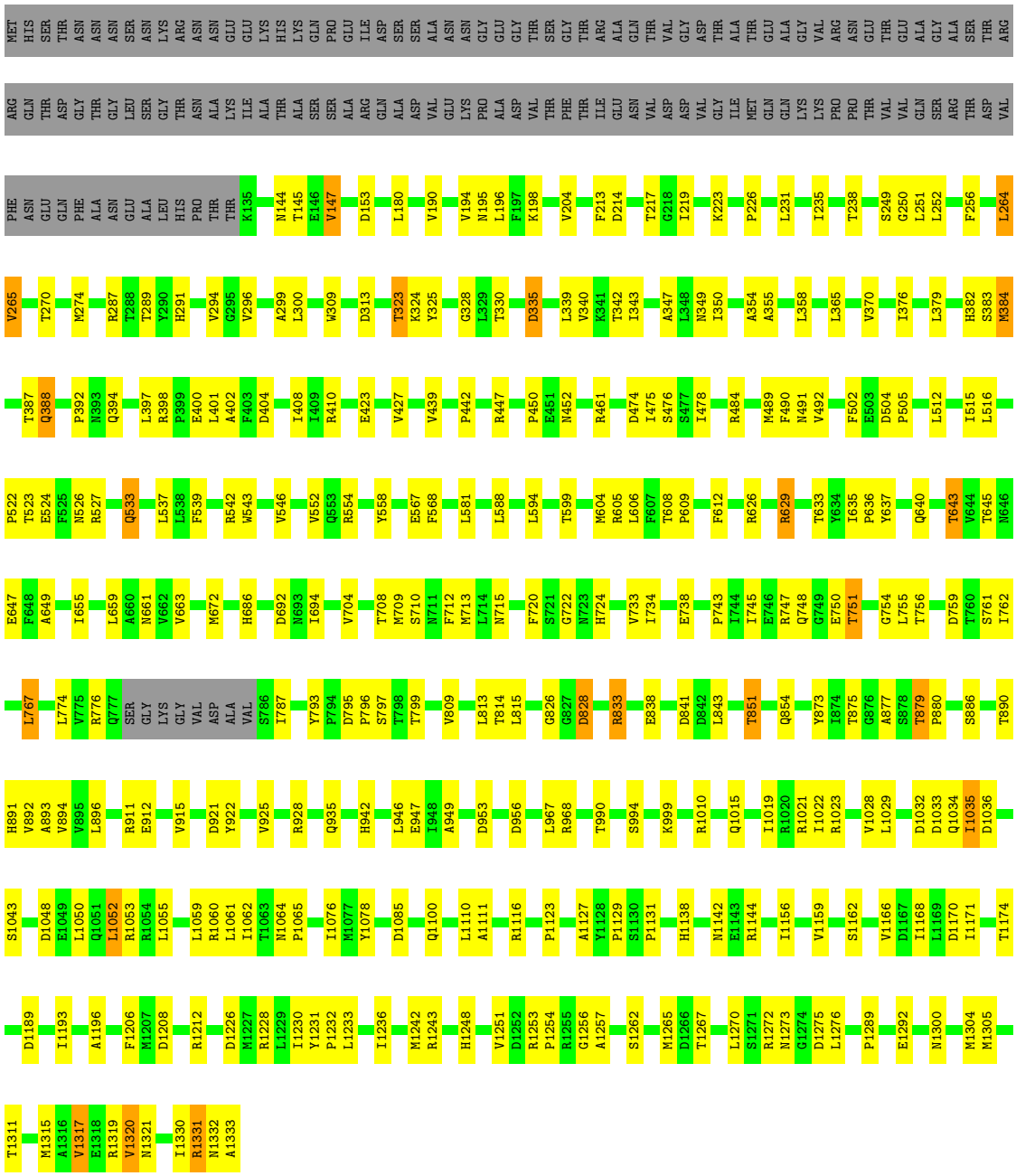
- Molecule 1: Structural protein VP3

Chain A: 69% 28% •



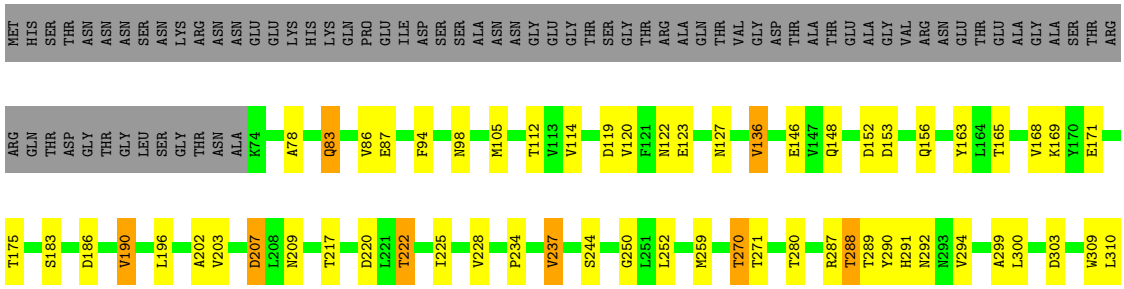
- Molecule 2: Capsid protein VP1

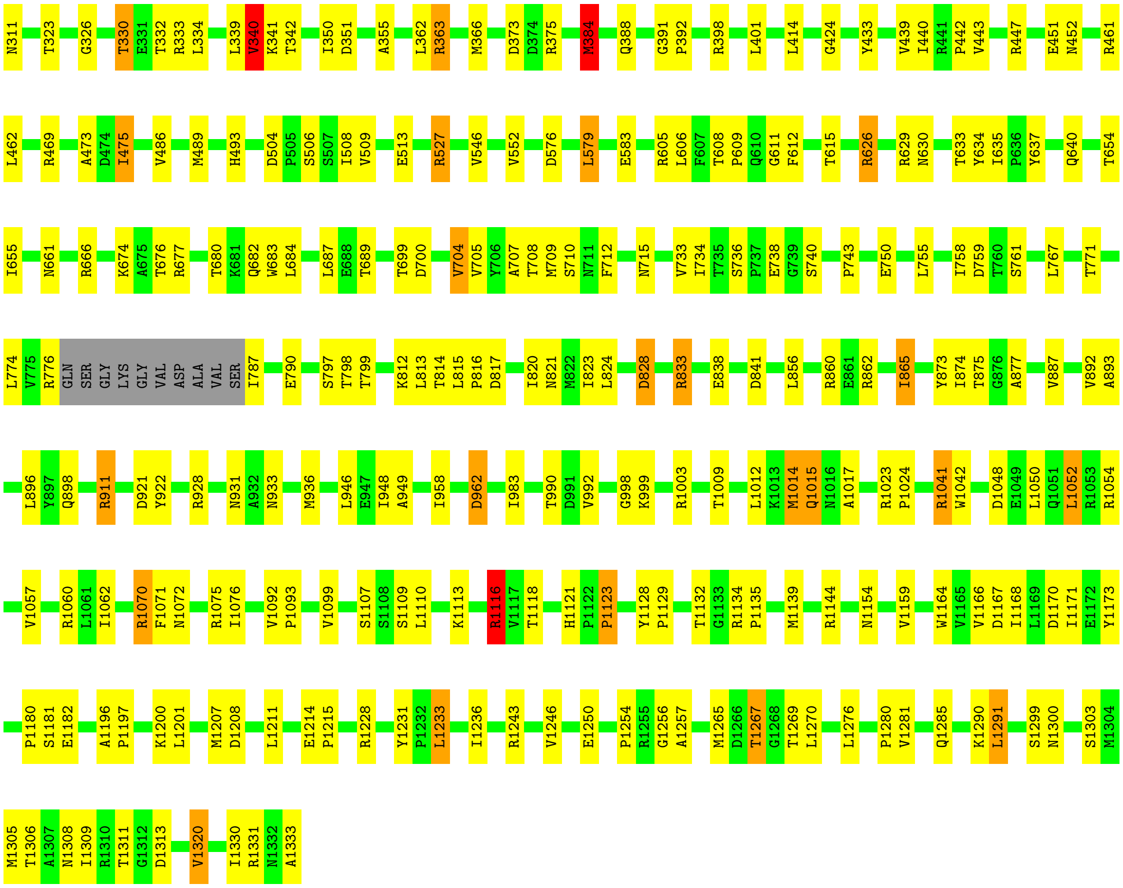
Chain B: 66% 22% • 11%



- Molecule 2: Capsid protein VP1

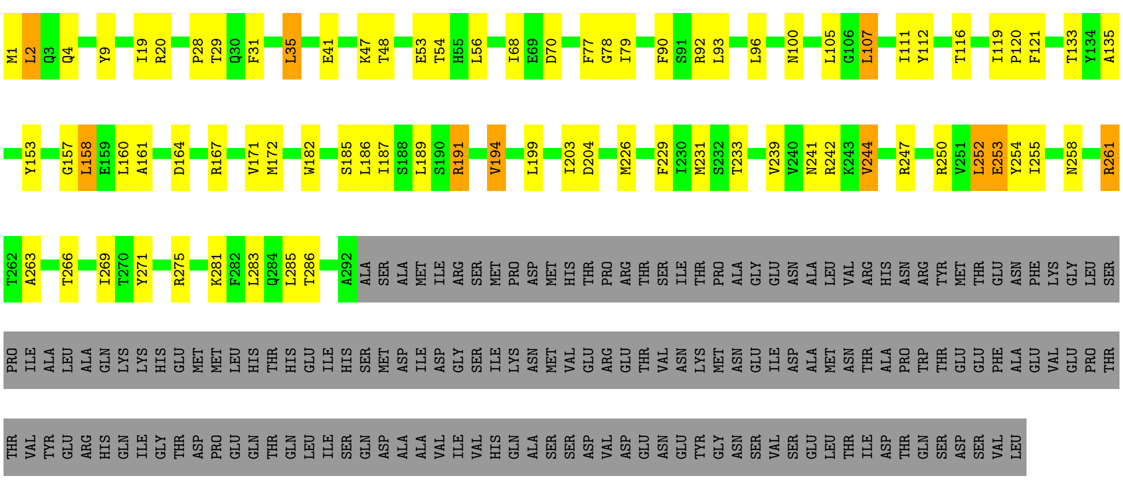
Chain C: 71% 21% • 6%





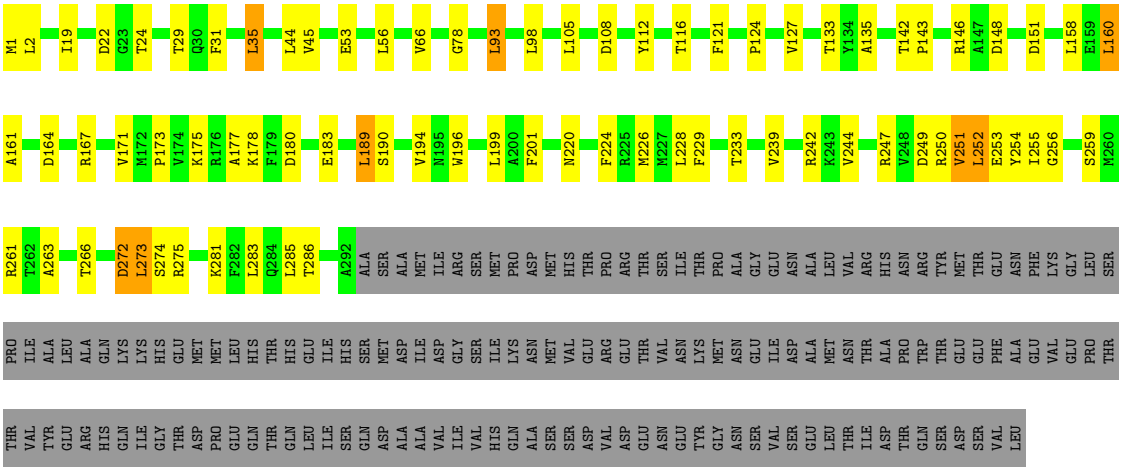
- Molecule 3: Viral structural protein 5

Chain D:



- Molecule 3: Viral structural protein 5

Chain E:


M1 L2 I19 D22 G23 T24 T29 Q30 F31 L35 L44 V45 E53 L56 V66 G78 L93 L98 L105 D108 Y112 T116 F121 P124 V127 T133 Y134 A135 T142 P143 R146 A147 D148 D151 L158 E159 L160
A161 D164 R167 V171 M172 P173 V174 K175 R176 A177 K178 F179 D180 E183 L189 S190 V194 N195 W196 L199 A200 F201 N220 F224 R225 M226 M227 L228 F229 T233 V239 R242 K243 V244 R247 V248 D249 R250 V251 L252 E253 Y254 I255 G256 S259 M260
R261 T262 A263 T266 D272 L273 S274 R275 K281 F282 L283 Q284 L285 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 GLU PHE ALA GLU VAL GLU PRO THR
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	71946	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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.28	0/8619	0.50	4/11737 (0.0%)
2	B	0.35	0/9590	0.55	0/13056
2	C	0.34	0/10052	0.56	1/13687 (0.0%)
3	D	0.33	0/2327	0.54	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.33	0/32915	0.54	5/44806 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ALA	C-N-CD	-8.43	102.05	120.60
1	A	78	TYR	C-N-CD	-6.39	106.53	120.60
1	A	186	ALA	C-N-CA	5.95	147.00	122.00
2	C	1116	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	78	TYR	C-N-CA	5.08	143.36	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	384	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8399	183	0
2	B	9397	0	9315	180	0
2	C	9851	0	9762	180	0
3	D	2281	0	2282	44	0
3	E	2281	0	2282	45	0
4	A	32	0	12	2	0
All	All	32276	0	32052	608	0

