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PDB ID	:	6U62
EMDB ID	:	EMD-20660
Title	:	Raptor-Rag-Ragulator complex
Authors	:	Rogala, K.B.; Sabatini, D.M.
Deposited on	:	2019-08-29
Resolution	:	3.18 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. dev 70
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	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.18 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)	$\mathop{\hbox{\rm EM}}_{(\#{\rm Entries})}$		
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	А	1392	64%	16% • 20%						
2	В	313	76%	17% •	5%					
3	С	400	58% 12%	o <u>30%</u>	_					
4	D	158	• 63% 65	% 32%						
5	Е	125	75%	23%	••					
6	F	162	56% 17%	· 26%	_					
7	G	100	74%	10% 16%						
8	Н	91	74%	24%	·					



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17036 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 Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	1110	Total 8739	$\begin{array}{c} \mathrm{C} \\ 5583 \end{array}$	N 1524	O 1574	S 58	1	0

There are 57 discrepancies between the modelled and reference seque	nces:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	1336	GLY	-	expression tag	UNP Q8N122
А	1337	GLY	-	expression tag	UNP Q8N122
А	1338	GLY	-	expression tag	UNP Q8N122
А	1339	SER	-	expression tag	UNP Q8N122
А	1340	LEU	-	expression tag	UNP Q8N122
A	1341	GLU	-	expression tag	UNP Q8N122
А	1342	VAL	-	expression tag	UNP Q8N122
A	1343	LEU	-	expression tag	UNP Q8N122
А	1344	PHE	-	expression tag	UNP Q8N122
А	1345	GLN	-	expression tag	UNP Q8N122
А	1346	GLY	-	expression tag	UNP Q8N122
А	1347	PRO	-	expression tag	UNP Q8N122
А	1348	GLY	-	expression tag	UNP Q8N122
А	1349	SER	-	expression tag	UNP Q8N122
А	1350	GLY	-	expression tag	UNP Q8N122
А	1351	GLY	-	expression tag	UNP Q8N122
А	1352	GLY	-	expression tag	UNP Q8N122
A	1353	SER	-	expression tag	UNP Q8N122
А	1354	ASP	-	expression tag	UNP Q8N122
А	1355	TYR	-	expression tag	UNP Q8N122
А	1356	LYS	-	expression tag	UNP Q8N122
А	1357	ASP	-	expression tag	UNP Q8N122
А	1358	ASP	-	expression tag	UNP Q8N122
A	1359	ASP	-	expression tag	UNP Q8N122
А	1360	ASP	-	expression tag	UNP Q8N122
А	1361	LYS	-	expression tag	UNP Q8N122
А	1362	SER	-	expression tag	UNP Q8N122
А	1363	SER	-	expression tag	UNP Q8N122



				0	DC
Chain	Residue	Modelled	Actual	Comment	Reference
А	1364	GLY	-	expression tag	UNP Q8N122
А	1365	TRP	-	expression tag	UNP Q8N122
А	1366	SER	-	expression tag	UNP Q8N122
А	1367	HIS	-	expression tag	UNP Q8N122
А	1368	PRO	-	expression tag	UNP Q8N122
А	1369	GLN	-	expression tag	UNP Q8N122
А	1370	PHE	-	expression tag	UNP Q8N122
А	1371	GLU	-	expression tag	UNP Q8N122
А	1372	LYS	-	expression tag	UNP Q8N122
А	1373	GLY	-	expression tag	UNP Q8N122
А	1374	GLY	-	expression tag	UNP Q8N122
А	1375	GLY	-	expression tag	UNP Q8N122
А	1376	ALA	-	expression tag	UNP Q8N122
А	1377	ARG	-	expression tag	UNP Q8N122
А	1378	GLY	-	expression tag	UNP Q8N122
А	1379	GLY	_	expression tag	UNP Q8N122
А	1380	SER	-	expression tag	UNP Q8N122
А	1381	GLY	-	expression tag	UNP Q8N122
А	1382	GLY	-	expression tag	UNP Q8N122
А	1383	GLY	_	expression tag	UNP Q8N122
А	1384	SER	_	expression tag	UNP Q8N122
А	1385	TRP	_	expression tag	UNP Q8N122
А	1386	SER	-	expression tag	UNP Q8N122
А	1387	HIS	_	expression tag	UNP Q8N122
А	1388	PRO	-	expression tag	UNP Q8N122
А	1389	GLN	-	expression tag	UNP Q8N122
А	1390	PHE	-	expression tag	UNP Q8N122
А	1391	GLU	-	expression tag	UNP Q8N122
А	1392	LYS	-	expression tag	UNP Q8N122

• Molecule 2 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	298	Total 2439	C 1548	N 424	O 450	${ m S}$ 17	0	0

• Molecule 3 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues		At	AltConf	Trace			
3	С	281	Total 2252	C 1451	N 368	0 421	S 12	1	0



Chain	Residue	Modelled	Actual	Comment	Reference
С	0	GLY	-	expression tag	UNP Q9HB90
С	1	PRO	-	expression tag	UNP Q9HB90
С	75	ASN	SER	engineered mutation	UNP Q9HB90
С	90	ASN	THR	engineered mutation	UNP Q9HB90

