

### Nov 21, 2022 – 06:11 PM JST

PDB II	D	:	7D73
EMDB II	D	:	EMD-30600
Titl	le	:	Cryo-EM structure of GMPPA/GMPPB complex bound to GTP (State I)
Author	rs	:	Zheng, L.; Liu, Z.; Wang, Y.; Yang, F.; Wang, J.; Qing, J.; Cai, X.; Mo, X.;
			Gao, N.; Jia, D.
Deposited o	n	:	2020-10-02
Resolutio	n	:	3.00  Å(reported)
This	is is a	a F	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 43
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 3.00 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	420	80%	16%	••
1	В	420	80%	16%	·
1	С	420	83%	13%	••
1	D	420	80%	16%	••
2	Е	360	69%	26%	••
2	F	360	41%	22%	••
2	G	360	46% 69%	29%	•
2	Н	360	52% 76%	23%	•



Mol	Chain	Length	Quality of chain				
			56%				
2	Ι	360	70%	26%	•		
			48%				
2	J	360	71%	28%	•		
			50%				
2	Κ	360	72%	24%	••		
			61%				
2	L	360	68%	28%	•		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	F	401	-	-	Х	-



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35292 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.

Mol	Chain	Residues		At	oms			AltConf	Trace	
1 A	Δ	407	Total	С	Ν	Ο	$\mathbf{S}$	0	0	
	407	3172	2031	561	569	11	0	0		
1	В	B	406	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	400	3167	2028	560	568	11	0	0		
1	С	406	Total	С	Ν	0	$\mathbf{S}$	0	0	
	400	3167	2028	560	568	11	0			
1	Л	406	Total	С	Ν	0	S	0	0	
	D	400	3167	2028	560	568	11	0	0	

• Molecule 1 is a protein called Mannose-1-phosphate guanyltransferase alpha.

• Molecule 2 is a protein called Mannose-1-phosphate guanyltransferase beta.

Mol	Chain	Residues		At		AltConf	Trace		
2	F	360	Total	С	Ν	0	$\mathbf{S}$	0	0
	500	2785	1769	487	507	22	0	0	
2	F	350	Total	С	Ν	0	S	0	0
	Ľ	550	2714	1728	473	492	21	0	0
0	С	260	Total	С	Ν	0	S	0	0
	G	500	2789	1772	488	507	22	0	0
0	т	I 360	Total	С	Ν	0	S	0	0
			2789	1772	488	507	22	0	
2	т	360	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	J	300	2789	1772	488	507	22	0	
2	K	360	Total	С	Ν	0	$\mathbf{S}$	0	0
2	IX	500	2783	1768	488	505	22	0	0
2	T	360	Total	$\mathbf{C}$	Ν	0	$\mathbf{S}$	0	0
	300	2783	1768	488	505	22	0	U	
2	н	Н 360	Total	C	N	0	S	0	0
	11		2789	1772	488	507	22	0	0

• Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>5</sub>O<sub>16</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			AltConf	
9	Δ	1	Total	С	Ν	Ο	Р	0	
$\left  \begin{array}{c} 3 \\ \mathbf{F} \end{array} \right  $	A	1	39	16	5	16	2	0	
2	2 C	1	Total	С	Ν	Ο	Р	0	
3	U	L	39	16	5	16	2	0	

• Molecule 4 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		
4	В	1	Total	С	N	0	Р	0	
-	_	D		32	10	5	14	3	



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Mol	Chain	Residues		Ate	oms			AltConf
4	F	1	Total	С	Ν	Ο	Р	0
4	Ľ	L	32	10	5	14	3	0
4		1	Total	С	Ν	Ο	Р	0
4	D	T	32	10	5	14	3	0
4	F	1	Total	С	Ν	Ο	Р	0
4	Ľ	T	32	10	5	14	3	0
4	С	1	Total	С	Ν	Ο	Р	0
4	G	T	32	10	5	14	3	0
4	T	1	Total	С	Ν	Ο	Р	0
	I	T	32	10	5	14	3	0
4	Т	1	Total	С	Ν	Ο	Р	0
т	5	I	32	10	5	14	3	0
4	K	1	Total	С	Ν	Ο	Р	0
т	17	I	32	10	5	14	3	0
4	T.	1	Total	С	Ν	Ο	Р	0
	+ L	1	32	10	5	14	3	0
4	н	1	Total	C	N	Ō	Р	0
4	11	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 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: Mannose-1-phosphate guanyltransferase alpha







# 332 GLN 333 GLN 339 GLN 339 GLN 401 PR0 405 GLN 406 CLN 406 CLN 406 CLN 406 CLN 419 CLN 419 CLN 421 CLN 421 CLN 421 CLN 421 CLN 421 CLN 4254 CLN 4264 CLN 4365 CLN

• Molecule 1: Mannose-1-phosphate guanyltransferase alpha

72%



22%

Chain F:



• Molecule 2: Mannose-1-phosphate guanyltransferase beta





• Molecule 2: Mannose-1-phosphate guanyltransferase beta





# 

• Molecule 2: Mannose-1-phosphate guanyltransferase beta





BANK

# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	64	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	0.280	Depositor
Minimum map value	-0.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0389	Depositor
Map size (Å)	252.48001, 252.48001, 252.48001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^{\circ}$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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, GDD

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).

Mal	Chain	Bond lengths		Bond angles		
WIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.53	0/3253	0.64	0/4427	
1	В	0.52	0/3248	0.61	1/4420~(0.0%)	
1	С	0.52	0/3248	0.63	0/4420	
1	D	0.51	0/3248	0.62	0/4420	
2	Е	0.39	0/2840	0.70	3/3850~(0.1%)	
2	F	0.46	0/2767	0.65	1/3748~(0.0%)	
2	G	0.41	0/2844	0.67	1/3854~(0.0%)	
2	Н	0.45	0/2844	0.65	0/3854	
2	Ι	0.45	0/2844	0.67	0/3854	
2	J	0.40	0/2844	0.65	0/3854	
2	Κ	0.44	0/2838	0.65	3/3846~(0.1%)	
2	L	0.39	0/2838	0.63	0/3846	
All	All	0.46	0/35656	0.65	9/48393~(0.0%)	

There are no bond length outliers.

•

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Κ	164	GLN	N-CA-C	-7.28	91.35	111.00
2	G	114	ASP	N-CA-C	-6.32	93.94	111.00
2	Е	114	ASP	N-CA-C	-6.07	94.61	111.00
2	Е	110	ASP	CB-CG-OD2	5.86	123.58	118.30
1	В	18	ARG	N-CA-C	5.46	125.74	111.00
2	F	14	LEU	CA-CB-CG	5.24	127.35	115.30
2	Κ	107	LEU	CA-CB-CG	5.11	127.05	115.30
2	Κ	188	LEU	CA-CB-CG	5.09	127.00	115.30
2	Е	160	VAL	N-CA-C	5.00	124.50	111.00

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	3172	0	3188	40	0
1	В	3167	0	3184	28	0
1	С	3167	0	3184	33	0
1	D	3167	0	3184	37	0
2	Е	2785	0	2828	84	0
2	F	2714	0	2769	70	0
2	G	2789	0	2840	70	0
2	Н	2789	0	2840	53	0
2	Ι	2789	0	2840	65	0
2	J	2789	0	2838	65	0
2	Κ	2783	0	2829	79	0
2	L	2783	0	2827	80	0
3	А	39	0	22	1	0
3	С	39	0	23	0	0
4	В	32	0	12	0	0
4	D	32	0	12	1	0
4	Е	32	0	12	1	0
4	F	32	0	12	16	0
4	G	32	0	10	2	0
4	Н	32	0	10	1	0
4	Ι	32	0	12	5	0
4	J	32	0	10	2	0
4	К	32	0	10	0	0
4	L	32	0	10	5	0
All	All	35292	0	35506	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (684) 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:I:163:PRO:HG2	2:I:167:VAL:CG2	1.25	1.54
2:I:163:PRO:CG	2:I:167:VAL:HG21	1.32	1.53
1:C:406:PRO:O	1:D:18:ARG:NH1	1.66	1.26