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

All (608) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD13	1:A:142:ASN:HB3	1.60	0.84
2:B:709:MET:O	2:B:715:ASN:ND2	2.13	0.82
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.44	0.82
2:B:461:ARG:HH21	2:B:504:ASP:HB2	1.48	0.79
1:A:255:ARG:NH2	4:A:1101:GTP:O2A	2.15	0.79
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.16	0.78
1:A:583:ARG:HH11	1:A:583:ARG:H	1.30	0.78
2:C:1116:ARG:HH11	2:C:1116:ARG:HG2	1.49	0.77
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.18	0.76
2:B:626:ARG:NH2	2:B:712:PHE:O	2.19	0.76
2:C:332:THR:HG22	2:C:334:LEU:H	1.50	0.76
2:C:709:MET:O	2:C:715:ASN:ND2	2.19	0.75
2:B:328:GLY:H	2:B:347:ALA:HB3	1.52	0.74
3:D:77:PHE:HB2	3:D:194:VAL:HG23	1.70	0.72
1:A:427:ASP:HA	1:A:703:PHE:HA	1.72	0.71
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.22	0.71
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.72	0.71
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.23	0.71
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.24	0.70
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.73	0.70
2:C:439:VAL:HG11	2:C:705:VAL:HG21	1.75	0.69
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.25	0.69
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.26	0.69
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.11	0.69
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.74	0.69
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.25	0.69
2:C:1208:ASP:OD2	2:C:1243:ARG:NH2	2.24	0.69
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.26	0.68
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.26	0.68
1:A:541:LYS:HG2	1:A:975:THR:HG21	1.75	0.68
1:A:680:THR:HG22	1:A:683:GLN:HG3	1.76	0.68
1:A:628:MET:SD	1:A:652:HIS:ND1	2.66	0.68
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.27	0.68
1:A:129:PRO:HB2	2:B:1332:ASN:HD22	1.57	0.67
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.24	0.67
2:B:814:THR:HA	2:B:1010:ARG:HH12	1.59	0.67
1:A:161:TYR:CE1	2:B:1333:ALA:HB1	2.29	0.67
2:C:443:VAL:HB	2:C:771:THR:HG23	1.76	0.67
2:C:812:LYS:NZ	2:C:990:THR:O	2.28	0.67
1:A:489:SER:OG	1:A:491:ASP:OD2	2.13	0.66
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.28	0.66
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.77	0.66
2:B:1021:ARG:NE	2:B:1036:ASP:OD1	2.28	0.66
2:C:704:VAL:O	2:C:708:THR:HG23	1.96	0.66
1:A:312:LEU:HD11	1:A:361:SER:HB3	1.78	0.65
2:B:1171:ILE:HD13	2:B:1193:ILE:HD12	1.78	0.65
2:B:145:THR:HB	2:B:1317:VAL:HG23	1.77	0.65
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.78	0.65
1:A:178:PRO:HB2	1:A:179:TYR:HD2	1.61	0.65
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.77	0.65
1:A:797:ARG:NH2	1:A:876:MET:O	2.30	0.65
2:C:736:SER:OG	2:C:738:GLU:OE1	2.13	0.65
2:B:704:VAL:O	2:B:708:THR:HG23	1.97	0.64
2:B:1023:ARG:HG3	2:B:1029:LEU:HD21	1.77	0.64
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.80	0.64
2:C:1116:ARG:HH11	2:C:1116:ARG:CG	2.11	0.64
1:A:73:ARG:HH11	1:A:73:ARG:HB2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.78	0.64
2:C:824:LEU:HB3	2:C:1015:GLN:HE21	1.63	0.63
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.80	0.63
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.81	0.63
2:C:633:THR:HG21	2:C:710:SER:HB2	1.80	0.63
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.79	0.63
1:A:317:ARG:NH1	3:D:41:GLU:OE1	2.32	0.63
3:E:78:GLY:O	3:E:275:ARG:NH2	2.30	0.63
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.79	0.62
2:B:328:GLY:HA3	2:B:347:ALA:H	1.62	0.62
2:C:183:SER:OG	2:C:186:ASP:OD2	2.17	0.62
1:A:979:THR:HG23	1:A:980:ILE:HG12	1.80	0.62
2:C:626:ARG:NH2	2:C:712:PHE:O	2.31	0.62
2:B:153:ASP:OD1	2:B:153:ASP:N	2.33	0.62
2:B:1131:PRO:O	2:B:1162:SER:OG	2.11	0.62
2:B:1100:GLN:OE1	2:B:1142:ASN:ND2	2.31	0.62
1:A:129:PRO:HG2	2:B:1332:ASN:HB2	1.81	0.62
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.33	0.62
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.82	0.62
1:A:531:LYS:HD3	1:A:683:GLN:HG2	1.81	0.61
2:C:388:GLN:HB3	2:C:1320:VAL:HG13	1.82	0.61
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.81	0.61
1:A:2:TRP:HD1	1:A:2:TRP:H	1.48	0.61
1:A:674:HIS:HB2	1:A:697:ILE:HD12	1.83	0.61
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.34	0.61
1:A:404:SER:OG	1:A:824:ARG:NH1	2.34	0.61
1:A:47:ARG:NH1	1:A:80:SER:OG	2.34	0.60
2:B:313:ASP:OD1	2:B:1253:ARG:NH1	2.34	0.60
3:E:242:ARG:HG3	3:E:251:VAL:HG21	1.83	0.60
1:A:234:LYS:HG2	1:A:260:LEU:HD22	1.84	0.60
1:A:563:ALA:O	1:A:565:ARG:NH1	2.35	0.60
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.84	0.60
1:A:658:ILE:HD12	1:A:712:ILE:HG12	1.84	0.60
2:B:335:ASP:OD2	2:B:340:VAL:N	2.32	0.60
1:A:419:TYR:HE1	1:A:421:LEU:HD23	1.66	0.59
1:A:541:LYS:HD3	1:A:550:TYR:HE2	1.65	0.59
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.36	0.59
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.84	0.59
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.84	0.59
1:A:887:ILE:HG13	1:A:899:VAL:HG21	1.84	0.59
2:B:474:ASP:OD1	2:B:476:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.84	0.58
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.36	0.58
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.84	0.58
1:A:541:LYS:NZ	1:A:545:PHE:O	2.36	0.58
1:A:477:TYR:HA	1:A:482:THR:HG22	1.86	0.58
3:D:164:ASP:OD2	3:D:167:ARG:NH2	2.31	0.58
3:D:283:LEU:HA	3:D:286:THR:HG22	1.86	0.58
3:E:283:LEU:HA	3:E:286:THR:HG22	1.86	0.57
2:B:223:LYS:HB3	2:B:1174:THR:HG21	1.86	0.57
2:B:512:LEU:HD13	2:B:659:LEU:HD12	1.86	0.57
2:B:264:LEU:HD11	2:B:365:LEU:HD22	1.85	0.57
1:A:59:TYR:HB3	4:A:1101:GTP:C6	2.38	0.57
1:A:420:VAL:HA	1:A:974:SER:HB2	1.86	0.57
2:B:410:ARG:HD3	2:B:1043:SER:HA	1.86	0.57
1:A:474:TYR:HD1	1:A:499:VAL:HG22	1.68	0.57
2:B:851:THR:HG22	2:B:854:GLN:HG2	1.87	0.57
1:A:42:PHE:HD1	1:A:49:HIS:HD2	1.52	0.57
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.27	0.57