There are 4 discrepancies between the modelled and reference sequences:

• Molecule 4 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	108	Total 710	C 449	N 121	O 140	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4	GLY	-	expression tag	UNP Q6IAA8
D	5	PRO	-	expression tag	UNP Q6IAA8

• Molecule 5 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	Е	124	Total 911	C 575	N 158	0 171	${ m S} 7$	0	0

• Molecule 6 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
6	F	120	Total 883	C 572	N 149	0 161	S 1	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	GLU	-	expression tag	UNP Q9UHA4
F	126	ASN	-	expression tag	UNP Q9UHA4
F	127	LEU	-	expression tag	UNP Q9UHA4
F	128	TYR	-	expression tag	UNP Q9UHA4
F	129	PHE	-	expression tag	UNP Q9UHA4
F	130	GLN	-	expression tag	UNP Q9UHA4
F	131	GLY	-	expression tag	UNP Q9UHA4
F	132	SER	-	expression tag	UNP Q9UHA4
F	133	SER	-	expression tag	UNP Q9UHA4



Chain	Residue	Modelled	Actual	Comment	Reference
F	134	GLY	-	expression tag	UNP Q9UHA4
F	135	TRP	-	expression tag	UNP Q9UHA4
F	136	SER	-	expression tag	UNP Q9UHA4
F	137	HIS	-	expression tag	UNP Q9UHA4
F	138	PRO	-	expression tag	UNP Q9UHA4
F	139	GLN	-	expression tag	UNP Q9UHA4
F	140	PHE	-	expression tag	UNP Q9UHA4
F	141	GLU	-	expression tag	UNP Q9UHA4
F	142	LYS	-	expression tag	UNP Q9UHA4
F	143	GLY	-	expression tag	UNP Q9UHA4
F	144	GLY	-	expression tag	UNP Q9UHA4
F	145	GLY	-	expression tag	UNP Q9UHA4
F	146	SER	-	expression tag	UNP Q9UHA4
F	147	GLY	-	expression tag	UNP Q9UHA4
F	148	GLY	-	expression tag	UNP Q9UHA4
F	149	GLY	-	expression tag	UNP Q9UHA4
F	150	SER	-	expression tag	UNP Q9UHA4
F	151	GLY	-	expression tag	UNP Q9UHA4
F	152	GLY	-	expression tag	UNP Q9UHA4
F	153	GLY	-	expression tag	UNP Q9UHA4
F	154	SER	-	expression tag	UNP Q9UHA4
F	155	TRP	-	expression tag	UNP Q9UHA4
F	156	SER	-	expression tag	UNP Q9UHA4
F	157	HIS	-	expression tag	UNP Q9UHA4
F	158	PRO	-	expression tag	UNP Q9UHA4
F	159	GLN	-	expression tag	UNP Q9UHA4
F	160	PHE	-	expression tag	UNP Q9UHA4
F	161	GLU	-	expression tag	UNP Q9UHA4
F	162	LYS	-	expression tag	UNP Q9UHA4

• Molecule 7 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms			AltConf	Trace	
7	G	84	Total 447	С 270	N 89	O 88	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q0VGL1
G	1	PRO	-	expression tag	UNP Q0VGL1



• Molecule 8 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
8	Н	89	Total 594	C 368	N 106	0 114	S 6	0	0

• Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf		
9	В	1	Total 32	C 10	N 5	0 14	Р 3	0

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	В	1	Total Mg 1 1	0

• Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf		
11	С	1	Total	С	Ν	Ο	Р	0
11	U	L	28	10	5	11	2	0



3 Residue-property plots (i)

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







• Molecule 2: Ras-related GTP-binding protein A

Chain B:	76%	17% · 5%
MET PRO ASN AISN AISN AIS AI AI AI TI21 S22 S22 S22 S22 S22	142 143 143 143 143 143 143 143 111 111 111	11 40 11 45 11 45 11 53 11 55 11 55 11 65 11 65 11 68 11 68 11 69 11 69 11 69 11 69 11 69
N183 V184 Q185 Q185 E198 E199 E199 L205 L205	F211 F215 F215 F215 F223 F224 F224 F224 F225 F224 F225 F225 F225	Y271 V272 S280 S280 A284 A284 A284 A294 A294 A294 A294 A294 A294 A294 A29
ARG		
• Molecule 3: Ra	as-related GTP-binding protein C	
Chain C:	58% 12%	30%
GLY PRO SER LEU GLN ALA GLU GLU GLU FHR PRO	LEU ALA SER TTR GLY GLY ALA ALA ALA ASP PHE PHE PTR CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALA ALA GLY GLY GLY GLY VAL ALA ALA ALA CLY GLY CLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA
L66 K79 H83 K84 ASR PR0 ASR CLU	ASN LEU CLEU CLEU CLEU CLEU TTRR ASP ASP ASP SER ASP ASP CLIY MIG6 CLIY MIG6 CLIY ASP ASP PHE PHE PHE PRE PRO PRO PRO PRO PRO PO CLIY PIC	THR ASP ASP E131 E131 E134 F134 F133 F133 F133 F133 F133 F133 F
V167 M171 E174 E174 D186 D186 M187 K188 K193	1196 1196 1237 1237 1237 1238 1238 1238 1238 1238 1238 1238 1238	M288 L301 L301 M315 M315 A316 A316 A316 A316 A329 F330 F3329 F332
L341 R342 R348 R348 R348 R348 R348 R348 R37 R1R R1R R1R R1R R1R R1R R2 R2 R2 R2 R37 CVS	HIS HIS SER SER ALA ALA ALA ALA ALA ASN ASN ASN ASN ALA ALA ALA ALA ALA ALA ALA	
• Molecule 4: Ra	agulator complex protein LAMTOR1	
Chain D:	63% 69	% 32%
GLY PRO SER SER SER GLU ASN ASP ASP CLN ASP ASP ASP	ARG GLU GLU ARG CLU ARG LLYS LLYS LLEU LLEU LLEU ARD PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	LEU PRO SER ALA ALA I57 161 161 161 161 161 161 161 161 162 166 172 SER 61 172 SER 61 172 SER 61 172 SER
897 SER LEU HH 01 H1 01 F1 05 P1 05	A120	
• Molecule 5: Ra	agulator complex protein LAMTOR2	
Chain E:	75%	23% •••