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:I:146:VAL:CG1	2:I:168:SER:O	1.88	1.20
2:J:9:GLY:N	4:J:401:GTP:N7	1.68	1.18
2:J:200:ILE:HA	2:J:203:LYS:HE2	1.25	1.16
2:F:7:VAL:CG2	2:F:24:PRO:CG	2.24	1.15
2:I:80:GLU:OE2	2:I:89:PRO:HB3	1.00	1.15
2:F:7:VAL:CG2	2:F:24:PRO:HG3	1.78	1.14
2:I:146:VAL:HG11	2:I:168:SER:O	1.43	1.14
2:K:162:LYS:HG3	2:K:163:PRO:HD2	1.15	1.14
2:I:80:GLU:OE2	2:I:89:PRO:CB	1.94	1.14
2:F:8:GLY:O	2:F:55:TYR:HB3	1.45	1.13
2:K:68:GLU:CA	2:K:75:ILE:HD11	1.81	1.10
1:A:16:ARG:HE	1:A:20:LEU:HD13	0.98	1.09
2:K:163:PRO:O	2:K:164:GLN:HG3	1.51	1.08
2:K:67:GLN:HE21	2:K:70:ARG:HD3	1.24	1.02
1:C:356:THR:HG23	1:C:401:ASN:HD21	1.24	1.02
2:F:7:VAL:CG2	2:F:24:PRO:HG2	1.90	1.00
2:G:105:PHE:CE1	2:G:117:PHE:HD1	1.79	1.00
2:E:145:GLY:HA2	2:E:160:VAL:HG23	1.39	0.99
2:K:163:PRO:O	2:K:164:GLN:CG	2.10	0.99
2:F:8:GLY:O	2:F:55:TYR:CB	2.10	0.99
2:K:68:GLU:HA	2:K:75:ILE:HD11	1.45	0.99
1:B:16:ARG:NH1	1:B:370:ASP:O	1.97	0.98
2:L:29:CYS:SG	2:L:255:LEU:HD12	2.05	0.96
1:A:16:ARG:NE	1:A:20:LEU:HD13	1.82	0.94
1:C:356:THR:CG2	1:C:401:ASN:HD21	1.80	0.94
1:A:16:ARG:HE	1:A:20:LEU:CD1	1.80	0.94
2:K:159:PHE:CZ	2:K:198:PHE:HB3	2.04	0.92
2:I:146:VAL:HG13	2:I:168:SER:O	1.67	0.92
2:F:7:VAL:HG21	2:F:24:PRO:CG	1.99	0.92
2:F:131:GLY:O	2:F:207:LEU:HA	1.70	0.91
2:K:163:PRO:C	2:K:164:GLN:HG3	1.85	0.91
2:E:320:MET:CE	2:E:338:LEU:HD12	1.99	0.91
2:K:162:LYS:HG3	2:K:163:PRO:CD	1.99	0.91
2:F:7:VAL:HG22	2:F:24:PRO:CG	1.99	0.91
1:C:356:THR:HG23	1:C:401:ASN:ND2	1.86	0.90
2:K:68:GLU:CB	2:K:75:ILE:HD11	2.02	0.90
2:I:94:ARG:O	2:I:98:SER:HB2	1.72	0.89
2:L:29:CYS:SG	2:L:255:LEU:CD1	2.60	0.88
2:K:162:LYS:CG	2:K:163:PRO:HD2	2.03	0.88
2:L:229:MET:HE3	2:L:271:ASN:O	1.74	0.87
2:E:142:SER:O	2:E:144:TYR:N	2.08	0.86



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:G:115:PHE:CE1	2:G:175:MET:CE	2.59	0.85
2:F:7:VAL:HG23	2:F:24:PRO:HG3	1.59	0.85
1:D:361:ASN:ND2	1:D:364:ASP:HB2	1.91	0.85
2:E:145:GLY:CA	2:E:160:VAL:HG23	2.08	0.84
1:C:359:ASP:HB3	1:C:360:PRO:HD2	1.59	0.84
2:K:159:PHE:HZ	2:K:198:PHE:HB3	1.39	0.83
2:E:320:MET:HE3	2:E:338:LEU:HD12	1.60	0.83
2:F:7:VAL:HG22	2:F:24:PRO:HG2	1.56	0.82
1:C:359:ASP:HB3	1:C:360:PRO:CD	2.08	0.82
2:K:158:ARG:HH21	2:K:158:ARG:HG3	1.44	0.82
2:E:324:THR:HG23	2:E:341:ALA:O	1.80	0.81
2:H:141:PRO:HB2	2:H:164:GLN:HE22	1.45	0.81
2:G:306:CYS:HB2	2:G:324:THR:HG23	1.63	0.81
2:G:105:PHE:CE1	2:G:117:PHE:CD1	2.68	0.79
2:G:115:PHE:CE1	2:G:175:MET:HE2	2.17	0.79
2:K:68:GLU:HG3	2:K:75:ILE:HG13	1.63	0.79
2:G:115:PHE:CD1	2:G:175:MET:CE	2.65	0.78
2:L:229:MET:SD	2:L:273:SER:OG	2.40	0.78
2:F:7:VAL:HG21	2:F:24:PRO:HG2	1.59	0.78
2:G:115:PHE:CE1	2:G:175:MET:HE1	2.18	0.77
2:L:31:LYS:HB2	2:L:31:LYS:NZ	2.00	0.77
2:E:44:ALA:HB2	2:E:117:PHE:CD2	2.20	0.76
1:D:276:HIS:CD2	1:D:283:ILE:H	2.03	0.76
2:G:94:ARG:O	2:G:98:SER:HB2	1.86	0.75
2:F:7:VAL:HG12	2:F:52:ALA:O	1.86	0.75
2:K:68:GLU:HB2	2:K:75:ILE:HD11	1.67	0.75
2:K:68:GLU:HB2	2:K:75:ILE:CD1	2.16	0.75
2:L:230:CYS:SG	2:L:271:ASN:OD1	2.44	0.74
2:L:9:GLY:HA3	4:L:401:GTP:O2B	1.88	0.74
2:H:84:LEU:HB3	2:H:88:GLY:HA3	1.68	0.73
1:C:359:ASP:CB	1:C:360:PRO:CD	2.67	0.73
2:F:120:MET:HG2	2:F:177:ILE:HD11	1.71	0.73
2:H:305:SER:O	2:H:323:VAL:HA	1.88	0.72
2:G:14:LEU:HB2	2:G:220:GLY:O	1.89	0.72
2:F:7:VAL:HA	4:F:401:GTP:O2'	1.90	0.71
2:F:12:THR:HA	2:F:15:ARG:HD3	1.72	0.71
2:J:7:VAL:CG2	2:J:53:VAL:HA	2.20	0.71
2:F:7:VAL:C	4:F:401:GTP:O2'	2.29	0.71
2:E:41:LEU:HB3	2:E:117:PHE:CE1	2.25	0.70
2:K:68:GLU:CG	2:K:75:ILE:HG13	2.20	0.70
2:E:320:MET:HE2	2:E:338:LEU:HD12	1.73	0.69



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		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:L:6:LEU:HB3	4:L:401:GTP:H1'	1.74	0.69
2:G:115:PHE:HE1	2:G:175:MET:CE	2.05	0.69
2:L:229:MET:SD	2:L:233:LEU:HD11	2.32	0.69
2:H:146:VAL:HB	2:H:160:VAL:HG11	1.74	0.69
2:F:7:VAL:CA	4:F:401:GTP:O2'	2.40	0.69
2:E:145:GLY:HA2	2:E:160:VAL:CG2	2.19	0.68
2:F:8:GLY:N	4:F:401:GTP:O2'	2.27	0.68
2:E:156:ILE:HD13	2:E:159:PHE:HE2	1.59	0.67
2:I:147:VAL:O	2:I:168:SER:HB2	1.94	0.67
2:L:80:GLU:OE2	4:L:401:GTP:N1	2.26	0.67
2:J:7:VAL:HG21	2:J:53:VAL:HB	1.76	0.67
2:I:80:GLU:CD	4:I:401:GTP:HN21	1.97	0.67
2:J:7:VAL:HG11	2:J:51:LEU:HD21	1.76	0.67
2:E:140:GLU:N	2:E:141:PRO:CD	2.58	0.66
2:K:163:PRO:C	2:K:164:GLN:CG	2.60	0.66
1:A:20:LEU:HD12	1:A:20:LEU:H	1.60	0.66
1:B:259:ARG:NH1	1:B:359:ASP:OD2	2.28	0.66
1:B:266:GLN:HE21	1:B:286:ASN:HD21	1.44	0.66
2:E:139:GLU:HB2	2:E:140:GLU:OE1	1.96	0.66
2:K:12:THR:HA	2:K:15:ARG:HD3	1.77	0.65
2:H:146:VAL:CB	2:H:160:VAL:HG11	2.26	0.65
2:L:140:GLU:O	2:L:140:GLU:HG2	1.97	0.64
2:H:161:GLU:HA	2:H:161:GLU:OE2	1.96	0.64
1:D:1:MET:HG2	1:D:51:GLN:HG3	1.80	0.64
2:K:163:PRO:O	2:K:164:GLN:HG2	1.96	0.64
2:I:163:PRO:CD	2:I:167:VAL:HG21	2.23	0.64
1:D:276:HIS:HD2	1:D:283:ILE:H	1.43	0.64
2:G:12:THR:HA	2:G:15:ARG:HD3	1.78	0.64
2:I:160:VAL:HG21	2:I:167:VAL:CG1	2.27	0.64
2:K:162:LYS:CG	2:K:163:PRO:CD	2.70	0.64
2:E:120:MET:HB3	2:E:177:ILE:HD11	1.77	0.64
2:E:142:SER:HB2	2:E:165:VAL:HG11	1.80	0.64
2:J:321:GLU:OE1	2:J:337:TYR:CE1	2.51	0.64
2:G:119:ALA:HB1	2:G:210:MET:CE	2.28	0.64
2:K:6:LEU:HA	2:K:52:ALA:HB3	1.80	0.64
2:K:68:GLU:CB	2:K:75:ILE:CD1	2.73	0.64
2:E:63:GLU:O	2:E:67:GLN:HB2	1.98	0.63
2:E:113:CYS:SG	2:E:114:ASP:N	2.71	0.63
2:J:57:SER:O	2:J:61:GLU:HB2	1.98	0.63
2:G:115:PHE:CD1	2:G:175:MET:HE2	2.30	0.63
2:L:229:MET:SD	2:L:233:LEU:CD1	2.87	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:159:PHE:HZ	2:K:198:PHE:CB	2.11	0.62
2:L:31:LYS:HB2	2:L:31:LYS:HZ2	1.62	0.62
2:F:8:GLY:O	2:F:55:TYR:HB2	2.00	0.62
2:E:305:SER:O	2:E:323:VAL:HA	1.99	0.62
2:J:7:VAL:HG21	2:J:53:VAL:HA	1.81	0.62
1:A:189:GLU:O	1:A:192:LYS:HB2	1.98	0.62
2:F:130:GLU:HB3	2:F:206:GLN:HB3	1.82	0.62
2:I:147:VAL:O	2:I:168:SER:CB	2.48	0.62
2:K:86:THR:HG23	2:K:193:ILE:H	1.64	0.62
1:D:325:LEU:HD12	1:D:342:GLY:HA2	1.82	0.62
2:J:323:VAL:HG23	2:J:323:VAL:O	2.00	0.62
2:H:323:VAL:HG23	2:H:323:VAL:O	2.00	0.62
2:E:75:ILE:HG22	2:E:75:ILE:O	2.00	0.62
2:L:195:LYS:HG2	2:L:196:GLU:HG3	1.81	0.62
2:F:12:THR:OG1	4:F:401:GTP:O3G	2.17	0.61
2:E:142:SER:C	2:E:144:TYR:H	2.04	0.61
2:G:1:MET:H3	2:G:46:VAL:HA	1.64	0.61
2:I:236:LEU:HD21	2:I:243:ARG:HD2	1.81	0.61
2:H:164:GLN:N	2:H:164:GLN:OE1	2.33	0.61
2:G:299:SER:HB2	2:G:316:GLN:HE21	1.64	0.61
2:E:1:MET:HB3	2:E:46:VAL:HG12	1.82	0.61
2:H:81:GLU:OE1	2:H:81:GLU:HA	2.00	0.61
2:E:138:VAL:HB	2:E:141:PRO:HD2	1.82	0.61
2:I:122:GLN:HA	2:I:125:ARG:HG2	1.82	0.61
2:G:115:PHE:CD1	2:G:175:MET:HE1	2.36	0.61
2:J:7:VAL:HG22	2:J:52:ALA:O	2.01	0.60
2:G:293:ARG:HB3	2:G:310:TRP:HD1	1.65	0.60
2:E:156:ILE:HG21	2:E:159:PHE:CD2	2.37	0.60
2:G:115:PHE:HE1	2:G:175:MET:HE1	1.61	0.60
2:G:13:ARG:O	2:G:14:LEU:HB3	2.01	0.60
2:L:1:MET:HB2	2:L:46:VAL:HG12	1.84	0.60
2:E:321:GLU:OE2	2:E:337:TYR:HE1	1.85	0.60
2:G:50:ILE:HA	2:G:76:SER:O	2.02	0.60
1:B:295:VAL:HG11	1:B:301:LEU:HD11	1.83	0.59
2:E:323:VAL:HG12	2:E:323:VAL:O	2.02	0.59
1:B:325:LEU:HD12	1:B:342:GLY:HA2	1.84	0.59
2:K:106:VAL:HG23	2:K:176:TYR:HB2	1.83	0.59
2:E:134:LEU:HB3	2:E:173:ALA:HB3	1.83	0.59
2:G:119:ALA:HB1	2:G:210:MET:HE3	1.84	0.59
2:I:70:ARG:HH21	2:I:71:LEU:HD21	1.68	0.59
2:I:106:VAL:HG13	2:I:176:TYR:HB2	1.84	0.59