2:C:163:TYR:N	2:C:351:ASP:OD1	2.38	0.57
2:B:712:PHE:HB2	2:B:715:ASN:ND2	2.20	0.56
3:D:78:GLY:O	3:D:275:ARG:NH2	2.38	0.56
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.87	0.56
1:A:288:LEU:HD22	1:A:368:THR:HG22	1.86	0.56
1:A:514:LEU:H	1:A:514:LEU:HD12	1.70	0.56
2:C:865:ILE:HD11	2:C:1041:ARG:O	2.05	0.56
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.23	0.56
1:A:203:THR:HG22	1:A:204:LEU:HG	1.88	0.56
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.33	0.56
1:A:13:VAL:HG21	1:A:146:PRO:HB3	1.87	0.56
2:B:492:VAL:HB	2:B:747:ARG:HG2	1.88	0.56
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	1.88	0.56
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.88	0.56
3:E:272:ASP:OD2	3:E:274:SER:OG	2.16	0.56
1:A:717:THR:HB	1:A:1020:SER:HB2	1.88	0.55
2:C:259:MET:O	2:C:1054:ARG:NH1	2.36	0.55
1:A:154:PHE:HE1	1:A:162:ILE:HG13	1.72	0.55
2:B:328:GLY:N	2:B:347:ALA:HB3	2.22	0.55
2:B:612:PHE:HZ	2:B:1330:ILE:HG22	1.71	0.55
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.89	0.55
2:C:114:VAL:HG22	2:C:136:VAL:HG12	1.88	0.55
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:148:ASP:OD2	3:E:151:ASP:N	2.34	0.55
1:A:275:ILE:HD12	1:A:301:SER:HA	1.88	0.55
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.22	0.55
3:D:239:VAL:HG12	3:D:250:ARG:HD2	1.88	0.55
1:A:466:LEU:HD23	1:A:530:MET:HG2	1.89	0.55
1:A:178:PRO:HB2	1:A:179:TYR:CD2	2.42	0.55
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.36	0.54
1:A:1020:SER:OG	1:A:1023:GLU:OE2	2.18	0.54
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.39	0.54
2:C:999:LYS:HG2	2:C:1009:THR:HG22	1.88	0.54
1:A:539:LEU:HG	1:A:647:LEU:HD12	1.90	0.54
2:B:270:THR:HG22	2:B:291:HIS:HA	1.88	0.54
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.89	0.54
2:B:252:LEU:HD23	2:B:967:LEU:HD21	1.90	0.54
2:B:1230:ILE:HG12	2:C:119:ASP:HA	1.90	0.54
1:A:218:THR:HG1	1:A:220:HIS:HE2	1.55	0.53
2:B:1076:ILE:HB	2:B:1166:VAL:HG22	1.90	0.53
1:A:409:MET:HE1	1:A:1036:GLY:HA2	1.90	0.53
2:B:370:VAL:HG12	2:B:400:GLU:HG3	1.90	0.53
1:A:12:ARG:NH2	1:A:16:ASP:OD2	2.41	0.53
1:A:189:MET:O	1:A:193:ASN:ND2	2.40	0.53
2:C:504:ASP:OD2	2:C:506:SER:OG	2.26	0.53
2:B:450:PRO:HG3	2:B:686:HIS:HB2	1.91	0.53
2:C:340:VAL:HG22	2:C:1309:ILE:HD12	1.90	0.53
2:C:439:VAL:HG23	2:C:440:ILE:HG22	1.90	0.53
2:C:736:SER:HB3	2:C:740:SER:HB3	1.90	0.53
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.34	0.53
2:C:78:ALA:HB2	2:C:1181:SER:HB2	1.90	0.53
2:C:666:ARG:O	2:C:677:ARG:NH1	2.39	0.53
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.90	0.53
1:A:858:VAL:HG23	1:A:876:MET:HE2	1.90	0.53
1:A:299:GLN:O	1:A:303:THR:HG23	2.08	0.52
2:B:384:MET:HA	2:B:708:THR:HG21	1.91	0.52
2:C:1116:ARG:HG2	2:C:1116:ARG:NH1	2.22	0.52
2:B:1032:ASP:HB3	2:B:1035:ILE:CG2	2.40	0.52
2:C:699:THR:OG1	2:C:700:ASP:OD2	2.24	0.52
3:E:124:PRO:HA	3:E:127:VAL:HG22	1.92	0.52
3:E:261:ARG:NH1	3:E:263:ALA:O	2.42	0.52
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.44	0.52
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.91	0.52
2:C:489:MET:SD	2:C:527:ARG:HD2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.92	0.52
1:A:39:LEU:HD23	1:A:54:LEU:HD11	1.92	0.52
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.44	0.52
1:A:163:ASP:OD2	1:A:182:ARG:NE	2.39	0.52
2:C:611:GLY:HA3	2:C:635:ILE:O	2.10	0.52
2:B:190:VAL:HG22	2:B:194:VAL:HG23	1.92	0.52
1:A:262:PRO:HG2	1:A:323:SER:HB2	1.91	0.52
1:A:951:LEU:O	1:A:1057:ARG:NH1	2.43	0.52
2:B:388:GLN:HB3	2:B:1320:VAL:HG13	1.92	0.52
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.25	0.52
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.92	0.51
2:B:324:LYS:O	2:B:1267:THR:HG22	2.10	0.51
2:B:748:GLN:HA	2:C:682:GLN:HE22	1.74	0.51
2:C:443:VAL:HG11	2:C:447:ARG:HH22	1.75	0.51
2:C:1305:MET:HE2	2:C:1309:ILE:HD11	1.92	0.51
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.45	0.51
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.92	0.51
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.92	0.51
2:C:962:ASP:OD1	2:C:962:ASP:N	2.43	0.51
1:A:157:LEU:HB3	1:A:159:ILE:HG23	1.93	0.51
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.90	0.51
2:B:190:VAL:HG23	2:B:300:LEU:HB3	1.92	0.51
2:B:833:ARG:HG3	2:B:922:TYR:CZ	2.45	0.51
2:C:1211:LEU:HD21	2:C:1246:VAL:HG21	1.93	0.51
1:A:129:PRO:CG	2:B:1332:ASN:HB2	2.41	0.51
2:C:424:GLY:HA2	2:C:755:LEU:HD11	1.92	0.51
1:A:246:ASP:OD1	1:A:331:ARG:NH2	2.43	0.51
1:A:572:LEU:HB3	1:A:584:ILE:HD13	1.91	0.51
2:B:1189:ASP:OD2	2:B:1189:ASP:N	2.42	0.51
2:C:156:GLN:HE22	2:C:1309:ILE:H	1.57	0.51
3:D:161:ALA:HB3	3:D:172:MET:HE1	1.93	0.51
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.92	0.51
2:C:828:ASP:OD1	2:C:862:ARG:NH2	2.44	0.51
1:A:613:ILE:HG21	1:A:639:CYS:HB3	1.93	0.51
2:B:226:PRO:HG2	2:B:251:LEU:HD23	1.92	0.51
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.92	0.50
2:C:1144:ARG:NH1	2:C:1170:ASP:OD1	2.43	0.50
1:A:775:ASP:OD1	1:A:776:SER:N	2.44	0.50
2:B:442:PRO:HB3	2:B:475:ILE:HG21	1.93	0.50
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.94	0.50
2:C:615:THR:H	2:C:1333:ALA:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1144:ARG:NH1	2:B:1170:ASP:OD2	2.45	0.50
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.92	0.50
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.94	0.50
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.94	0.50
1:A:491:ASP:O	1:A:494:THR:HG22	2.11	0.50
1:A:923:ALA:N	1:A:961:SER:OG	2.31	0.50
1:A:379:VAL:HG21	1:A:794:LEU:HD13	1.92	0.50
2:B:1289:PRO:HG2	3:D:191:ARG:NH2	2.26	0.50
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.43	0.50
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.23	0.50
2:B:1144:ARG:HD2	2:B:1168:ILE:HG21	1.93	0.50
3:D:9:TYR:H	3:D:204:ASP:CG	2.16	0.50
3:E:252:LEU:HD12	3:E:255:ILE:HD11	1.93	0.50
2:B:828:ASP:OD2	2:B:1015:GLN:NE2	2.45	0.49
2:C:207:ASP:OD1	2:C:207:ASP:N	2.45	0.49
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.94	0.49