• Molecule 6: Ragulator complex protein LAMTOR3



• Molecule 7: Ragulator complex protein LAMTOR4



• Molecule 8: Ragulator complex protein LAMTOR5





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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, GDP, MG

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	А	0.27	0/8951	0.44	0/12178
2	В	0.32	0/2484	0.44	0/3346
3	С	0.29	0/2298	0.42	0/3101
4	D	0.25	0/720	0.39	0/991
5	Ε	0.26	0/921	0.44	0/1249
6	F	0.27	0/899	0.45	0/1224
7	G	0.23	0/448	0.47	0/619
8	Н	0.23	0/600	0.45	0/821
All	All	0.28	0/17321	0.43	0/23529

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 (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	А	8739	0	8626	134	0
2	В	2439	0	2421	41	0
3	С	2252	0	2235	30	0
4	D	710	0	593	6	0
5	Е	911	0	919	21	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	883	0	878	20	0
7	G	447	0	268	6	0
8	Н	594	0	560	18	0
9	В	32	0	12	7	0
10	В	1	0	0	0	0
11	С	28	0	12	0	0
All	All	17036	0	16524	259	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 8.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:250:GLN:HB2	2:B:265:ILE:HD11	1.59	0.85
2:B:162:THR:HA	2:B:168:THR:HG23	1.60	0.84
1:A:192:PHE:HB2	1:A:242:GLN:HB3	1.64	0.79
2:B:162:THR:HA	2:B:168:THR:CG2	2.13	0.78
2:B:22:SER:HB3	9:B:401:GTP:O1A	1.85	0.77
1:A:1310:HIS:HD2	1:A:1312:HIS:H	1.34	0.74
7:G:17:GLY:HA3	7:G:32:ASP:H	1.52	0.73
1:A:660:ARG:NH2	1:A:821:ASP:OD2	2.21	0.73
2:B:17:GLY:CA	9:B:401:GTP:O1B	2.36	0.73
1:A:165:TRP:HB3	1:A:174:TYR:HB2	1.71	0.73
1:A:428:ASN:ND2	1:A:429:PRO:O	2.22	0.72
2:B:17:GLY:HA2	9:B:401:GTP:O1B	1.89	0.72
2:B:42:THR:N	9:B:401:GTP:O3G	2.20	0.72
1:A:1043:LYS:HB2	1:A:1069:ARG:HB2	1.74	0.69
1:A:1062:ASN:HD22	1:A:1064:ASN:HD22	1.40	0.69
6:F:86:LEU:HB2	6:F:87:PRO:HD3	1.75	0.69
3:C:331:VAL:HG12	3:C:332:THR:HG23	1.75	0.68
1:A:158:PRO:HB2	1:A:201:LEU:HD11	1.76	0.67
2:B:224:ASP:HB3	2:B:227:ARG:HB3	1.77	0.66
2:B:162:THR:HG22	2:B:169:LEU:HA	1.79	0.65
1:A:558:LEU:HD23	1:A:584:ILE:HD12	1.77	0.65
1:A:53:ASP:OD2	1:A:339:GLN:NE2	2.30	0.64
2:B:145:GLU:HG3	2:B:159:CYS:HB2	1.79	0.64
1:A:59:SER:HB2	1:A:137:LEU:HD22	1.80	0.63
2:B:199:GLU:OE2	5:E:3:ARG:NH1	2.31	0.63
2:B:181:ILE:HB	2:B:184:VAL:HG22	1.81	0.62
1:A:988:ARG:NH1	1:A:1080:ASP:OD2	2.32	0.62