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:I:135:VAL:HA	2:I:171:ILE:O	2.02	0.59
2:K:68:GLU:HA	2:K:75:ILE:CD1	2.25	0.59
2:H:141:PRO:HB2	2:H:164:GLN:NE2	2.15	0.59
2:I:95:ASP:OD1	2:I:95:ASP:N	2.34	0.59
2:I:24:PRO:HB3	2:I:34:LEU:HB2	1.85	0.59
2:J:321:GLU:OE1	2:J:337:TYR:HE1	1.86	0.58
2:K:160:VAL:O	2:K:160:VAL:HG13	2.01	0.58
2:H:162:LYS:HB3	2:H:163:PRO:HD2	1.84	0.58
2:H:162:LYS:CB	2:H:163:PRO:HD2	2.32	0.58
2:I:87:ALA:HB3	2:I:191:THR:HB	1.83	0.58
2:L:292:LEU:HD12	2:L:309:GLY:HA2	1.85	0.58
2:L:324:THR:HG22	2:L:324:THR:O	2.03	0.58
2:G:120:MET:HG2	2:G:177:ILE:HG13	1.84	0.58
2:F:94:ARG:HE	2:F:184:GLN:HA	1.69	0.58
2:L:87:ALA:HB3	2:L:191:THR:HG23	1.85	0.58
2:E:50:ILE:HD11	2:E:96:LEU:HD22	1.86	0.58
2:E:142:SER:C	2:E:144:TYR:N	2.56	0.58
2:E:156:ILE:HG21	2:E:159:PHE:CE2	2.38	0.58
2:I:30:ASN:ND2	2:I:257:ASP:OD1	2.37	0.58
2:K:17:LEU:HD11	2:K:307:ILE:HG21	1.86	0.58
2:J:127:HIS:HE2	2:J:132:SER:HB2	1.69	0.58
2:J:32:PRO:HD2	2:J:35:LEU:HD22	1.86	0.58
2:K:158:ARG:HH21	2:K:158:ARG:CG	2.14	0.57
2:E:64:MET:HG3	2:E:75:ILE:HG21	1.86	0.57
2:E:130:GLU:HB3	2:E:206:GLN:HB3	1.86	0.57
2:G:32:PRO:HD2	2:G:35:LEU:HD22	1.87	0.57
1:A:363:ASN:ND2	2:G:142:SER:OG	2.37	0.57
2:K:49:VAL:HG12	2:K:75:ILE:HG22	1.85	0.57
2:L:240:GLN:OE1	2:L:243:ARG:NH2	2.37	0.57
2:H:80:GLU:OE2	2:H:84:LEU:HB2	2.04	0.57
2:J:168:SER:OG	2:J:169:ASN:N	2.37	0.57
2:E:68:GLU:HB3	2:E:75:ILE:HB	1.85	0.57
2:I:160:VAL:HG21	2:I:167:VAL:HG11	1.85	0.57
2:E:140:GLU:H	2:E:141:PRO:CD	2.18	0.57
2:L:215:PHE:HD1	2:L:231:LEU:HD13	1.70	0.57
2:H:306:CYS:SG	2:H:307:ILE:N	2.77	0.57
2:F:9:GLY:H	4:F:401:GTP:C2'	2.16	0.57
2:H:239:LYS:HE3	2:H:240:GLN:HG3	1.85	0.57
2:H:311:ARG:NH1	2:H:329:ASP:OD1	2.38	0.57
1:A:155:ILE:HG23	1:A:164:VAL:HG13	1.87	0.56
1:D:6:ILE:HG12	1:D:113:LEU:HD12	1.86	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:96:LEU:HA	2:F:99:GLU:HG3	1.86	0.56
2:H:108:ASN:ND2	4:H:401:GTP:O2B	2.38	0.56
2:E:44:ALA:CB	2:E:117:PHE:CD2	2.87	0.56
2:F:9:GLY:HA3	4:F:401:GTP:O2B	2.05	0.56
2:I:323:VAL:HG12	2:I:323:VAL:O	2.04	0.56
2:K:94:ARG:NH2	2:K:186:ILE:O	2.38	0.56
1:B:168:VAL:HG21	1:B:175:ILE:HG13	1.86	0.56
2:J:156:ILE:HD11	2:J:209:ALA:HB2	1.87	0.56
2:K:134:LEU:HA	2:K:210:MET:O	2.05	0.56
1:C:20:LEU:H	1:C:20:LEU:HD12	1.70	0.56
2:K:273:SER:O	2:K:273:SER:OG	2.24	0.56
2:F:323:VAL:HG12	2:F:323:VAL:O	2.06	0.56
2:H:12:THR:HA	2:H:15:ARG:HD3	1.87	0.56
2:E:140:GLU:H	2:E:141:PRO:HD3	1.70	0.56
2:J:7:VAL:CG2	2:J:52:ALA:O	2.54	0.56
2:G:115:PHE:HD1	2:G:175:MET:CE	2.17	0.56
2:I:33:ILE:HG12	2:I:219:ILE:HD11	1.88	0.56
2:E:32:PRO:HD2	2:E:35:LEU:HD22	1.88	0.55
2:F:7:VAL:HA	4:F:401:GTP:HO2'	1.71	0.55
2:K:35:LEU:O	2:K:39:GLU:HB2	2.06	0.55
1:C:356:THR:CG2	1:C:401:ASN:ND2	2.56	0.55
2:G:105:PHE:HE1	2:G:117:PHE:HD1	1.46	0.55
2:L:337:TYR:OH	2:L:339:ASN:ND2	2.40	0.55
1:C:320:ARG:NH1	2:I:335:GLU:OE1	2.39	0.55
2:K:305:SER:O	2:K:323:VAL:HA	2.06	0.55
1:A:158:ASN:ND2	1:A:161:THR:OG1	2.39	0.55
2:I:204:GLU:HB3	2:I:206:GLN:HG2	1.88	0.55
2:H:146:VAL:HB	2:H:160:VAL:CG1	2.36	0.55
1:B:156:VAL:HB	1:B:166:HIS:HB3	1.89	0.55
2:J:7:VAL:HG21	2:J:53:VAL:CA	2.37	0.55
2:F:87:ALA:HB2	2:F:193:ILE:HB	1.88	0.55
2:I:148:VAL:HG13	2:I:168:SER:OG	2.05	0.55
1:D:16:ARG:O	1:D:16:ARG:HG3	2.05	0.55
1:A:325:LEU:HD12	1:A:342:GLY:HA2	1.87	0.55
2:I:311:ARG:NH2	2:I:328:GLU:OE1	2.40	0.55
2:G:84:LEU:HB3	2:G:88:GLY:HA3	1.88	0.55
2:L:337:TYR:H	2:L:352:SER:HB3	1.72	0.55
2:H:94:ARG:NH2	2:H:186:ILE:O	2.38	0.55
2:G:116:PRO:HB2	2:G:119:ALA:HB3	1.89	0.55
2:L:282:ASP:OD1	2:L:282:ASP:N	2.40	0.55
2:F:9:GLY:HA3	4:F:401:GTP:H2'	1.88	0.54