2:C:366:MET:HG2	3:E:266:THR:HG21	1.94	0.49
2:B:484:ARG:O	2:B:527:ARG:NH2	2.46	0.49
1:A:588:GLY:H	1:A:598:VAL:HG23	1.76	0.49
2:C:119:ASP:OD1	2:C:119:ASP:N	2.45	0.49
2:C:817:ASP:OD1	2:C:821:ASN:ND2	2.45	0.49
1:A:771:THR:HG22	1:A:783:ILE:HG23	1.93	0.49
2:B:342:THR:OG1	2:B:343:ILE:N	2.45	0.49
2:B:759:ASP:OD2	2:B:761:SER:OG	2.31	0.49
2:B:813:LEU:HG	2:B:1010:ARG:NH1	2.27	0.49
1:A:533:LEU:HD21	1:A:571:ILE:HG21	1.95	0.49
2:C:326:GLY:H	2:C:1267:THR:HG21	1.77	0.49
2:C:759:ASP:OD1	2:C:761:SER:OG	2.28	0.49
2:C:1075:ARG:NH2	2:C:1167:ASP:OD2	2.32	0.49
1:A:680:THR:HG23	1:A:682:SER:H	1.77	0.49
2:B:704:VAL:HB	2:B:1330:ILE:HD11	1.93	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.94	0.49
1:A:595:ASN:HD22	1:A:595:ASN:H	1.61	0.49
1:A:882:ASP:OD1	1:A:882:ASP:N	2.45	0.49
2:C:287:ARG:HH11	2:C:330:THR:HB	1.76	0.49
1:A:12:ARG:HH21	1:A:15:LEU:HB3	1.78	0.48
1:A:420:VAL:HA	1:A:974:SER:CB	2.43	0.48
2:B:606:LEU:HD13	2:B:655:ILE:HG23	1.94	0.48
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.47	0.48
1:A:628:MET:HG3	1:A:629:PHE:N	2.28	0.48
1:A:651:ASN:HA	1:A:689:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.13	0.48
1:A:658:ILE:O	1:A:662:ILE:HG12	2.13	0.48
2:B:1171:ILE:CD1	2:B:1193:ILE:HG23	2.44	0.48
3:D:4:GLN:NE2	3:D:204:ASP:OD1	2.46	0.48
1:A:586:GLY:HA3	1:A:595:ASN:OD1	2.13	0.48
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.48	0.48
1:A:251:VAL:HG12	1:A:253:ALA:H	1.79	0.48
1:A:664:ARG:HD2	1:A:667:GLN:HE21	1.78	0.48
1:A:830:HIS:HB2	1:A:1034:ARG:CZ	2.44	0.48
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.94	0.48
2:B:355:ALA:HB3	2:B:1276:LEU:HD11	1.94	0.48
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.35	0.48
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.46	0.48
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.95	0.48
1:A:302:ASP:O	1:A:306:GLN:HB2	2.13	0.48
2:C:1057:VAL:HG22	2:C:1291:LEU:HD21	1.94	0.48
2:C:1311:THR:HB	2:C:1313:ASP:OD2	2.13	0.48
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.48	0.48
2:C:398:ARG:HG2	2:C:398:ARG:HH11	1.79	0.48
1:A:560:LEU:HD22	1:A:560:LEU:H	1.78	0.48
2:B:720:PHE:CE1	2:B:722:GLY:HA2	2.49	0.48
3:E:253:GLU:HA	3:E:254:TYR:HA	1.55	0.48
1:A:377:LEU:HB3	1:A:763:LYS:HB3	1.94	0.48
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.96	0.48
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.14	0.48
2:C:252:LEU:HD22	2:C:823:ILE:HD13	1.95	0.48
3:D:1:MET:HB2	3:D:121:PHE:CE1	2.49	0.48
1:A:544:ASN:HB3	1:A:547:THR:OG1	2.14	0.47
2:B:640:GLN:OE1	2:B:647:GLU:N	2.37	0.47
1:A:882:ASP:OD2	1:A:885:THR:OG1	2.29	0.47
2:C:165:THR:HG23	2:C:209:ASN:HB2	1.95	0.47
3:D:105:LEU:HD23	3:D:203:ILE:HD11	1.96	0.47
3:E:44:LEU:HD11	3:E:256:GLY:HA3	1.96	0.47
1:A:154:PHE:CE1	1:A:162:ILE:HG13	2.49	0.47
2:B:633:THR:HG21	2:B:710:SER:CB	2.45	0.47
2:C:342:THR:O	2:C:1306:THR:HG23	2.14	0.47
2:C:605:ARG:O	2:C:608:THR:HG23	2.13	0.47
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.96	0.47
1:A:528:SER:O	1:A:532:MET:HG2	2.15	0.47
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.44	0.47
1:A:164:ILE:HB	1:A:181:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:THR:O	2:B:527:ARG:HG3	2.15	0.47
2:B:843:LEU:HG	2:B:942:HIS:HB2	1.96	0.47
3:E:239:VAL:HG12	3:E:250:ARG:HD2	1.97	0.47
1:A:42:PHE:HD1	1:A:49:HIS:CD2	2.32	0.47
1:A:419:TYR:CE1	1:A:421:LEU:HD23	2.50	0.47
2:B:522:PRO:HB3	2:B:609:PRO:HB3	1.95	0.47
2:B:925:VAL:HA	2:B:928:ARG:HD2	1.97	0.47
2:B:1305:MET:HE2	2:B:1305:MET:HB3	1.72	0.47
2:C:1159:VAL:HA	2:C:1164:TRP:HB2	1.97	0.47
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.96	0.47
1:A:977:HIS:HB2	1:A:981:ARG:HB3	1.97	0.47
2:C:640:GLN:N	2:C:700:ASP:OD1	2.46	0.47
2:C:865:ILE:HD11	2:C:1041:ARG:C	2.35	0.47
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.14	0.47
1:A:967:ILE:HG13	1:A:1045:VAL:HG12	1.96	0.47
2:B:558:TYR:HB3	2:B:568:PHE:CD1	2.49	0.47
2:C:384:MET:HA	2:C:708:THR:CG2	2.44	0.47
1:A:206:SER:HB3	1:A:227:MET:HE3	1.95	0.47
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.80	0.47
1:A:653:PRO:HB3	1:A:658:ILE:HD11	1.97	0.46
2:B:879:THR:HG22	2:B:880:PRO:HD2	1.96	0.46
1:A:129:PRO:HA	1:A:132:GLN:HG2	1.97	0.46
1:A:242:LYS:NZ	1:A:246:ASP:OD2	2.32	0.46
1:A:265:SER:HB2	1:A:269:VAL:HB	1.97	0.46
2:B:147:VAL:HG22	2:B:379:LEU:HD11	1.96	0.46
2:C:1267:THR:HB	2:C:1299:SER:HB3	1.96	0.46
3:E:281:LYS:O	3:E:285:LEU:HG	2.15	0.46
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.97	0.46
1:A:970:ARG:NH1	1:A:1049:TYR:OH	2.49	0.46
2:C:384:MET:SD	2:C:433:TYR:OH	2.70	0.46
2:C:1211:LEU:HD23	2:C:1211:LEU:HA	1.60	0.46
1:A:560:LEU:HD23	1:A:569:VAL:HG22	1.96	0.46
2:C:220:ASP:OD1	2:C:222:THR:OG1	2.34	0.46
2:C:375:ARG:O	2:C:375:ARG:HD3	2.16	0.46
2:C:1139:MET:HB3	2:C:1166:VAL:HG12	1.96	0.46
2:C:1228:ARG:HG2	2:C:1231:TYR:CZ	2.50	0.46
3:E:19:ILE:HD13	3:E:189:LEU:HD11	1.98	0.46
2:B:502:PHE:CE1	2:B:539:PHE:HB2	2.51	0.46
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.96	0.46
2:C:824:LEU:HB3	2:C:1015:GLN:NE2	2.27	0.46
2:C:384:MET:HA	2:C:708:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:HIS:HB3	2:C:758:ILE:HD13	1.98	0.46
2:C:816:PRO:HB2	2:C:983:ILE:HG23	1.96	0.46
3:E:229:PHE:O	3:E:233:THR:HG23	2.15	0.46
1:A:914:GLU:N	1:A:919:TYR:OH	2.49	0.46
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.50	0.46
2:C:609:PRO:HB2	2:C:634:TYR:HE2	1.81	0.46
1:A:895:LYS:HA	1:A:895:LYS:HD3	1.76	0.46
3:E:253:GLU:HB2	3:E:254:TYR:CD1	2.51	0.46
1:A:309:ASN:OD1	1:A:311:GLN:HG3	2.15	0.46
2:C:169:LYS:O	2:C:202:ALA:N	2.42	0.46
2:C:856:LEU:HD23	2:C:860:ARG:HD3	1.98	0.46
2:C:1076:ILE:HG22	2:C:1159:VAL:HG11	1.97	0.46
3:E:178:LYS:HA	3:E:250:ARG:O	2.16	0.46
1:A:426:ARG:HG3	1:A:707:SER:HB3	1.98	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:776:ARG:HD3	2:B:787:ILE:HB	1.97	0.45
2:B:833:ARG:HG3	2:B:922:TYR:CE2	2.51	0.45
1:A:257:ILE:HG22	1:A:259:ARG:H	1.81	0.45
1:A:404:SER:O	1:A:826:PHE:HA	2.16	0.45
2:B:1228:ARG:HB3	2:B:1231:TYR:OH	2.16	0.45