	the page	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
6:F:94:ALA:HB1	6:F:98:ALA:HB3	1.81	0.62	
1:A:660:ARG:NH1	1:A:1111:ALA:O	2.32	0.62	
1:A:1103:GLU:N	1:A:1103:GLU:OE1	2.33	0.61	
5:E:59:ASN:ND2	6:F:52:THR:OG1	2.33	0.60	
1:A:423:GLY:O	1:A:426:ASN:ND2	2.35	0.59	
3:C:148:ASP:OD1	3:C:149:ASP:N	2.33	0.59	
6:F:99:ASN:HD22	6:F:102:LEU:H	1.49	0.59	
1:A:38:LYS:NZ	1:A:40:GLU:OE1	2.35	0.58	
1:A:1047:CYS:SG	1:A:1049:TRP:NE1	2.76	0.58	
3:C:165:TYR:HB2	3:C:211:LEU:HD21	1.84	0.58	
2:B:17:GLY:N	9:B:401:GTP:O1B	2.37	0.58	
1:A:1247:VAL:HG12	1:A:1248:ASN:HD22	1.68	0.57	
1:A:158:PRO:HG2	1:A:202:ILE:HD11	1.86	0.57	
1:A:1313:TRP:HB3	1:A:1315:HIS:HD2	1.69	0.56	
4:D:71:ALA:HB1	5:E:58:ARG:HH22	1.70	0.56	
6:F:102:LEU:HD22	8:H:47:VAL:HG21	1.87	0.56	
2:B:197:ILE:O	5:E:3:ARG:NH2	2.38	0.56	
2:B:204:LEU:HD23	2:B:216:HIS:HB2	1.88	0.56	
2:B:280:SER:O	5:E:43:ARG:NH1	2.33	0.56	
6:F:9:LEU:HD23	6:F:35:VAL:HG23	1.88	0.56	
5:E:20:GLN:NE2	5:E:40:THR:OG1	2.39	0.55	
1:A:665:VAL:HG21	1:A:957:THR:HG23	1.88	0.55	
2:B:110:LEU:HD11	2:B:122:ILE:HD13	1.89	0.55	
6:F:79:GLN:NE2	6:F:100:THR:OG1	2.39	0.55	
1:A:1062:ASN:HD22	1:A:1064:ASN:ND2	2.05	0.55	
1:A:1043:LYS:HA	1:A:1070:VAL:H	1.71	0.55	
2:B:266:PHE:O	2:B:294:ARG:HG3	2.07	0.55	
1:A:71:ASP:O	1:A:73:PRO:HD3	2.07	0.55	
6:F:16:VAL:HG22	6:F:102:LEU:HD23	1.89	0.54	
1:A:1218:SER:OG	1:A:1219:LEU:N	2.41	0.54	
8:H:20:GLY:O	8:H:87:HIS:N	2.41	0.54	
1:A:1191:ARG:HB3	1:A:1203:ARG:HD2	1.90	0.54	
6:F:44:ALA:HB1	6:F:93:ILE:HG12	1.88	0.54	
3:C:185:ASP:HA	3:C:188:LYS:HE3	1.91	0.53	
6:F:32:VAL:HG12	6:F:33:ILE:HG23	1.89	0.53	
7:G:15:GLN:HA	7:G:89:ARG:HA	1.90	0.53	
1:A:1259:LEU:HD12	1:A:1270:CYS:HB3	1.90	0.53	
8:H:74:ILE:HB	8:H:87:HIS:ND1	2.24	0.53	
1:A:156:PRO:HG2	1:A:165:TRP:CD1	2.44	0.53	
5:E:16:THR:OG1	5:E:17:GLY:N	2.42	0.52	
1:A:266:CYS:HA	1:A:273:ILE:HG21	1.91	0.52	



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:298:ILE:HD13	1:A:393:LEU:HD11	1.91	0.52
1:A:163:GLU:HB2	1:A:176:PRO:HB3	1.92	0.51
1:A:41:GLY:HA3	1:A:961:ASP:HB3	1.93	0.51
5:E:86:VAL:HG12	5:E:87:ALA:H	1.76	0.51
1:A:47:GLN:HG3	1:A:49:TRP:CD1	2.46	0.51
1:A:1091:GLY:HA2	1:A:1127:MET:SD	2.50	0.51
2:B:255:ARG:HB3	3:C:315:MET:HG3	1.91	0.51
8:H:46:SER:HA	8:H:83:THR:HG21	1.92	0.51
1:A:1047:CYS:HB2	1:A:1059:TYR:HD1	1.76	0.51
3:C:135:ARG:NH1	3:C:167:VAL:O	2.44	0.51
4:D:57:ILE:O	4:D:61:THR:HG22	2.11	0.51
3:C:348:ARG:HD3	4:D:68:VAL:HB	1.92	0.51
1:A:444:VAL:HG13	1:A:445:HIS:ND1	2.26	0.50
1:A:57:THR:HG22	1:A:145:ARG:HB2	1.91	0.50
3:C:310:TYR:OH	3:C:335:LEU:O	2.30	0.50
2:B:23:MET:HB2	2:B:169:LEU:HD11	1.93	0.50
3:C:154:LEU:HD21	3:C:195:ILE:HG23	1.93	0.50
5:E:80:ARG:NH1	5:E:99:VAL:O	2.44	0.50
1:A:105:ASN:O	1:A:109:GLN:N	2.42	0.50
1:A:611:PRO:HB3	1:A:1154:ARG:HD2	1.92	0.50
1:A:1262:HIS:HD2	1:A:1264:GLN:H	1.60	0.50
3:C:322:ASN:OD1	3:C:322:ASN:N	2.45	0.50
6:F:85:ARG:O	6:F:88:LEU:N	2.45	0.50
1:A:184:THR:HG22	1:A:213:ARG:NH1	2.26	0.50
1:A:1237:ARG:HD3	1:A:1249:VAL:HG13	1.94	0.50
3:C:79:LYS:HA	3:C:83:HIS:HB2	1.93	0.50
3:C:237:ILE:HG13	3:C:237:ILE:O	2.12	0.49
1:A:241:ILE:HG22	1:A:368:PRO:HD3	1.94	0.49
2:B:211:PHE:HE2	2:B:239:LYS:HD2	1.76	0.49
1:A:1230:VAL:HG11	1:A:1259:LEU:HD13	1.95	0.49
1:A:35:HIS:HB3	1:A:1109:VAL:HG13	1.95	0.49
1:A:114:GLN:O	1:A:119:TYR:OH	2.31	0.49
1:A:1310:HIS:CD2	1:A:1313:TRP:H	2.31	0.49
5:E:84:THR:HG22	5:E:85:ARG:H	1.76	0.49
1:A:652:VAL:HG11	1:A:796:LEU:HD13	1.95	0.48
3:C:239:GLN:O	3:C:243:LEU:HG	2.14	0.48
2:B:52:PHE:CZ	2:B:177:VAL:HG11	2.49	0.48
1:A:1058:ASP:OD1	1:A:1059:TYR:N	2.47	0.48
1:A:1013:LEU:HD23	1:A:1279:ILE:HD13	1.95	0.48
3:C:273:ASP:OD1	3:C:273:ASP:N	2.47	0.48
1:A:605:TYR:HD1	1:A:608:LEU:HD12	1.79	0.48