	ious puye	International	Clash
Atom-1	Atom-2	distance $(\hat{A})$	$\alpha$ overlap $(\text{\AA})$
2·F·134·LEU·HB3	2·F·173·ALA·HB3	1.89	0.54
2:H:134:LEU:HG	2:H:212:LEU:HD22	1.89	0.54
1:A:20:LEU:HD12	1:A:20:LEU:N	2.22	0.54
1:A:142:THR:HG1	1:A:181:CYS:HG	1.49	0.54
2:K:51:LEU:HD12	2:K:77:MET:HB3	1.89	0.54
1:B:148:GLN:NE2	1:B:367:ALA:O	2.40	0.54
1:C:20:LEU:HD23	1:C:254:ALA:HB2	1.87	0.54
2:I:141:PRO:HB3	2:I:146:VAL:HG21	1.89	0.54
2:G:34:LEU:HD21	2:G:51:LEU:HD13	1.90	0.54
2:L:192:SER:HB3	2:L:195:LYS:HE2	1.90	0.54
1:C:337:LEU:HD12	1:C:354:GLU:HG3	1.90	0.54
2:K:158:ARG:HG3	2:K:158:ARG:NH2	2.20	0.54
2:L:94:ARG:O	2:L:98:SER:HB2	2.08	0.54
1:C:379:LYS:NZ	1:D:377:ASP:O	2.39	0.54
2:J:7:VAL:O	4:J:401:GTP:O2'	2.22	0.54
1:D:276:HIS:NE2	1:D:282:TRP:HB2	2.23	0.53
2:I:6:LEU:HD22	4:I:401:GTP:H1'	1.89	0.53
2:L:308:VAL:HG13	2:L:326:LEU:HD12	1.90	0.53
1:B:96:TYR:O	1:B:99:ARG:NH1	2.41	0.53
2:I:129:GLN:HG3	2:I:208:TYR:HE2	1.73	0.53
2:G:246:SER:HA	2:G:250:ILE:HG21	1.89	0.53
2:G:156:ILE:HD11	2:G:209:ALA:HB2	1.90	0.53
2:J:146:VAL:HG12	2:J:171:ILE:HG22	1.88	0.53
2:E:12:THR:N	4:E:401:GTP:O3G	2.41	0.53
2:K:68:GLU:OE2	2:K:69:GLN:NE2	2.41	0.53
2:L:17:LEU:HD11	2:L:307:ILE:HG21	1.90	0.53
2:I:163:PRO:CG	2:I:167:VAL:CG2	2.22	0.53
2:J:7:VAL:HG11	2:J:51:LEU:CD2	2.39	0.53
1:A:290:HIS:ND1	1:A:292:THR:OG1	2.42	0.53
2:F:233:LEU:HD21	2:F:255:LEU:HB2	1.91	0.53
2:K:68:GLU:N	2:K:75:ILE:HD11	2.24	0.53
2:K:91:ALA:HB2	2:K:186:ILE:HG23	1.89	0.53
2:K:147:VAL:HA	2:K:159:PHE:HB2	1.90	0.53
2:E:299:SER:OG	2:E:316:GLN:NE2	2.41	0.53
2:E:84:LEU:HB3	2:E:88:GLY:HA3	1.91	0.53
2:K:87:ALA:HB3	2:K:191:THR:HB	1.90	0.53
2:I:17:LEU:HD11	2:I:307:ILE:HG21	1.90	0.52
2:E:156:ILE:HD13	2:E:159:PHE:CE2	2.43	0.52
2:E:328:GLU:H	2:E:345:PRO:HB3	1.75	0.52
2:K:94:ARG:NH2	2:K:183:LEU:O	2.43	0.52
1:D:341:VAL:HG13	1:D:387:LEU:HD12	1.91	0.52



	lous puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:33:ILE:HD12	2:K:219:ILE:HD11	1.92	0.52
2:H:257:ASP:OD2	2:H:259:SER:OG	2.25	0.52
1:C:178:ILE:HD13	1:C:240:LEU:HD21	1.91	0.52
2:F:9:GLY:H	4:F:401:GTP:H2'	1.73	0.52
1:A:142:THR:OG1	1:A:181:CYS:SG	2.58	0.52
1:D:347:VAL:HA	1:D:393:ILE:HB	1.90	0.52
2:J:233:LEU:HD21	2:J:255:LEU:HB2	1.91	0.52
2:G:332:VAL:HG22	2:G:349:ILE:HD12	1.92	0.52
2:I:178:LEU:HD22	2:I:182:VAL:HG11	1.91	0.52
2:J:200:ILE:HA	2:J:203:LYS:CE	2.18	0.52
2:L:156:ILE:HD11	2:L:159:PHE:HA	1.90	0.52
2:E:138:VAL:HG21	2:E:141:PRO:O	2.10	0.52
1:C:356:THR:HG22	1:C:401:ASN:HD21	1.72	0.52
1:D:120:ASP:N	1:D:120:ASP:OD1	2.41	0.52
2:F:198:PHE:HA	2:F:201:MET:HB2	1.90	0.51
2:J:153:THR:OG1	2:J:154:GLY:N	2.43	0.51
2:L:289:CYS:SG	2:L:306:CYS:N	2.84	0.51
2:E:180:PRO:HA	2:E:183:LEU:HB3	1.92	0.51
2:G:44:ALA:HA	2:G:118:GLN:HE22	1.75	0.51
2:G:269:GLY:N	2:G:286:ILE:O	2.43	0.51
2:G:107:LEU:HD23	2:G:175:MET:HG2	1.92	0.51
2:G:120:MET:HG2	2:G:177:ILE:CG1	2.39	0.51
2:J:262:ILE:HD13	2:J:268:ILE:HG13	1.92	0.51
2:L:22:PRO:HG3	2:L:56:MET:HB3	1.92	0.51
1:D:303:PRO:HD2	1:D:320:ARG:HG3	1.92	0.51
2:L:239:LYS:HD3	2:L:240:GLN:HE21	1.75	0.51
2:E:142:SER:O	2:E:143:LYS:C	2.47	0.51
2:I:130:GLU:HB2	2:I:206:GLN:HB3	1.93	0.51
2:E:86:THR:HB	2:E:193:ILE:H	1.74	0.51
2:E:204:GLU:HB3	2:E:206:GLN:HG2	1.91	0.51
2:J:51:LEU:HD13	2:J:64:MET:HE1	1.92	0.51
2:E:212:LEU:HD13	2:E:214:GLY:H	1.76	0.51
2:H:155:ARG:HA	2:H:208:TYR:HA	1.93	0.51
1:A:403:ILE:HD12	1:A:418:ILE:HG12	1.92	0.51
2:F:84:LEU:N	4:F:401:GTP:O6	2.44	0.51
2:G:13:ARG:O	2:G:14:LEU:CB	2.59	0.51
2:J:4:LEU:HD11	2:J:52:ALA:HB2	1.93	0.51
2:J:313:ARG:HB2	2:J:331:ILE:HD13	1.93	0.51
2:K:5:ILE:HD13	2:K:34:LEU:HD11	1.92	0.51
2:E:320:MET:HE3	2:E:326:LEU:HD21	1.93	0.50
2:F:146:VAL:HG22	2:F:163:PRO:HG3	1.94	0.50



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	loue page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:295:VAL:HG11	1:A:301:LEU:HD11	1.93	0.50
2:I:160:VAL:CG2	2:I:167:VAL:HG11	2.42	0.50
2:J:135:VAL:HG11	2:J:147:VAL:HG21	1.94	0.50
1:B:376:LYS:HB2	1:B:381:LEU:HD21	1.94	0.50
2:L:101:ALA:HA	2:L:180:PRO:HG2	1.92	0.50
2:L:142:SER:OG	2:L:143:LYS:N	2.44	0.50
2:L:148:VAL:HG22	2:L:168:SER:HB2	1.93	0.50
2:H:304:GLU:O	2:H:321:GLU:HA	2.11	0.50
2:I:250:ILE:HD13	2:I:268:ILE:HB	1.92	0.50
2:J:22:PRO:HG3	2:J:56:MET:HB3	1.93	0.50
1:B:59:TYR:O	1:B:82:TYR:OH	2.24	0.50
2:E:37:GLN:NE2	2:E:108:ASN:O	2.44	0.50
2:E:12:THR:HA	2:E:15:ARG:HD3	1.93	0.50
1:D:92:GLY:HA2	1:D:95:LEU:HD12	1.93	0.50
2:F:9:GLY:CA	4:F:401:GTP:H2'	2.42	0.50
2:F:9:GLY:N	4:F:401:GTP:H2'	2.26	0.50
2:F:33:ILE:HD11	2:F:112:ILE:HB	1.93	0.50
2:J:324:THR:O	2:J:324:THR:HG23	2.11	0.50
2:E:320:MET:HE3	2:E:338:LEU:CD1	2.36	0.50
2:L:134:LEU:HD11	2:L:212:LEU:HG	1.94	0.50
1:D:3:LYS:O	1:D:110:PHE:HA	2.12	0.50
1:D:284:ARG:HH21	1:D:300:VAL:HG11	1.77	0.50
2:J:310:TRP:HE3	2:J:328:GLU:HB3	1.77	0.50
1:D:396:GLU:OE2	2:K:287:ARG:NH2	2.43	0.49
2:I:163:PRO:HB2	2:I:165:VAL:HG23	1.94	0.49
2:I:332:VAL:HG22	2:I:349:ILE:HD12	1.93	0.49
1:C:359:ASP:OD2	1:C:360:PRO:HD3	2.12	0.49
2:K:162:LYS:HD3	2:K:163:PRO:HD3	1.93	0.49
2:L:180:PRO:O	2:L:183:LEU:HB3	2.12	0.49
2:F:168:SER:OG	2:F:169:ASN:N	2.45	0.49
2:J:67:GLN:O	2:J:71:LEU:HB2	2.13	0.49
2:G:247:GLY:H	2:G:250:ILE:HB	1.77	0.49
2:K:116:PRO:HB2	2:K:119:ALA:HB3	1.95	0.49
2:J:7:VAL:HG21	2:J:53:VAL:CB	2.41	0.49
2:K:94:ARG:NH1	2:K:184:GLN:OE1	2.45	0.49
2:K:138:VAL:HB	2:K:141:PRO:HD2	1.94	0.49
2:L:54:SER:HB3	2:L:80:GLU:OE2	2.12	0.49
2:H:194:GLU:HA	2:H:198:PHE:HB2	1.95	0.49
2:K:95:ASP:OD1	2:K:95:ASP:N	2.46	0.49
2:I:360:MET:HB3	2:J:358:ILE:HD13	1.94	0.49
2:K:39:GLU:OE1	2:K:70:ARG:NH2	2.41	0.49