2:C:828:ASP:OD2	2:C:828:ASP:N	2.49	0.45
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.56	0.45
2:C:1233:LEU:HD13	2:C:1233:LEU:HA	1.76	0.45
3:E:253:GLU:HB2	3:E:254:TYR:CE1	2.51	0.45
1:A:161:TYR:CD1	2:B:1333:ALA:HB1	2.52	0.45
1:A:963:TYR:CD2	1:A:987:LEU:HD21	2.52	0.45
2:C:303:ASP:N	2:C:311:ASN:OD1	2.45	0.45
2:C:931:ASN:HD21	2:C:936:MET:HB3	1.81	0.45
2:B:886:SER:O	2:B:890:THR:HG23	2.16	0.45
2:C:152:ASP:OD1	2:C:152:ASP:N	2.49	0.45
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.99	0.45
3:D:281:LYS:O	3:D:285:LEU:HG	2.17	0.45
2:C:362:LEU:HD11	2:C:1305:MET:SD	2.57	0.45
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.45
2:B:370:VAL:HG21	2:B:402:ALA:HB2	1.99	0.45
2:B:392:PRO:HG2	2:B:394:GLN:HG3	1.98	0.45
2:B:774:LEU:HD23	2:B:774:LEU:HA	1.79	0.45
2:B:838:GLU:C	2:B:935:GLN:HG2	2.36	0.45
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.74	0.45
2:B:649:ALA:HB1	2:B:692:ASP:OD1	2.17	0.45
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:TRP:CD1	1:A:2:TRP:N	2.78	0.45
2:B:515:ILE:HG21	2:B:655:ILE:HG21	1.99	0.45
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.98	0.45
2:C:270:THR:HG22	2:C:291:HIS:HA	1.99	0.45
2:C:1144:ARG:HD2	2:C:1168:ILE:CG2	2.47	0.45
1:A:271:ARG:HE	1:A:271:ARG:HB3	1.63	0.45
1:A:419:TYR:O	1:A:974:SER:HB2	2.16	0.45
2:B:196:LEU:HD22	2:B:296:VAL:HG11	1.98	0.45
2:B:581:LEU:HD11	2:B:745:ILE:HG22	1.97	0.45
2:B:659:LEU:O	2:B:663:VAL:HG23	2.17	0.45
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.98	0.45
2:B:1033:ASP:OD1	2:B:1033:ASP:N	2.50	0.45
2:B:489:MET:SD	2:B:527:ARG:HD2	2.57	0.44
1:A:267:THR:OG1	1:A:320:TYR:OH	2.14	0.44
1:A:282:GLU:HB2	1:A:363:ASN:HB3	1.99	0.44
1:A:944:ARG:HG3	1:A:1010:ILE:HD11	1.99	0.44
1:A:752:VAL:HG13	1:A:779:ASN:O	2.17	0.44
2:B:635:ILE:HA	2:B:636:PRO:HD3	1.80	0.44
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.99	0.44
2:C:169:LYS:HB2	2:C:203:VAL:HG22	2.00	0.44
3:D:153:TYR:CD2	3:D:258:ASN:HB2	2.53	0.44
3:D:157:GLY:HA2	3:D:255:ILE:HG22	2.00	0.44
1:A:967:ILE:HG12	1:A:971:LEU:HD23	2.00	0.44
1:A:797:ARG:HD2	1:A:869:ILE:HD11	1.99	0.44
2:B:354:ALA:O	2:B:358:LEU:HG	2.17	0.44
2:B:751:THR:HB	2:B:754:GLY:H	1.82	0.44
1:A:222:ARG:HA	1:A:222:ARG:HD3	1.71	0.44
1:A:746:PHE:HB2	1:A:785:ALA:HB3	2.00	0.44
1:A:878:TYR:HD2	1:A:897:ILE:HD12	1.83	0.44
1:A:886:ARG:HD3	1:A:886:ARG:H	1.83	0.44
2:B:1144:ARG:HD2	2:B:1168:ILE:CG2	2.47	0.44
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.53	0.44
2:C:865:ILE:HD12	2:C:1042:TRP:HE3	1.82	0.44
1:A:384:GLU:HA	1:A:802:THR:HG22	2.00	0.44
2:B:1053:ARG:HD3	2:B:1053:ARG:HA	1.75	0.44
2:C:1168:ILE:HG21	2:C:1171:ILE:HD12	1.99	0.44
1:A:26:THR:OG1	1:A:28:PRO:HG3	2.18	0.44
1:A:474:TYR:CE2	1:A:522:PRO:HG3	2.52	0.44
2:C:127:ASN:O	2:C:127:ASN:ND2	2.51	0.44
1:A:675:THR:HA	1:A:693:TYR:O	2.18	0.43
1:A:913:LEU:O	1:A:953:ARG:NE	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ASP:OD2	2:B:339:LEU:N	2.51	0.43
2:B:694:ILE:HD13	2:B:767:LEU:HD23	1.99	0.43
2:C:475:ILE:H	2:C:475:ILE:HG13	1.51	0.43
2:B:478:ILE:HG13	2:B:762:ILE:HD11	2.00	0.43
2:C:469:ARG:O	2:C:761:SER:HB2	2.18	0.43
1:A:811:TYR:O	1:A:815:GLY:N	2.42	0.43
2:B:1226:ASP:OD2	2:C:122:ASN:ND2	2.41	0.43
3:D:158:LEU:HD13	3:D:158:LEU:HA	1.81	0.43
3:D:253:GLU:HA	3:D:254:TYR:HA	1.55	0.43
1:A:936:ALA:HB1	1:A:998:LEU:HD23	2.01	0.43
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.18	0.43
1:A:277:ALA:HB3	1:A:319:MET:CE	2.49	0.43
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	2.01	0.43
3:E:173:PRO:O	3:E:175:LYS:HG3	2.18	0.43
1:A:42:PHE:CE1	1:A:47:ARG:HA	2.53	0.43
1:A:157:LEU:HD23	1:A:159:ILE:HD13	2.01	0.43
2:B:795:ASP:HA	2:B:796:PRO:HD2	1.84	0.43
2:C:146:GLU:O	2:C:148:GLN:NE2	2.52	0.43
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.78	0.43
2:C:1118:THR:HA	2:C:1129:PRO:HA	1.99	0.43
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.53	0.43
1:A:373:ILE:HG12	1:A:817:GLY:N	2.33	0.43
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.18	0.43
3:D:182:TRP:NE1	3:D:185:SER:HA	2.34	0.43
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.84	0.43
2:C:1012:LEU:HD23	2:C:1012:LEU:HA	1.83	0.43
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	2.00	0.43
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.51	0.43
3:E:201:PHE:HE1	3:E:220:ASN:HB3	1.82	0.43
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.54	0.43
1:A:180:ASN:HD22	1:A:180:ASN:C	2.19	0.43
1:A:557:SER:HB3	1:A:583:ARG:HB2	2.00	0.43
2:B:554:ARG:HD3	2:B:594:LEU:HD13	2.00	0.43
1:A:561:LEU:HD22	1:A:587:MET:HB2	2.00	0.43
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.84	0.43
2:B:299:ALA:HB2	2:B:1265:MET:HB3	2.01	0.43
2:B:490:PHE:O	2:B:745:ILE:HA	2.19	0.43
2:B:526:ASN:HB2	2:B:724:HIS:CE1	2.54	0.43
2:C:271:THR:HB	2:C:290:TYR:CE2	2.53	0.43
2:C:707:ALA:HB2	2:C:1330:ILE:HG23	2.01	0.43
2:C:1267:THR:HB	2:C:1299:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:GLU:OE1	3:E:281:LYS:NZ	2.52	0.43
3:E:142:THR:HA	3:E:143:PRO:HD3	1.85	0.43
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.42
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.54	0.42
2:C:1214:GLU:HG2	2:C:1215:PRO:HD2	2.01	0.42
1:A:616:ASP:OD1	1:A:691:TYR:OH	2.31	0.42
2:B:309:TRP:CH2	2:B:1257:ALA:HB1	2.54	0.42
1:A:154:PHE:HD1	1:A:159:ILE:HG13	1.85	0.42
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	2.01	0.42
2:C:153:ASP:OD2	2:C:401:LEU:N	2.42	0.42
2:C:733:VAL:HG12	2:C:743:PRO:CA	2.46	0.42
1:A:860:SER:HA	1:A:920:LEU:HB2	2.00	0.42
2:B:213:PHE:HB3	2:B:219:ILE:HD12	2.01	0.42
2:B:404:ASP:O	2:B:408:ILE:HG12	2.19	0.42
2:B:1050:LEU:HD23	2:B:1050:LEU:HA	1.66	0.42
3:E:19:ILE:HG23	3:E:196:TRP:HZ2	1.84	0.42
1:A:36:THR:OG1	1:A:37:ASP:N	2.52	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.00	0.42
2:C:309:TRP:CZ2	2:C:1257:ALA:HB1	2.55	0.42
2:C:633:THR:HG21	2:C:710:SER:CB	2.49	0.42
3:D:261:ARG:NH1	3:D:263:ALA:O	2.52	0.42
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.67	0.42