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:1024:GLY:HA2	1:A:1323:TYR:CD2	2.49	0.48	
8:H:66:CYS:SG	8:H:67:LEU:N	2.87	0.47	
1:A:1315:HIS:ND1	1:A:1329:SER:HB3	2.29	0.47	
1:A:155:VAL:HB	1:A:165:TRP:HB2	1.96	0.47	
1:A:120:LYS:HB3	1:A:133:LEU:HD11	1.96	0.47	
1:A:347:PHE:HD2	1:A:370:LEU:HD11	1.78	0.47	
2:B:255:ARG:HG3	2:B:255:ARG:O	2.15	0.47	
8:H:8:HIS:O	8:H:12:THR:OG1	2.22	0.47	
1:A:1029:VAL:HG22	1:A:1040:VAL:HG22	1.96	0.47	
5:E:73:LEU:HB3	5:E:101:PHE:CE1	2.50	0.47	
1:A:1250:LEU:HG	1:A:1283:SER:O	2.14	0.47	
4:D:66:ILE:HD12	5:E:48:ILE:HD12	1.97	0.47	
5:E:16:THR:HG21	8:H:1:MET:HB2	1.97	0.47	
1:A:1146:ILE:HD13	1:A:1162:PRO:HA	1.98	0.46	
1:A:1310:HIS:CD2	1:A:1312:HIS:H	2.25	0.46	
3:C:137:THR:OG1	3:C:171:MET:SD	2.73	0.46	
3:C:186:ASP:OD1	3:C:187:HIS:N	2.48	0.46	
7:G:67:SER:HB3	8:H:66:CYS:HB3	1.97	0.46	
1:A:147:LEU:HD22	1:A:342:LEU:HD21	1.97	0.46	
1:A:1187:ASP:OD1	1:A:1188:GLY:N	2.48	0.46	
7:G:68:VAL:HG22	8:H:65:VAL:HG13	1.97	0.46	
1:A:180:TYR:HE2	1:A:212:GLN:HE22	1.64	0.46	
8:H:17:SER:O	8:H:89:MET:N	2.44	0.46	
1:A:528:PRO:HG2	1:A:531:HIS:HD2	1.80	0.46	
2:B:205:LEU:HD12	2:B:205:LEU:HA	1.80	0.46	
8:H:22:LEU:HD22	8:H:37:LEU:HD13	1.97	0.46	
1:A:109:GLN:OE1	1:A:268:THR:OG1	2.34	0.46	
1:A:458:ASP:HA	1:A:497:LYS:HE2	1.98	0.46	
1:A:1139:MET:HE3	1:A:1139:MET:HB2	1.84	0.46	
1:A:376:HIS:HD2	1:A:378:MET:H	1.63	0.45	
8:H:74:ILE:HB	8:H:87:HIS:CE1	2.52	0.45	
1:A:326:ASN:HD21	1:A:431:GLU:HB2	1.80	0.45	
1:A:778:ILE:HD12	I:A:778:ILE:H	1.80	0.45	
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.88	0.45	
2:B:136:GLN:O	2:B:140:1LE:HG13	2.16	0.45	
1:A:935:GLU:HG2	1:A:936:GLN:N	2.32	0.45	
7:G:54:AKG:H	7:G:b2:PRO:HB2	1.81	0.45	
1:A:457:LEU:HG	1:A:404:VAL:HG22	1.98	0.45	
1:A:/91:SER:OG	1:A:/92:SEK:N	2.49	0.45	
1:A:1048:PHE:HZ	1:A:1084:LEU:HD22	1.82	0.45	
1:A:1208:AKG:HA	1:A:1208:ARG:HD3	1.77	0.45	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:1072:ALA:HB3	1:A:1087:ALA:HB3	1.99	0.45
1:A:582:GLY:O	1:A:625:THR:HG21	2.17	0.45
1:A:784:ILE:HD12	1:A:831:MET:SD	2.57	0.45
3:C:304:ASP:N	3:C:304:ASP:OD1	2.50	0.45
1:A:959:PHE:O	1:A:963:SER:OG	2.31	0.45
5:E:23:LEU:HD22	5:E:46:ALA:HB2	1.98	0.45
1:A:566:LEU:HD22	1:A:607:LEU:HD11	1.99	0.44
4:D:105:LEU:O	4:D:107:PRO:HD3	2.16	0.44
6:F:118:ARG:O	6:F:121:VAL:HG12	2.17	0.44
1:A:1047:CYS:HB2	1:A:1059:TYR:CD1	2.52	0.44
2:B:266:PHE:HB2	2:B:272:VAL:HB	1.98	0.44
5:E:25:LEU:HD11	5:E:46:ALA:HB1	1.99	0.44
1:A:1240:ASP:HB3	1:A:1243:MET:HB2	2.00	0.44
6:F:99:ASN:OD1	8:H:46:SER:OG	2.28	0.44
3:C:262:PHE:HE1	3:C:282:TYR:HE1	1.65	0.44
6:F:27:ARG:HB3	6:F:27:ARG:HH11	1.82	0.44
1:A:159:THR:OG1	1:A:163:GLU:OE1	2.26	0.44
1:A:1148:ARG:HD2	1:A:1150:TRP:NE1	2.32	0.44
3:C:174:GLU:OE1	3:C:214:SER:OG	2.35	0.44
1:A:1313:TRP:CB	1:A:1315:HIS:HD2	2.31	0.44
2:B:284:ALA:O	2:B:288:ILE:HG13	2.17	0.44
1:A:72:PRO:HB2	1:A:174:TYR:HE2	1.83	0.44
3:C:131:GLU:HG2	3:C:167:VAL:HG13	2.00	0.44
1:A:57:THR:O	1:A:114:GLN:NE2	2.33	0.44
2:B:122:ILE:HD11	2:B:155:LEU:HD23	2.00	0.44
1:A:799:LEU:HB2	1:A:802:VAL:HG12	1.98	0.43
5:E:82:ALA:O	5:E:92:CYS:HA	2.18	0.43
5:E:108:ALA:O	5:E:112:VAL:HG23	2.18	0.43
2:B:132:VAL:HG11	2:B:140:ILE:HD12	2.00	0.43
2:B:253:GLU:O	3:C:316:ALA:HA	2.18	0.43
1:A:184:THR:HG22	1:A:213:ARG:HH12	1.82	0.43
1:A:547:HIS:NE2	1:A:551:GLU:OE2	2.52	0.43
1:A:1128:VAL:HG22	1:A:1141:SER:O	2.18	0.43
1:A:1194:ASP:HB3	1:A:1197:MET:HG3	2.01	0.43
1:A:183:GLN:HB2	1:A:237:MET:HG3	1.99	0.43
2:B:128:LYS:HG2	9:B:401:GTP:C6	2.53	0.43
6:F:79:GLN:HB2	6:F:96:SER:HA	2.01	0.43
1:A:97:LYS:O	1:A:101:THR:HG23	2.18	0.43
2:B:188:GLU:HG2	2:B:215:SER:HB2	2.01	0.43
1:A:199:ALA:HB3	1:A:245:ALA:H	1.83	0.43
1:A:1093:ILE:HD11	1:A:1127:MET:HE1	2.00	0.43