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:406:PRO:O	1:B:18:ARG:NH1	2.25	0.49
2:L:84:LEU:HB3	2:L:88:GLY:HA3	1.95	0.49
1:B:178:ILE:HD13	1:B:240:LEU:HD21	1.95	0.49
2:G:308:VAL:HG13	2:G:326:LEU:HD12	1.94	0.49
2:G:342:SER:HB3	2:H:360:MET:HE1	1.94	0.49
2:K:345:PRO:O	2:L:15:ARG:NH2	2.35	0.49
2:E:113:CYS:SG	2:E:114:ASP:O	2.71	0.48
2:E:138:VAL:HG11	2:E:141:PRO:HB2	1.94	0.48
2:K:15:ARG:NH2	2:L:345:PRO:O	2.32	0.48
2:H:42:ALA:HB2	2:H:73:ILE:HD13	1.95	0.48
1:A:16:ARG:HG2	1:A:20:LEU:CD1	2.43	0.48
1:B:303:PRO:HD2	1:B:320:ARG:HG3	1.94	0.48
1:B:331:GLN:HG3	1:B:348:GLY:HA2	1.94	0.48
1:D:290:HIS:CE1	1:D:309:LYS:HB3	2.47	0.48
2:K:2:LYS:HG2	2:K:48:HIS:HB3	1.94	0.48
2:L:52:ALA:O	4:L:401:GTP:N2	2.46	0.48
2:F:22:PRO:HB2	2:F:24:PRO:HD2	1.95	0.48
2:L:116:PRO:HG3	2:L:212:LEU:HD21	1.93	0.48
1:A:417:GLN:HE22	1:B:375:PHE:H	1.60	0.48
1:B:122:PRO:HG3	1:B:241:THR:HG21	1.94	0.48
2:F:24:PRO:HB3	2:F:34:LEU:HB2	1.95	0.48
2:F:27:ASP:OD2	2:F:27:ASP:N	2.37	0.48
2:G:57:SER:O	2:G:61:GLU:HB3	2.12	0.48
2:I:269:GLY:N	2:I:286:ILE:O	2.41	0.48
2:G:106:VAL:HB	2:G:176:TYR:HD1	1.78	0.48
2:I:110:ASP:OD2	2:I:110:ASP:N	2.33	0.48
1:B:277:THR:O	1:B:277:THR:OG1	2.27	0.48
2:J:10:TYR:O	2:J:11:GLY:C	2.50	0.48
2:J:14:LEU:HG	2:J:17:LEU:HD12	1.96	0.48
2:J:186:ILE:HG12	2:J:197:VAL:HG21	1.94	0.48
2:L:14:LEU:O	2:L:14:LEU:HG	2.13	0.48
1:B:392:ARG:HB2	1:B:409:GLU:HG2	1.96	0.48
2:F:94:ARG:O	2:F:98:SER:OG	2.31	0.48
2:E:124:HIS:HA	2:E:127:HIS:CD2	2.49	0.48
1:C:362:PRO:HB3	2:J:164:GLN:HA	1.95	0.48
1:D:364:ASP:OD2	1:D:365:PRO:N	2.47	0.48
2:J:49:VAL:HB	2:J:75:ILE:HG23	1.94	0.48
1:A:3:LYS:O	1:A:110:PHE:HA	2.12	0.48
1:C:37:ILE:HA	1:C:40:HIS:CD2	2.49	0.48
2:I:311:ARG:NH1	2:I:329:ASP:OD2	2.46	0.48
2:E:37:GLN:HE22	2:E:109:SER:HA	1.79	0.48