1:A:402:THR:HG23	1:A:824:ARG:HB3	2.01	0.42
2:B:235:ILE:HG21	2:C:774:LEU:HA	2.01	0.42
2:C:310:LEU:HD12	2:C:310:LEU:HA	1.82	0.42
2:C:1109:SER:OG	2:C:1118:THR:HB	2.19	0.42
2:C:1236:ILE:HD13	2:C:1236:ILE:HA	1.87	0.42
1:A:11:THR:OG1	1:A:254:ASP:OD2	2.37	0.42
1:A:293:LEU:HD22	1:A:297:LEU:HG	2.01	0.42
2:B:1048:ASP:O	2:B:1052:LEU:HD22	2.20	0.42
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.19	0.42
2:C:190:VAL:HG23	2:C:300:LEU:HB3	2.00	0.42
2:C:776:ARG:HB3	2:C:787:ILE:HG13	2.02	0.42
2:C:874:ILE:HG12	2:C:896:LEU:O	2.19	0.42
1:A:773:ARG:O	1:A:818:PHE:HA	2.19	0.42
2:B:384:MET:O	2:B:387:THR:HG23	2.20	0.42
2:B:1064:ASN:HA	2:B:1065:PRO:HD3	1.94	0.42
2:B:1206:PHE:CE1	2:B:1232:PRO:HD3	2.55	0.42
2:B:1236:ILE:HD13	2:B:1236:ILE:HA	1.90	0.42
2:C:1071:PHE:HB2	2:C:1173:TYR:CZ	2.54	0.42
2:C:1121:HIS:CD2	2:C:1123:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:28:PRO:HB3	3:D:226:MET:HG3	2.01	0.42
2:B:231:LEU:HB3	2:B:249:SER:HB3	2.01	0.42
2:C:83:GLN:HG3	2:C:165:THR:HB	2.01	0.42
2:C:674:LYS:HA	2:C:674:LYS:HD2	1.82	0.42
2:C:1134:ARG:NH1	2:C:1154:ASN:OD1	2.50	0.42
3:D:244:VAL:HG13	3:D:247:ARG:HB2	2.02	0.42
3:E:178:LYS:HB2	3:E:249:ASP:OD2	2.20	0.42
1:A:290:LEU:O	1:A:293:LEU:HB2	2.20	0.42
2:C:332:THR:HG23	2:C:1270:LEU:HD12	2.02	0.41
2:C:355:ALA:HB3	2:C:1276:LEU:HD11	2.02	0.41
2:C:674:LYS:HE3	2:C:677:ARG:HH21	1.84	0.41
2:B:325:TYR:OH	2:B:349:ASN:OD1	2.22	0.41
2:B:484:ARG:HE	2:B:524:GLU:CD	2.23	0.41
2:B:537:LEU:HD23	2:B:537:LEU:HA	1.80	0.41
2:B:643:THR:HG22	2:B:645:THR:H	1.84	0.41
2:B:748:GLN:H	2:B:748:GLN:HG2	1.65	0.41
2:B:793:TYR:CD2	2:B:1321:ASN:HB3	2.55	0.41
2:B:994:SER:O	2:B:999:LYS:HE3	2.20	0.41
2:C:234:PRO:HB2	2:C:237:VAL:HG23	2.02	0.41
2:C:288:THR:OG1	2:C:289:THR:N	2.53	0.41
3:D:96:LEU:HD21	3:D:111:ILE:HG23	2.02	0.41
2:B:323:THR:HG21	2:B:1262:SER:HB2	2.03	0.41
2:B:588:LEU:O	2:B:604:MET:HG3	2.20	0.41
2:B:605:ARG:O	2:B:608:THR:HG23	2.20	0.41
2:C:875:THR:HG23	2:C:877:ALA:H	1.85	0.41
2:C:1048:ASP:O	2:C:1052:LEU:HD22	2.21	0.41
1:A:70:PRO:HA	1:A:73:ARG:NH1	2.36	0.41
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.95	0.41
1:A:794:LEU:O	1:A:797:ARG:HG3	2.20	0.41
3:D:2:LEU:HD12	3:D:107:LEU:HD21	2.01	0.41
3:D:79:ILE:HA	3:D:269:ILE:HG22	2.03	0.41
1:A:268:TYR:HD2	1:A:271:ARG:HD2	1.86	0.41
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.79	0.41
3:D:229:PHE:CE2	3:D:252:LEU:HD11	2.55	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.20	0.41
1:A:572:LEU:O	1:A:576:ASN:ND2	2.33	0.41
2:B:873:TYR:HA	2:B:896:LEU:O	2.20	0.41
2:B:1156:ILE:O	2:B:1159:VAL:HB	2.20	0.41
2:C:168:VAL:HG11	2:C:196:LEU:HG	2.02	0.41
2:C:509:VAL:HG22	2:C:683:TRP:CZ3	2.55	0.41
2:C:1076:ILE:HB	2:C:1166:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:LEU:HD12	3:E:35:LEU:HA	1.82	0.41
1:A:519:ILE:HA	1:A:520:PRO:HD2	1.97	0.41
1:A:726:ILE:H	1:A:726:ILE:HG12	1.64	0.41
1:A:862:GLY:HA2	1:A:882:ASP:HB3	2.03	0.41
2:B:287:ARG:HD2	2:B:328:GLY:HA2	2.02	0.41
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.90	0.41
2:B:505:PRO:HB3	2:B:663:VAL:HG13	2.02	0.41
2:B:762:ILE:HD12	2:B:762:ILE:HA	1.89	0.41
2:B:814:THR:HA	2:B:1010:ARG:NH1	2.33	0.41
2:B:875:THR:HG23	2:B:877:ALA:H	1.85	0.41
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.92	0.41
2:C:1099:VAL:O	2:C:1139:MET:HA	2.21	0.41
1:A:268:TYR:HA	1:A:271:ARG:HG2	2.01	0.41
1:A:371:GLY:N	1:A:818:PHE:O	2.51	0.41
2:B:195:ASN:O	2:B:198:LYS:HE3	2.21	0.41
2:B:447:ARG:O	2:B:686:HIS:NE2	2.52	0.41
2:B:505:PRO:HA	2:B:543:TRP:CH2	2.56	0.41
2:B:581:LEU:HD23	2:B:581:LEU:HA	1.85	0.41
2:C:169:LYS:NZ	2:C:1182:GLU:OE2	2.32	0.41
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.83	0.41
3:E:259:SER:OG	3:E:261:ARG:HB2	2.20	0.41
1:A:583:ARG:HH11	1:A:583:ARG:N	2.08	0.41
1:A:763:LYS:HE2	1:A:803:SER:HB3	2.03	0.41
1:A:767:SER:N	1:A:788:ASP:OD1	2.54	0.41
2:B:383:SER:HB3	2:B:387:THR:HG21	2.03	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.90	0.41
2:B:516:LEU:HD23	2:B:516:LEU:HA	1.92	0.41
3:D:187:ILE:HD13	3:D:187:ILE:HA	1.91	0.41
1:A:27:LYS:NZ	1:A:37:ASP:OD1	2.37	0.40
1:A:500:ASP:OD1	1:A:574:ARG:NH2	2.53	0.40
2:B:382:HIS:HE2	2:B:713:MET:H	1.69	0.40
2:C:339:LEU:C	2:C:341:LYS:H	2.25	0.40
2:C:583:GLU:H	2:C:583:GLU:CD	2.24	0.40
3:E:108:ASP:OD2	3:E:112:TYR:OH	2.22	0.40
2:B:892:VAL:HG12	2:B:894:VAL:HB	2.04	0.40
3:D:231:MET:HG3	3:D:271:TYR:OH	2.21	0.40
2:B:214:ASP:OD2	2:B:217:THR:OG1	2.40	0.40
2:B:1289:PRO:CD	3:D:20:ARG:HD2	2.49	0.40
2:C:375:ARG:HH11	2:C:375:ARG:HD2	1.74	0.40
2:C:504:ASP:OD1	2:C:504:ASP:N	2.52	0.40
2:C:576:ASP:O	2:C:579:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:160:LEU:HB3	3:E:161:ALA:H	1.77	0.40
3:E:189:LEU:HD13	3:E:189:LEU:HA	1.92	0.40
1:A:272:LEU:HD21	1:A:297:LEU:HB3	2.02	0.40
1:A:563:ALA:HA	1:A:589:ASP:O	2.22	0.40
1:A:722:ASP:OD1	1:A:722:ASP:N	2.49	0.40
1:A:887:ILE:HG22	1:A:891:THR:HB	2.04	0.40
2:B:226:PRO:HB2	2:B:250:GLY:HA3	2.04	0.40
2:B:394:GLN:HB3	2:B:398:ARG:HG3	2.03	0.40
2:C:225:ILE:HD13	2:C:1070:ARG:HB2	2.03	0.40
2:C:414:LEU:HD23	2:C:814:THR:HB	2.03	0.40
2:C:813:LEU:HA	2:C:992:VAL:HG11	2.03	0.40
2:C:1050:LEU:HD12	2:C:1050:LEU:HA	1.78	0.40
3:D:239:VAL:CG1	3:D:250:ARG:HD2	2.52	0.40
3:E:239:VAL:CG1	3:E:250:ARG:HD2	2.51	0.40
1:A:83:ILE:H	1:A:83:ILE:HG13	1.64	0.40
2:C:712:PHE:HB2	2:C:715:ASN:ND2	2.36	0.40
3:E:1:MET:HB2	3:E:121:PHE:CZ	2.56	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%)	1012 (96%)	40 (4%)	3 (0%)	41	71
2	B	1187/1333 (89%)	1145 (96%)	39 (3%)	3 (0%)	41	71
2	C	1246/1333 (94%)	1197 (96%)	41 (3%)	8 (1%)	25	58
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	41	71
3	E	290/448 (65%)	284 (98%)	6 (2%)	0	100	100
All	All	4068/4620 (88%)	3919 (96%)	134 (3%)	15 (0%)	38	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	C	288	THR
2	C	1267	THR
1	A	483	MET
2	B	738	GLU
2	C	87	GLU
2	C	1041	ARG
2	C	1123	PRO
2	C	340	VAL
2	B	1123	PRO
2	C	1014	MET
3	D	244	VAL
2	C	1281	VAL
1	A	728	PRO