	Atom 2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (\AA)		
1:A:262:LEU:HD23	1:A:357:MET:SD	2.59	0.43	
1:A:1205:MET:HG3	1:A:1241:PRO:O	2.19	0.43	
1:A:1235:ASP:OD1	1:A:1235:ASP:N	2.52	0.43	
2:B:185:GLN:CD	2:B:185:GLN:H	2.22	0.43	
1:A:71:ASP:C	1:A:73:PRO:HD3	2.40	0.42	
1:A:1021:ARG:HB2	1:A:1324:TYR:HE1	1.84	0.42	
1:A:299:PRO:HG2	1:A:308:PRO:HG2	2.01	0.42	
1:A:1187:ASP:OD1	1:A:1189:SER:OG	2.35	0.42	
4:D:148:VAL:HG21	5:E:10:VAL:HG13	2.00	0.42	
1:A:23:ASP:HA	1:A:26:LEU:HG	2.01	0.42	
1:A:128:ASP:HA	1:A:131:LYS:HD3	2.01	0.42	
1:A:790:ALA:O	1:A:794:SER:OG	2.26	0.42	
5:E:84:THR:HG22	5:E:85:ARG:N	2.34	0.42	
1:A:1101:ASP:N	1:A:1101:ASP:OD1	2.52	0.42	
1:A:1008:LYS:HB2	1:A:1008:LYS:HE3	1.85	0.42	
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.90	0.42	
1:A:105:ASN:OD1	1:A:106:LEU:N	2.51	0.42	
1:A:1069:ARG:HG2	1:A:1089:ASP:OD2	2.20	0.42	
2:B:129:MET:HG3	2:B:161:ARG:HB2	2.01	0.42	
7:G:65:ARG:HH11	7:G:76:LEU:HD13	1.85	0.42	
8:H:33:CYS:HB2	8:H:38:SER:HA	2.01	0.42	
1:A:439:VAL:CG1	1:A:445:HIS:HB2	2.50	0.42	
1:A:479:LEU:HB3	1:A:491:LEU:HD11	2.01	0.42	
2:B:264:ASP:O	2:B:271:TYR:HD1	2.02	0.42	
3:C:272:THR:OG1	3:C:273:ASP:N	2.52	0.42	
1:A:158:PRO:HB3	1:A:164:VAL:HG12	2.02	0.41	
2:B:88:LEU:HD22	2:B:113:ILE:HG13	2.02	0.41	
1:A:183:GLN:H	1:A:183:GLN:HG2	1.62	0.41	
3:C:145:ASP:OD1	3:C:145:ASP:N	2.35	0.41	
5:E:102:GLY:HA3	8:H:31:LEU:HD12	2.02	0.41	
1:A:155:VAL:HG11	1:A:165:TRP:O	2.20	0.41	
1:A:202:ILE:O	1:A:206:PHE:HB2	2.21	0.41	
1:A:201:LEU:HD12	1:A:202:ILE:N	2.35	0.41	
6:F:88:LEU:HD23	6:F:88:LEU:HA	1.83	0.41	
1:A:341:LEU:HD13	1:A:341:LEU:HA	1.92	0.41	
1:A:581:LEU:O	1:A:584:ILE:HG22	2.20	0.41	
8:H:47:VAL:HA	8:H:50:GLN:HG2	2.00	0.41	
8:H:74:ILE:HA	8:H:86:VAL:O	2.20	0.41	
1:A:308:PRO:HG3	1:A:403:PHE:CZ	2.55	0.41	
1:A:1043:LYS:O	1:A:1069:ARG:HA	2.21	0.41	
1:A:80:PRO:HG2	1:A:256:PRO:HG3	2.01	0.41	



Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)			
3:C:263:ASP:O	3:C:267:LYS:N	2.50	0.41			
5:E:117:GLU:HB3	5:E:118:PRO:HD3	2.03	0.41			
2:B:75:THR:OG1	2:B:76:SER:N	2.54	0.41			
2:B:183:ASN:OD1	2:B:183:ASN:N	2.48	0.41			
1:A:424:VAL:HG12	1:A:462:TRP:HZ2	1.86	0.41			
2:B:20:LYS:HE3	9:B:401:GTP:O2B	2.21	0.41			
3:C:262:PHE:CE1	3:C:282:TYR:HE1	2.39	0.41			
6:F:20:HIS:NE2	6:F:95:SER:HB2	2.35	0.41			
1:A:439:VAL:HG13	1:A:445:HIS:HB2	2.02	0.41			
1:A:669:HIS:O	1:A:673:GLN:HG2	2.20	0.41			
1:A:1322:ASP:O	1:A:1323:TYR:HB2	2.21	0.41			
2:B:153:ARG:NE	2:B:153:ARG:HA	2.35	0.41			
3:C:133:ILE:O	3:C:137:THR:HG23	2.21	0.41			
6:F:101:GLY:C	8:H:43:GLY:HA3	2.42	0.41			
6:F:86:LEU:HD12	6:F:86:LEU:H	1.85	0.40			
1:A:202:ILE:H	1:A:202:ILE:HG13	1.76	0.40			
3:C:193:ARG:HE	3:C:193:ARG:HB2	1.71	0.40			
1:A:466:LEU:O	1:A:470:VAL:HG23	2.21	0.40			
1:A:1201:GLU:HG2	1:A:1202:CYS:H	1.86	0.40			
3:C:329:LYS:HE3	3:C:329:LYS:HB3	1.93	0.40			
1:A:238:LYS:HE3	1:A:238:LYS:HB3	1.92	0.40			
3:C:257:GLU:OE2	3:C:342:ARG:HG3	2.22	0.40			
3:C:301:LEU:HD13	3:C:305:GLY:HA2	2.04	0.40			
1:A:84:LEU:HA	1:A:89:ASP:HA	2.03	0.40			
1:A:326:ASN:ND2	1:A:431:GLU:HB2	2.37	0.40			
2:B:43:ILE:HD13	2:B:43:ILE:HA	1.82	0.40			
6:F:20:HIS:HB3	6:F:40:ALA:HB2	2.02	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	Perce	ntiles
1	А	1095/1392~(79%)	993~(91%)	102 (9%)	0	100	100
2	В	296/313~(95%)	275~(93%)	21 (7%)	0	100	100
3	С	276/400~(69%)	258~(94%)	18 (6%)	0	100	100
4	D	102/158~(65%)	98~(96%)	4 (4%)	0	100	100
5	Ε	122/125~(98%)	118 (97%)	4 (3%)	0	100	100
6	F	118/162~(73%)	105~(89%)	13 (11%)	0	100	100
7	G	80/100 (80%)	71~(89%)	9 (11%)	0	100	100
8	Н	87/91 (96%)	82 (94%)	5(6%)	0	100	100
All	All	2176/2741 (79%)	2000 (92%)	176 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	946/1202~(79%)	917~(97%)	29~(3%)	40	71
2	В	271/287~(94%)	257~(95%)	14~(5%)	23	56
3	С	251/340~(74%)	245~(98%)	6 (2%)	49	76
4	D	55/138~(40%)	54 (98%)	1 (2%)	59	81
5	Ε	90/98~(92%)	87~(97%)	3~(3%)	38	70
6	F	91/135~(67%)	87~(96%)	4 (4%)	28	62
7	G	12/83~(14%)	12 (100%)	0	100	100
8	Н	58/77~(75%)	58 (100%)	0	100	100
All	All	1774/2360~(75%)	1717 (97%)	57(3%)	42	70