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:273:SER:O	2:F:273:SER:OG	2.31	0.48
2:H:266:CYS:HB2	2:H:284:VAL:H	1.78	0.48
1:A:394:PRO:HG2	1:A:397:VAL:HG21	1.95	0.47
2:G:150:GLU:OE1	2:G:153:THR:OG1	2.32	0.47
2:H:169:ASN:OD1	2:H:169:ASN:N	2.35	0.47
1:A:373:SER:O	1:A:373:SER:OG	2.32	0.47
1:B:100:ASP:OD1	1:C:99:ARG:NH2	2.47	0.47
2:E:17:LEU:HD11	2:E:307:ILE:HG21	1.95	0.47
1:B:393:ILE:HD12	1:B:399:ILE:HG13	1.96	0.47
2:E:19:LEU:HD22	2:F:19:LEU:HD22	1.96	0.47
2:E:194:GLU:HA	2:E:198:PHE:HB2	1.96	0.47
2:F:85:GLY:O	4:F:401:GTP:C5	2.67	0.47
2:I:87:ALA:HB2	2:I:193:ILE:HB	1.95	0.47
2:E:321:GLU:HG3	2:E:339:ASN:HD22	1.80	0.47
2:J:193:ILE:HA	2:J:197:VAL:HB	1.97	0.47
1:A:133:GLN:HB3	1:A:135:HIS:CD2	2.49	0.47
2:E:311:ARG:NH2	2:E:328:GLU:OE1	2.43	0.47
2:L:106:VAL:HB	2:L:176:TYR:HD1	1.79	0.47
1:D:364:ASP:OD2	1:D:365:PRO:HD2	2.15	0.47
2:K:16:PRO:HA	2:K:19:LEU:HD12	1.96	0.47
2:L:320:MET:HB3	2:L:320:MET:HE2	1.75	0.47
1:C:37:ILE:HA	1:C:40:HIS:HD2	1.79	0.47
2:I:6:LEU:CD2	4:I:401:GTP:H1'	2.44	0.47
2:I:321:GLU:OE1	2:I:337:TYR:HE1	1.98	0.47
2:J:7:VAL:HG23	2:J:8:GLY:H	1.80	0.47
2:F:10:TYR:O	4:F:401:GTP:O1B	2.34	0.46
2:G:129:GLN:NE2	2:G:206:GLN:OE1	2.42	0.46
2:G:134:LEU:HB3	2:G:173:ALA:HB3	1.95	0.46
1:C:15:THR:O	1:C:15:THR:HG22	2.15	0.46
2:F:94:ARG:HG3	2:F:183:LEU:HG	1.97	0.46
2:I:37:GLN:NE2	2:I:108:ASN:O	2.49	0.46
2:I:80:GLU:CD	4:I:401:GTP:N2	2.66	0.46
2:L:230:CYS:HG	2:L:271:ASN:CG	2.09	0.46
2:L:276:PRO:HD2	2:L:293:ARG:HG2	1.97	0.46
2:E:160:VAL:HG13	2:E:160:VAL:O	2.14	0.46
2:K:158:ARG:CG	2:K:158:ARG:NH2	2.73	0.46
2:L:1:MET:N	2:L:47:ASP:OD2	2.39	0.46
1:D:318:ARG:HB2	2:K:317:TRP:CE2	2.51	0.46
2:G:8:GLY:HA2	4:G:401:GTP:C4	2.51	0.46
2:I:306:CYS:HB3	2:I:324:THR:HG23	1.97	0.46
2:J:64:MET:HA	2:J:67:GLN:HB2	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:87:ALA:HB1	2:J:186:ILE:HG21	1.97	0.46
2:J:110:ASP:OD2	2:J:110:ASP:N	2.39	0.46
2:L:31:LYS:HB2	2:L:31:LYS:HZ3	1.78	0.46
1:A:302:GLY:N	1:A:318:ARG:HH12	2.13	0.46
2:I:292:LEU:HD12	2:I:309:GLY:HA2	1.96	0.46
2:E:302:TRP:HE3	2:E:319:ARG:HG3	1.80	0.46
2:G:310:TRP:HE3	2:G:328:GLU:HB2	1.81	0.46
2:J:7:VAL:HG23	2:J:53:VAL:HA	1.97	0.46
2:L:12:THR:HA	2:L:15:ARG:HD3	1.98	0.46
2:L:103:PRO:HA	2:L:178:LEU:O	2.16	0.46
1:C:5:VAL:HG11	1:C:95:LEU:HD21	1.98	0.45
2:I:1:MET:H2	2:I:46:VAL:HA	1.81	0.45
2:I:35:LEU:HD11	2:I:67:GLN:HG2	1.98	0.45
2:K:148:VAL:N	2:K:158:ARG:O	2.46	0.45
2:E:8:GLY:HA3	2:E:54:SER:H	1.81	0.45
2:E:360:MET:HG2	2:F:358:ILE:HD13	1.97	0.45
2:L:180:PRO:O	2:L:183:LEU:CB	2.64	0.45
2:H:146:VAL:CB	2:H:160:VAL:CG1	2.92	0.45
1:C:393:ILE:HD12	1:C:399:ILE:HG13	1.98	0.45
2:L:133:ILE:HG22	2:L:176:TYR:HD2	1.81	0.45
2:H:162:LYS:HG3	2:H:163:PRO:HD2	1.97	0.45
2:G:35:LEU:HA	2:G:38:VAL:HG22	1.99	0.45
2:K:49:VAL:HG12	2:K:75:ILE:CG2	2.45	0.45
2:K:133:ILE:HD11	2:K:207:LEU:HD22	1.98	0.45
2:L:230:CYS:SG	2:L:271:ASN:CG	2.95	0.45
2:I:273:SER:O	2:I:273:SER:OG	2.34	0.45
2:H:321:GLU:OE1	2:H:337:TYR:HE1	1.99	0.45
1:D:13:LYS:HA	1:D:13:LYS:HD3	1.73	0.45
1:D:242:ASP:OD1	1:D:242:ASP:N	2.50	0.45
2:G:135:VAL:HG11	2:G:147:VAL:HG21	1.99	0.45
2:H:91:ALA:HB1	2:H:188:LEU:HA	1.99	0.45
2:G:12:THR:HB	2:H:347:LYS:HD2	1.99	0.45
2:G:186:ILE:HG12	2:G:197:VAL:HG22	1.98	0.45
2:K:133:ILE:HG23	2:K:176:TYR:HD2	1.82	0.45
2:L:219:ILE:HB	2:L:225:PHE:HD2	1.80	0.45
2:E:148:VAL:HB	2:E:158:ARG:HB3	1.99	0.45
1:D:37:ILE:HA	1:D:40:HIS:CD2	2.52	0.45
2:F:120:MET:SD	2:F:134:LEU:HG	2.57	0.45
2:F:184:GLN:H	2:F:184:GLN:HG3	1.52	0.45
2:I:240:GLN:OE1	2:I:243:ARG:NH2	2.49	0.45
2:J:112:ILE:HD13	2:J:112:ILE:HA	1.83	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:6:LEU:H	2:K:6:LEU:HG	1.43	0.45
2:L:9:GLY:N	4:L:401:GTP:C4	2.85	0.45
2:H:127:HIS:CD2	2:H:129:GLN:H	2.35	0.45
2:K:11:GLY:O	2:K:18:THR:OG1	2.28	0.45
2:K:135:VAL:HG11	2:K:147:VAL:HG21	1.99	0.45
2:E:294:ASP:HB3	2:E:311:ARG:HG2	1.98	0.44
2:L:29:CYS:SG	2:L:255:LEU:HD11	2.53	0.44
2:L:68:GLU:HB3	2:L:75:ILE:HD12	1.98	0.44
2:E:27:ASP:HB3	2:E:292:LEU:HD22	2.00	0.44
2:G:25:LEU:HD11	2:G:60:LEU:HA	1.99	0.44
2:K:86:THR:HG23	2:K:193:ILE:HG22	1.99	0.44
1:A:358:SER:O	1:A:369:MET:CE	2.65	0.44
3:A:501:GDD:H8	3:A:501:GDD:H2'	1.75	0.44
2:E:116:PRO:HG2	2:E:134:LEU:HD21	1.99	0.44
2:G:12:THR:N	4:G:401:GTP:O2G	2.46	0.44
2:G:173:ALA:O	2:G:216:TRP:NE1	2.47	0.44
2:L:229:MET:SD	2:L:233:LEU:HD12	2.58	0.44
2:E:158:ARG:HD2	2:E:158:ARG:HA	1.80	0.44
1:C:113:LEU:HD23	1:C:183:ILE:HG23	2.00	0.44
1:C:376:LYS:HB3	1:C:381:LEU:HD21	1.99	0.44
2:F:110:ASP:OD1	4:F:401:GTP:O1A	2.35	0.44
2:J:93:ALA:HB1	2:J:97:LEU:HD23	1.99	0.44
2:K:103:PRO:HB2	2:K:177:ILE:HG22	1.99	0.44
2:L:54:SER:OG	2:L:55:TYR:N	2.51	0.44
1:A:13:LYS:HB2	1:A:58:PHE:HZ	1.83	0.44
2:F:17:LEU:HD11	2:F:307:ILE:HG21	1.98	0.44
2:G:182:VAL:HG21	2:G:201:MET:HE1	1.99	0.44
2:L:52:ALA:O	2:L:80:GLU:OE1	2.36	0.44
1:A:73:GLN:HE21	1:A:79:PRO:HA	1.82	0.44
2:E:41:LEU:HB2	2:E:46:VAL:HG22	1.99	0.44
2:E:60:LEU:O	2:E:64:MET:HB2	2.18	0.44
2:I:136:THR:HG22	2:I:212:LEU:HB3	1.99	0.44
2:H:15:ARG:HD2	2:H:15:ARG:HA	1.83	0.44
1:A:176:SER:OG	1:A:177:ASP:N	2.51	0.44
1:B:28:LEU:HA	1:B:35:PRO:HB3	2.00	0.44
2:E:134:LEU:HD12	2:E:134:LEU:HA	1.82	0.44
2:F:342:SER:O	2:F:342:SER:OG	2.36	0.44
2:I:185:ARG:HE	2:I:185:ARG:HB2	1.63	0.44
2:J:321:GLU:OE1	2:J:337:TYR:OH	2.33	0.44
1:A:16:ARG:HG2	1:A:20:LEU:HD12	2.00	0.44
2:E:39:GLU:HG2	2:E:71:LEU:HD21	1.98	0.44



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:344:LEU:HD13	2:E:360:MET:HB3	1.99	0.44
2:G:97:LEU:HB2	2:G:183:LEU:HD11	1.99	0.44
2:G:307:ILE:HD12	2:G:325:VAL:HG22	2.00	0.44
2:I:266:CYS:HB2	2:I:284:VAL:H	1.83	0.44
1:B:376:LYS:HA	1:B:376:LYS:HD3	1.74	0.43
1:D:114:ASN:CG	4:D:501:GTP:H4'	2.38	0.43
2:G:22:PRO:HD2	2:G:25:LEU:HD12	2.00	0.43
2:E:207:LEU:HD23	2:E:207:LEU:HA	1.82	0.43
2:F:50:ILE:HD12	2:F:97:LEU:HD13	2.00	0.43
2:J:269:GLY:N	2:J:286:ILE:O	2.51	0.43
2:H:32:PRO:HD2	2:H:35:LEU:HD22	1.99	0.43
2:H:233:LEU:HD23	2:H:233:LEU:HA	1.88	0.43
1:A:156:VAL:HB	1:A:166:HIS:HB3	1.99	0.43
2:G:6:LEU:H	2:G:6:LEU:HG	1.68	0.43
2:I:13:ARG:NH2	4:I:401:GTP:O3G	2.49	0.43
2:J:243:ARG:HD2	2:J:255:LEU:HD11	2.00	0.43
1:A:20:LEU:CD1	1:A:20:LEU:H	2.28	0.43
2:F:182:VAL:HG23	2:F:185:ARG:HD2	2.00	0.43
2:G:105:PHE:CD1	2:G:117:PHE:CD1	3.04	0.43
2:J:52:ALA:HB1	2:J:89:PRO:HB3	1.99	0.43
1:A:405:LEU:HD22	1:A:420:LEU:HA	2.00	0.43
1:C:52:GLU:HG3	1:C:79:PRO:HG2	2.00	0.43
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.91	0.43
2:I:251:VAL:HB	2:I:269:GLY:HA2	2.01	0.43
2:J:12:THR:HA	2:J:15:ARG:HD3	1.99	0.43
2:J:307:ILE:HB	2:J:325:VAL:HG13	2.01	0.43
2:L:172:ASN:HD21	2:L:176:TYR:HE2	1.65	0.43
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.85	0.43
1:A:376:LYS:HG3	1:A:381:LEU:HD11	2.00	0.43
2:L:52:ALA:HB1	2:L:80:GLU:OE1	2.18	0.43
2:L:215:PHE:HA	2:L:231:LEU:HD13	1.99	0.43
2:H:13:ARG:HE	2:H:221:GLN:HG2	1.83	0.43
1:D:42:GLU:OE2	1:D:269:HIS:NE2	2.51	0.43
1:D:376:LYS:HB2	1:D:381:LEU:HD21	1.99	0.43
2:H:146:VAL:CG1	2:H:160:VAL:HG11	2.49	0.43
1:D:400:LEU:HD23	1:D:415:THR:HG23	2.01	0.43
2:L:94:ARG:HE	2:L:94:ARG:HB2	1.60	0.43
1:C:140:LEU:HB3	1:C:181:CYS:HB2	2.01	0.43
2:F:84:LEU:HA	2:F:190:PRO:HB3	2.01	0.43
2:G:63:GLU:HG3	2:G:67:GLN:HE21	1.84	0.43
2:J:212:LEU:HD23	2:J:212:LEU:HA	1.84	0.43