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%)	849 (90%)	93 (10%)	8 24
2	B	1038/1153 (90%)	980 (94%)	58 (6%)	21 52
2	C	1089/1153 (94%)	1018 (94%)	71 (6%)	17 45
3	D	240/379 (63%)	219 (91%)	21 (9%)	10 30
3	E	240/379 (63%)	220 (92%)	20 (8%)	11 32
All	All	3549/4007 (89%)	3286 (93%)	263 (7%)	17 38

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	12	ARG
1	A	13	VAL

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Mol	Chain	Res	Type
1	A	36	THR
1	A	41	THR
1	A	73	ARG
1	A	76	LEU
1	A	77	LYS
1	A	78	TYR
1	A	88	LEU
1	A	97	ARG
1	A	99	VAL
1	A	104	VAL
1	A	117	LEU
1	A	130	VAL
1	A	133	LEU
1	A	157	LEU
1	A	163	ASP
1	A	166	ILE
1	A	180	ASN
1	A	199	MET
1	A	207	THR
1	A	210	SER
1	A	234	LYS
1	A	260	LEU
1	A	264	SER
1	A	267	THR
1	A	272	LEU
1	A	275	ILE
1	A	293	LEU
1	A	300	LEU
1	A	312	LEU
1	A	314	ARG
1	A	337	LEU
1	A	360	THR
1	A	377	LEU
1	A	402	THR
1	A	444	LEU
1	A	465	LEU
1	A	466	LEU
1	A	493	LEU
1	A	504	THR
1	A	506	VAL
1	A	523	MET
1	A	530	MET

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Mol	Chain	Res	Type
1	A	534	SER
1	A	543	GLU
1	A	547	THR
1	A	583	ARG
1	A	598	VAL
1	A	611	ASP
1	A	613	ILE
1	A	619	SER
1	A	622	ASP
1	A	628	MET
1	A	647	LEU
1	A	648	VAL
1	A	680	THR
1	A	697	ILE
1	A	711	MET
1	A	714	ARG
1	A	721	ASP
1	A	726	ILE
1	A	740	THR
1	A	757	LEU
1	A	762	LEU
1	A	763	LYS
1	A	770	THR
1	A	782	ASN
1	A	784	ILE
1	A	794	LEU
1	A	800	SER
1	A	816	LEU
1	A	823	THR
1	A	832	GLU
1	A	855	MET
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	902	ARG
1	A	910	ASN
1	A	914	GLU
1	A	926	MET
1	A	934	THR
1	A	941	ASP
1	A	970	ARG
1	A	981	ARG

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Mol	Chain	Res	Type
1	A	1007	LEU
1	A	1013	THR
1	A	1018	ARG
1	A	1025	ILE
1	A	1034	ARG
1	A	1035	LEU
2	B	144	ASN
2	B	147	VAL
2	B	180	LEU
2	B	238	THR
2	B	264	LEU
2	B	265	VAL
2	B	274	MET
2	B	289	THR
2	B	294	VAL
2	B	323	THR
2	B	330	THR
2	B	335	ASP
2	B	384	MET
2	B	388	GLN
2	B	397	LEU
2	B	439	VAL
2	B	452	ASN
2	B	533	GLN
2	B	542	ARG
2	B	546	VAL
2	B	552	VAL
2	B	567	GLU
2	B	599	THR
2	B	629	ARG
2	B	637	TYR
2	B	643	THR
2	B	661	ASN
2	B	672	MET
2	B	751	THR
2	B	755	LEU
2	B	767	LEU
2	B	797	SER
2	B	799	THR
2	B	809	VAL
2	B	815	LEU
2	B	828	ASP