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	25	ASN
1	А	43	LYS
	<i>a</i>	-	



Mol	Chain	Res	Type
1	А	56	LYS
1	А	127	VAL
1	А	139	ARG
1	А	174	TYR
1	А	213	ARG
1	А	242	GLN
1	А	283	CYS
1	А	339	GLN
1	А	356	ILE
1	А	358	ARG
1	А	391	SER
1	А	403	PHE
1	А	437	LEU
1	А	633	ARG
1	А	635	ASP
1	А	668	SER
1	А	916	TYR
1	А	931	ASP
1	А	1067	TYR
1	А	1135	THR
1	А	1139	MET
1	А	1145	ARG
1	А	1196	ARG
1	А	1242	ARG
1	А	1246	SER
1	А	1259	LEU
1	А	1283	SER
2	В	66	GLN
2	В	67	ASP
2	В	129	MET
2	В	132	VAL
2	В	135	ASP
2	В	162	THR
2	В	168	THR
2	В	188	GLU
2	В	223	ARG
2	В	224	ASP
2	В	249	PHE
2	В	264	ASP
2	В	268	SER
2	В	269	ASN
3	С	66	LEU



\mathbf{Mol}	Chain	Res	Type
3	С	202	ASP
3	С	273	ASP
3	С	288	MET
3	С	330	GLU
3	С	341	LEU
4	D	147	ARG
5	Е	13	GLN
5	Е	23	LEU
5	Е	44	VAL
6	F	28	ASP
6	F	49	PHE
6	F	71	ILE
6	F	85	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	212	GLN
1	А	281	GLN
1	А	361	ASN
1	А	376	HIS
1	А	417	GLN
1	А	428	ASN
1	А	531	HIS
1	А	557	ASN
1	А	636	HIS
1	А	835	ASN
1	А	1061	HIS
1	А	1064	ASN
1	А	1098	ASN
1	А	1177	HIS
1	А	1251	GLN
1	А	1262	HIS
1	А	1310	HIS
1	А	1315	HIS
2	В	107	GLN
2	В	115	GLN
2	В	179	GLN
2	В	233	ASN
2	В	258	ASN
3	С	196	HIS
3	С	200	ASN



Continued from previous page...

Mol	Chain	Res	Type
5	Е	20	GLN
5	Е	59	ASN
5	Е	109	GLN
6	F	79	GLN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
WIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GTP	В	401	10	26,34,34	0.95	2 (7%)	32,54,54	0.73	0
11	GDP	С	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)

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
9	GTP	В	401	10	-	6/18/38/38	0/3/3/3
11	GDP	С	401	-	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
11	С	401	GDP	C6-N1	-2.70	1.33	1.37
9	В	401	GTP	C5-C6	-2.50	1.42	1.47
9	В	401	GTP	C8-N7	-2.10	1.31	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
11	С	401	GDP	PA-O3A-PB	-3.43	121.06	132.83
11	С	401	GDP	C5-C6-N1	2.51	118.39	113.95
11	С	401	GDP	C3'-C2'-C1'	2.41	104.61	100.98
11	С	401	GDP	C8-N7-C5	2.34	107.45	102.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	В	401	GTP	PB-O3A-PA-O5'
9	В	401	GTP	C5'-O5'-PA-O1A
11	С	401	GDP	C5'-O5'-PA-O1A
11	С	401	GDP	C5'-O5'-PA-O2A
9	В	401	GTP	O4'-C4'-C5'-O5'
9	В	401	GTP	C3'-C4'-C5'-O5'
9	В	401	GTP	C5'-O5'-PA-O3A
9	В	401	GTP	C5'-O5'-PA-O2A
11	С	401	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	В	401	GTP	7	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 similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20660. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

6.2Central slices (i)

6.2.1Primary map



X Index: 176

Y Index: 176



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: 192

Y Index: 202

Z Index: 174

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 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)



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 (i)



The volume at the recommended contour level is 174 $\rm nm^3;$ this corresponds to an approximate mass of 157 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 0.314 \AA^{-1}



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20660 and PDB model 6U62. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).



9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



1.0

Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.9450	0.5130	
А	0.9460	0.5150	
В	0.9620	0.5580	
С	0.9590	0.5420	
D	0.9060	0.4370	
E	0.9400	0.5200	
F	0.9320	0.4720	
G	0.8900	0.3880	0.0
Н	0.9220	0.4410	— <0.