	ious page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:320:MET:HG2	2:K:338:LEU:HD12	2.01	0.43
2:E:54:SER:O	2:E:54:SER:OG	2.34	0.43
2:F:269:GLY:HA3	2:F:287:ARG:HG3	2.01	0.43
2:F:305:SER:O	2:F:323:VAL:HA	2.18	0.43
2:G:115:PHE:HA	2:G:116:PRO:HD3	1.69	0.43
2:J:184:GLN:H	2:J:184:GLN:HG3	1.67	0.43
1:A:347:VAL:HA	1:A:393:ILE:HB	2.00	0.42
1:D:78:LEU:HD12	1:D:79:PRO:HD2	2.00	0.42
2:K:37:GLN:NE2	2:K:108:ASN:O	2.46	0.42
2:L:287:ARG:O	2:L:304:GLU:HA	2.19	0.42
2:L:305:SER:O	2:L:323:VAL:HA	2.19	0.42
2:H:22:PRO:HD2	2:H:25:LEU:HD12	2.00	0.42
1:C:4:ALA:HB3	1:C:53:ILE:HG12	2.00	0.42
1:D:265:TYR:CE2	1:D:272:ARG:HD3	2.54	0.42
2:I:233:LEU:HD22	2:I:233:LEU:HA	1.87	0.42
2:K:132:SER:O	2:K:176:TYR:HA	2.18	0.42
2:L:320:MET:HG2	2:L:338:LEU:HB2	2.01	0.42
2:H:165:VAL:HG23	2:H:166:PHE:H	1.84	0.42
2:E:254:VAL:HG12	2:E:272:VAL:HB	2.01	0.42
2:E:310:TRP:HB2	2:E:328:GLU:HG3	2.00	0.42
1:C:359:ASP:HA	1:C:369:MET:CE	2.49	0.42
2:H:162:LYS:HD2	2:H:162:LYS:HA	1.68	0.42
2:J:7:VAL:CG2	2:J:53:VAL:CA	2.94	0.42
2:H:162:LYS:CB	2:H:163:PRO:CD	2.97	0.42
2:G:178:LEU:HD13	2:G:182:VAL:HG11	2.01	0.42
2:J:289:CYS:SG	2:J:306:CYS:N	2.93	0.42
2:H:74:ARG:HH21	2:H:76:SER:HB3	1.84	0.42
2:G:105:PHE:CD1	2:G:117:PHE:HD1	2.29	0.42
2:F:5:ILE:HD13	2:F:107:LEU:HB2	2.01	0.42
1:D:15:THR:O	1:D:18:ARG:HD3	2.20	0.42
2:K:14:LEU:O	2:K:18:THR:OG1	2.37	0.42
2:L:298:ARG:HD3	2:L:315:GLY:HA2	2.02	0.42
2:I:25:LEU:HD11	2:I:63:GLU:HG3	2.02	0.42
2:J:28:PHE:N	2:J:31:LYS:O	2.47	0.42
2:H:146:VAL:HG12	2:H:160:VAL:HG11	2.02	0.42
2:E:116:PRO:O	2:E:120:MET:HB2	2.19	0.42
2:F:142:SER:HA	2:F:164:GLN:HA	2.01	0.42
2:F:267:SER:OG	2:F:287:ARG:NH1	2.53	0.42
1:C:389:CYS:H	1:C:406:PRO:HB3	1.84	0.41
2:F:203:LYS:HA	2:F:203:LYS:HD2	1.85	0.41
2:I:173:ALA:O	2:I:216:TRP:NE1	2.53	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:276:PRO:HG2	2:H:293:ARG:HB2	2.01	0.41
1:A:13:LYS:HD2	1:A:13:LYS:HA	1.78	0.41
2:E:182:VAL:HA	2:E:185:ARG:HB2	2.00	0.41
1:C:127:LEU:HD12	1:C:127:LEU:HA	1.93	0.41
2:F:14:LEU:HD22	2:F:17:LEU:HD12	2.01	0.41
2:F:15:ARG:HD2	2:F:15:ARG:HA	1.78	0.41
2:G:60:LEU:O	2:G:64:MET:HG2	2.20	0.41
2:J:276:PRO:HG2	2:J:293:ARG:HG3	2.02	0.41
2:K:110:ASP:OD2	2:K:110:ASP:N	2.43	0.41
2:L:129:GLN:HG3	2:L:208:TYR:CE2	2.55	0.41
1:A:318:ARG:HB2	2:H:317:TRP:CE2	2.56	0.41
2:E:264:GLN:H	2:E:264:GLN:HG3	1.43	0.41
1:C:404:VAL:HG22	1:C:419:ILE:HD12	2.02	0.41
2:F:292:LEU:HD12	2:F:309:GLY:HA2	2.02	0.41
2:G:320:MET:HB3	2:G:324:THR:HG21	2.02	0.41
2:I:84:LEU:H	2:I:190:PRO:HG3	1.86	0.41
2:J:237:ARG:HE	2:J:237:ARG:HB2	1.76	0.41
1:B:18:ARG:O	1:B:18:ARG:HG3	2.20	0.41
1:D:156:VAL:HB	1:D:166:HIS:HB3	2.02	0.41
2:F:97:LEU:HB3	2:F:183:LEU:HD21	2.02	0.41
2:J:335:GLU:OE1	2:L:287:ARG:NH2	2.53	0.41
2:L:231:LEU:HD23	2:L:231:LEU:HA	1.55	0.41
2:E:321:GLU:OE2	2:E:337:TYR:CE1	2.70	0.41
2:F:260:ALA:HB1	2:F:278:VAL:HG22	2.03	0.41
2:I:163:PRO:HG2	2:I:167:VAL:HG21	0.47	0.41
2:J:33:ILE:HG12	2:J:219:ILE:HD11	2.02	0.41
2:J:189:GLN:H	2:J:189:GLN:HG3	1.64	0.41
2:K:358:ILE:HD13	2:L:360:MET:HB2	2.02	0.41
2:L:229:MET:O	2:L:232:PHE:HB3	2.20	0.41
2:H:291:VAL:HG13	2:H:308:VAL:HB	2.02	0.41
1:A:37:ILE:HA	1:A:40:HIS:CD2	2.56	0.41
1:B:196:ASP:HB3	1:B:200:ARG:HH21	1.86	0.41
1:D:364:ASP:OD2	1:D:365:PRO:CD	2.69	0.41
2:G:27:ASP:HA	2:G:32:PRO:HA	2.03	0.41
2:K:49:VAL:CG1	2:K:75:ILE:HG22	2.51	0.41
2:K:67:GLN:HA	2:K:70:ARG:HB2	2.03	0.41
2:K:221:GLN:O	2:K:225:PHE:N	2.50	0.41
2:L:223:LYS:HE3	2:L:223:LYS:HB2	1.82	0.41
2:H:27:ASP:HA	2:H:32:PRO:HA	2.02	0.41
2:F:134:LEU:HB2	2:F:175:MET:HB2	2.03	0.41
2:F:186:ILE:H	2:F:186:ILE:HG13	1.75	0.41



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:312:THR:O	1:B:312:THR:OG1	2.38	0.40
2:E:70:ARG:HH11	2:E:70:ARG:HD2	1.75	0.40
2:G:7:VAL:HG21	2:G:51:LEU:HD12	2.02	0.40
2:J:268:ILE:HG22	2:J:272:VAL:HG11	2.02	0.40
1:A:386:ILE:HB	1:A:403:ILE:HG23	2.03	0.40
2:L:14:LEU:O	2:L:14:LEU:CG	2.70	0.40
1:A:198:PHE:CZ	1:D:100:ASP:HB3	2.56	0.40
1:B:186:PHE:HZ	1:B:222:LEU:HD21	1.86	0.40
2:E:71:LEU:HD23	2:E:71:LEU:HA	1.89	0.40
1:C:361:ASN:HA	1:C:362:PRO:HD3	1.97	0.40
2:G:15:ARG:HD2	2:G:15:ARG:HA	1.89	0.40
2:H:141:PRO:CB	2:H:164:GLN:HE22	2.25	0.40
2:H:236:LEU:HB3	2:H:244:LEU:HD21	2.02	0.40
2:G:107:LEU:HD21	2:G:117:PHE:HE1	1.86	0.40
2:J:7:VAL:HG23	2:J:8:GLY:N	2.35	0.40
2:L:110:ASP:OD2	2:L:110:ASP:N	2.46	0.40
2:L:237:ARG:HD3	2:L:237:ARG:HA	1.88	0.40
2:H:70:ARG:HH11	2:H:70:ARG:HD2	1.77	0.40
1:A:358:SER:O	1:A:369:MET:HE2	2.21	0.40
1:B:170:LYS:HE3	1:B:170:LYS:HB2	1.94	0.40
1:D:10:GLY:H	1:D:13:LYS:HB2	1.86	0.40
2:K:14:LEU:HD12	2:K:222:PRO:HG3	2.03	0.40
2:K:118:GLN:HA	2:K:121:VAL:HG12	2.03	0.40
2:L:25:LEU:HA	2:L:32:PRO:HB3	2.03	0.40
2:L:139:GLU:HB3	2:L:140:GLU:OE2	2.20	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	Percent	tiles
1	А	403/420~(96%)	383~(95%)	20~(5%)	0	100 1	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	402/420~(96%)	381 (95%)	20~(5%)	1 (0%)	47	82
1	С	402/420~(96%)	381 (95%)	21 (5%)	0	100	100
1	D	402/420~(96%)	387~(96%)	15 (4%)	0	100	100
2	Ε	358/360~(99%)	325 (91%)	31 (9%)	2(1%)	25	64
2	F	346/360~(96%)	322~(93%)	24 (7%)	0	100	100
2	G	358/360~(99%)	331 (92%)	26~(7%)	1 (0%)	41	76
2	Н	358/360~(99%)	333~(93%)	24 (7%)	1 (0%)	41	76
2	Ι	358/360~(99%)	333~(93%)	24 (7%)	1 (0%)	41	76
2	J	358/360~(99%)	343~(96%)	14 (4%)	1 (0%)	41	76
2	Κ	358/360~(99%)	323 (90%)	31 (9%)	4 (1%)	14	50
2	L	358/360~(99%)	326 (91%)	31 (9%)	1 (0%)	41	76
All	All	4461/4560 (98%)	4168 (93%)	281 (6%)	12 (0%)	44	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Е	143	LYS
2	G	116	PRO
2	Κ	72	GLY
2	Κ	164	GLN
2	J	11	GLY
2	Κ	160	VAL
1	В	360	PRO
2	Ι	167	VAL
2	Н	162	LYS
2	Κ	167	VAL
2	Е	141	PRO
2	L	8	GLY