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Mol	Chain	Res	Type
2	B	833	ARG
2	B	851	THR
2	B	879	THR
2	B	912	GLU
2	B	946	LEU
2	B	1052	LEU
2	B	1060	ARG
2	B	1061	LEU
2	B	1062	ILE
2	B	1085	ASP
2	B	1110	LEU
2	B	1138	HIS
2	B	1212	ARG
2	B	1233	LEU
2	B	1270	LEU
2	B	1292	GLU
2	B	1311	THR
2	B	1315	MET
2	B	1317	VAL
2	B	1319	ARG
2	B	1320	VAL
2	B	1331	ARG
2	C	83	GLN
2	C	86	VAL
2	C	98	ASN
2	C	112	THR
2	C	120	VAL
2	C	136	VAL
2	C	175	THR
2	C	190	VAL
2	C	207	ASP
2	C	217	THR
2	C	222	THR
2	C	237	VAL
2	C	244	SER
2	C	270	THR
2	C	280	THR
2	C	294	VAL
2	C	323	THR
2	C	330	THR
2	C	340	VAL
2	C	363	ARG

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Mol	Chain	Res	Type
2	C	373	ASP
2	C	384	MET
2	C	451	GLU
2	C	475	ILE
2	C	486	VAL
2	C	508	ILE
2	C	527	ARG
2	C	546	VAL
2	C	552	VAL
2	C	579	LEU
2	C	626	ARG
2	C	629	ARG
2	C	630	ASN
2	C	637	TYR
2	C	654	THR
2	C	661	ASN
2	C	684	LEU
2	C	687	LEU
2	C	689	THR
2	C	704	VAL
2	C	767	LEU
2	C	790	GLU
2	C	797	SER
2	C	798	THR
2	C	799	THR
2	C	815	LEU
2	C	828	ASP
2	C	833	ARG
2	C	865	ILE
2	C	892	VAL
2	C	911	ARG
2	C	946	LEU
2	C	948	ILE
2	C	962	ASP
2	C	1014	MET
2	C	1015	GLN
2	C	1052	LEU
2	C	1062	ILE
2	C	1070	ARG
2	C	1072	ASN
2	C	1107	SER
2	C	1110	LEU

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Mol	Chain	Res	Type
2	C	1113	LYS
2	C	1116	ARG
2	C	1132	THR
2	C	1233	LEU
2	C	1250	GLU
2	C	1269	THR
2	C	1291	LEU
2	C	1320	VAL
2	C	1331	ARG
3	D	2	LEU
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	48	THR
3	D	54	THR
3	D	92	ARG
3	D	93	LEU
3	D	100	ASN
3	D	107	LEU
3	D	116	THR
3	D	133	THR
3	D	158	LEU
3	D	160	LEU
3	D	171	VAL
3	D	189	LEU
3	D	191	ARG
3	D	194	VAL
3	D	252	LEU
3	D	253	GLU
3	D	261	ARG
3	E	2	LEU
3	E	24	THR
3	E	29	THR
3	E	35	LEU
3	E	66	VAL
3	E	93	LEU
3	E	98	LEU
3	E	116	THR
3	E	133	THR
3	E	158	LEU
3	E	160	LEU
3	E	189	LEU

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Mol	Chain	Res	Type
3	E	190	SER
3	E	194	VAL
3	E	226	MET
3	E	244	VAL
3	E	251	VAL
3	E	252	LEU
3	E	272	ASP
3	E	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	180	ASN
1	A	595	ASN
2	B	491	ASN
2	B	1138	HIS
2	B	1332	ASN
2	C	156	GLN
2	C	981	HIS
2	C	1138	HIS

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)

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	GTP	A	1101	-	26,34,34	1.14	2 (7%)	32,54,54	1.55	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	1101	-	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	GTP	C5-C6	-3.98	1.39	1.47
4	A	1101	GTP	C2-N3	2.26	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	GTP	PB-O3B-PG	-3.76	119.91	132.83
4	A	1101	GTP	C8-N7-C5	3.57	109.78	102.99
4	A	1101	GTP	C5-C6-N1	3.07	119.38	113.95
4	A	1101	GTP	C2-N1-C6	-2.93	119.69	125.10
4	A	1101	GTP	PA-O3A-PB	-2.07	125.72	132.83
4	A	1101	GTP	O6-C6-C5	-2.06	120.36	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	GTP	C5'-O5'-PA-O3A
4	A	1101	GTP	C4'-C5'-O5'-PA
4	A	1101	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	1101	GTP	O4'-C4'-C5'-O5'
4	A	1101	GTP	PB-O3A-PA-O1A
4	A	1101	GTP	PB-O3B-PG-O1G

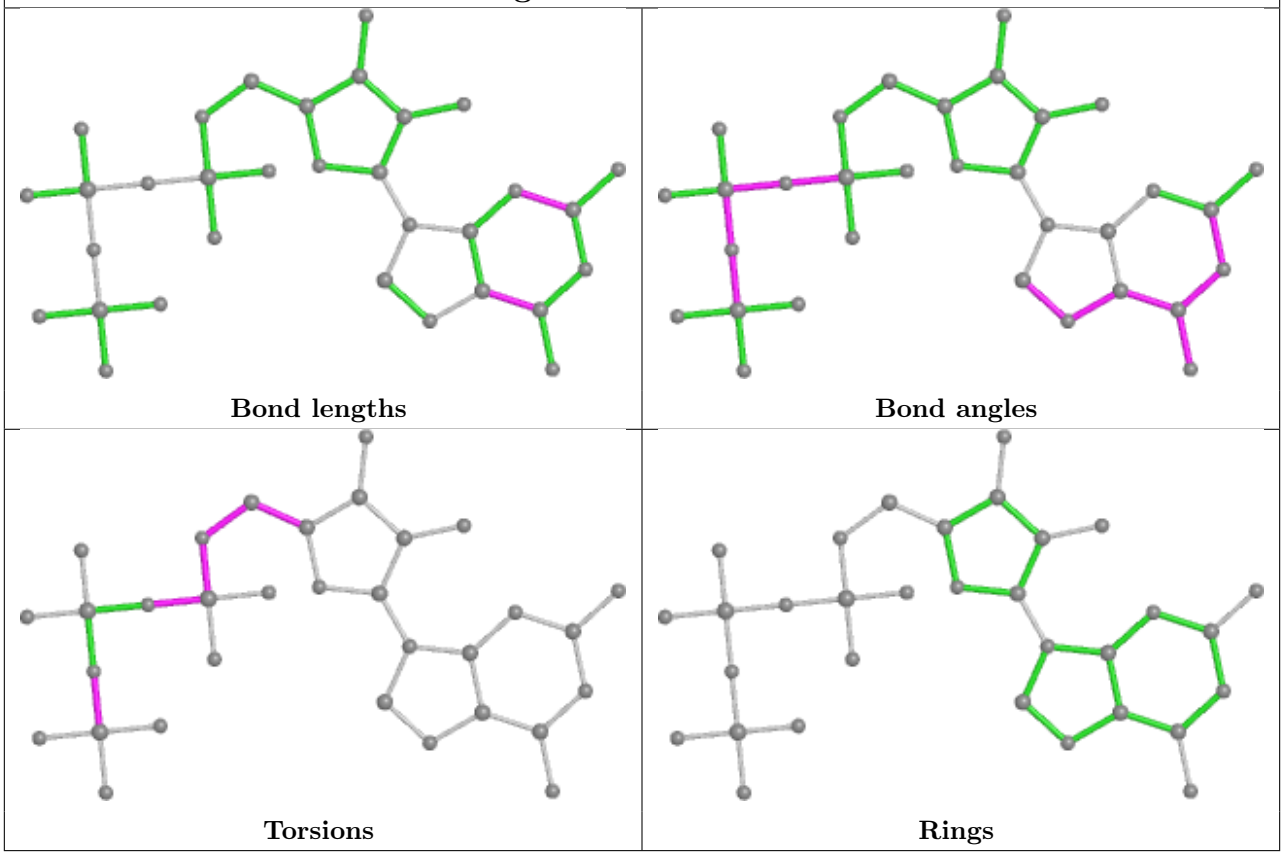
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	GTP	2	0

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

Ligand GTP A 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 (i)

This section contains visualisations of the EMDB entry EMD-6374. 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 (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.