### 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	entiles
1	А	344/354~(97%)	320~(93%)	24 (7%)	15	47
1	В	344/354~(97%)	321 (93%)	23~(7%)	16	49
1	С	344/354~(97%)	323 (94%)	21 (6%)	18	53
1	D	344/354~(97%)	323 (94%)	21 (6%)	18	53
2	Е	310/311 (100%)	278 (90%)	32 (10%)	7	28
2	F	303/311~(97%)	269~(89%)	34 (11%)	6	24
2	G	311/311~(100%)	280 (90%)	31 (10%)	7	29
2	Н	311/311 (100%)	284 (91%)	27 (9%)	10	37
2	Ι	311/311~(100%)	273~(88%)	38 (12%)	5	21
2	J	311/311 (100%)	279~(90%)	32 (10%)	7	28
2	K	309/311~(99%)	275~(89%)	34 (11%)	6	25
2	L	309/311~(99%)	273 (88%)	36 (12%)	5	22
All	All	3851/3904 (99%)	3498 (91%)	353 (9%)	13	34

All (353) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	12	GLN
1	А	13	LYS
1	А	15	THR
1	А	20	LEU
1	А	118	CYS
1	А	120	ASP
1	А	142	THR
1	А	169	GLU
1	А	172	SER
1	А	173	THR
1	А	238	VAL
1	А	247	GLN
1	А	253	SER
1	А	258	SER
1	А	264	ARG
1	А	276	HIS
1	А	298	SER
1	А	306	SER
1	А	337	LEU
1	А	356	THR
1	А	359	ASP
1	А	376	LYS



Mol	Chain	Res	Type
1	А	411	SER
1	А	413	SER
1	В	1	MET
1	В	2	LEU
1	В	18	ARG
1	В	118	CYS
1	В	142	THR
1	В	143	THR
1	В	160	GLN
1	В	168	VAL
1	В	219	THR
1	В	221	ARG
1	В	225	ASP
1	В	238	VAL
1	В	264	ARG
1	В	275	LYS
1	В	309	LYS
1	В	358	SER
1	В	373	SER
1	В	377	ASP
1	В	389	CYS
1	В	390	ARG
1	В	397	VAL
1	В	398	LEU
1	В	411	SER
2	Е	51	LEU
2	Е	54	SER
2	Е	64	MET
2	Е	68	GLU
2	Е	75	ILE
2	Е	78	SER
2	Е	86	THR
2	Е	109	SER
2	Е	114	ASP
2	E	122	GLN
2	E	126	HIS
2	Е	134	LEU
2	Е	140	GLU
2	E	147	VAL
2	Е	149	CYS
2	Е	158	ARG
2	Е	159	PHE



Mol	Chain	Res	Type
2	Е	160	VAL
2	Е	188	LEU
2	Е	192	SER
2	Е	194	GLU
2	Е	199	PRO
2	Е	203	LYS
2	Е	235	SER
2	Е	240	GLN
2	Е	257	ASP
2	Е	264	GLN
2	Е	267	SER
2	Е	279	VAL
2	E	299	SER
2	Е	348	SER
2	Е	359	ILE
1	C	1	MET
1	С	2	LEU
1	С	63	GLU
1	С	142	THR
1	С	149	SER
1	С	160	GLN
1	С	172	SER
1	С	173	THR
1	С	187	SER
1	С	219	THR
1	С	253	SER
1	С	264	ARG
1	С	298	SER
1	C	329	THR
1	С	356	THR
1	С	361	ASN
1	С	370	ASP
1	С	374	LEU
1	С	389	CYS
1	С	392	ARG
1	С	408	LYS
1	D	1	MET
1	D	18	ARG
1	D	62	ASP
1	D	118	CYS
1	D	142	THR
1	D	168	VAL



Mol	Chain	Res	Type
1	D	187	SER
1	D	219	THR
1	D	228	SER
1	D	238	VAL
1	D	246	SER
1	D	253	SER
1	D	258	SER
1	D	276	HIS
1	D	292	THR
1	D	312	THR
1	D	354	GLU
1	D	366	ARG
1	D	371	SER
1	D	392	ARG
1	D	397	VAL
2	F	7	VAL
2	F	13	ARG
2	F	27	ASP
2	F	35	LEU
2	F	62	LYS
2	F	65	LYS
2	F	78	SER
2	F	86	THR
2	F	95	ASP
2	F	96	LEU
2	F	109	SER
2	F	113	CYS
2	F	120	MET
2	F	130	GLU
2	F	132	SER
2	F	138	VAL
2	F	139	GLU
2	F	168	SER
2	F	175	MET
2	F	177	ILE
2	F	184	GLN
2	F	186	ILE
2	F	199	PRO
2	F	211	GLU
2	F	227	THR
2	F	243	ARG
2	F	246	SER



Mol	Chain	Res	Type
2	F	257	ASP
2	F	261	ARG
2	F	273	SER
2	F	306	CYS
2	F	334	ASP
2	F	347	LYS
2	F	348	SER
2	G	6	LEU
2	G	20	SER
2	G	31	LYS
2	G	39	GLU
2	G	47	ASP
2	G	48	HIS
2	G	55	TYR
2	G	81	GLU
2	G	82	GLU
2	G	86	THR
2	G	96	LEU
2	G	98	SER
2	G	102	ASP
2	G	152	ASP
2	G	157	HIS
2	G	164	GLN
2	G	179	SER
2	G	184	GLN
2	G	186	ILE
2	G	191	THR
2	G	192	SER
2	G	199	PRO
2	G	207	LEU
2	G	212	LEU
2	G	237	ARG
2	G	267	SER
2	G	279	VAL
2	G	294	ASP
2	G	306	CYS
2	G	324	THR
2	G	344	LEU
2	Ι	6	LEU
2	Ι	10	TYR
2	Ι	20	SER
2	Ι	63	GLU



Mol	Chain	Res	Type
2	Ι	65	LYS
2	Ι	75	ILE
2	Ι	80	GLU
2	Ι	90	LEU
2	Ι	92	LEU
2	Ι	95	ASP
2	Ι	98	SER
2	Ι	106	VAL
2	Ι	143	LYS
2	Ι	149	CYS
2	Ι	152	ASP
2	Ι	155	ARG
2	Ι	157	HIS
2	Ι	158	ARG
2	Ι	165	VAL
2	Ι	175	MET
2	Ι	179	SER
2	Ι	184	GLN
2	Ι	191	THR
2	Ι	199	PRO
2	Ι	200	ILE
2	Ι	207	LEU
2	Ι	224	ASP
2	Ι	233	LEU
2	Ι	234	GLN
2	Ι	235	SER
2	Ι	236	LEU
2	Ι	253	ASN
2	Ι	257	ASP
2	Ι	266	CYS
2	Ι	279	VAL
2	Ι	296	ARG
2	Ι	319	ARG
2	I	360	MET
2	J	31	LYS
2	J	34	LEU
2	J	54	SER
2	J	60	LEU
2	J	62	LYS
2	J	77	MET
2	J	100	THR
2	J	107	LEU



Mol	Chain	Res	Type
2	J	109	SER
2	J	114	ASP
2	J	129	GLN
2	J	139	GLU
2	J	152	ASP
2	J	153	THR
2	J	160	VAL
2	J	161	GLU
2	J	172	ASN
2	J	177	ILE
2	J	179	SER
2	J	186	ILE
2	J	188	LEU
2	J	198	PHE
2	J	223	LYS
2	J	237	ARG
2	J	240	GLN
2	J	272	VAL
2	J	288	ARG
2	J	290	THR
2	J	299	SER
2	J	305	SER
2	J	323	VAL
2	J	352	SER
2	K	5	ILE
2	K	6	LEU
2	K	13	ARG
2	K	20	SER
2	K	54	SER
2	К	57	SER
2	Κ	71	LEU
2	K	75	ILE
2	К	76	SER
2	Κ	92	LEU
2	Κ	94	ARG
2	K	95	ASP
2	K	106	VAL
2	K	109	SER
2	K	113	CYS
2	К	118	GLN
2	Κ	125	ARG
2	K	138	VAL



Mol	Chain	Res	Type
2	K	146	VAL
2	K	158	ARG
2	K	159	PHE
2	K	160	VAL
2	K	162	LYS
2	K	171	ILE
2	K	177	ILE
2	K	194	GLU
2	K	201	MET
2	K	243	ARG
2	K	266	CYS
2	K	273	SER
2	K	282	ASP
2	K	301	SER
2	Κ	342	SER
2	K	348	SER
2	L	14	LEU
2	L	20	SER
2	L	21	THR
2	L	31	LYS
2	L	33	ILE
2	L	54	SER
2	L	60	LEU
2	L	78	SER
2	L	86	THR
2	L	90	LEU
2	L	98	SER
2	L	100	THR
2	L	120	MET
2	L	142	SER
2	L	148	VAL
2	L	149	CYS
2	L	152	ASP
2	L	156	ILE
2	L	159	PHE
2	L	169	ASN
2	L	175	MET
2	L	176	TYR
2	L	199	PRO
2	L	210	MET
2	L	212	LEU
2	L	231	LEU



Mol	Chain	Res	Type
2	L	255	LEU
2	L	257	ASP
2	L	261	ARG
2	L	266	CYS
2	L	282	ASP
2	L	288	ARG
2	L	324	THR
2	L	342	SER
2	L	347	LYS
2	L	352	SER
2	Н	54	SER
2	Н	57	SER
2	Н	60	LEU
2	Н	69	GLN
2	Н	84	LEU
2	Н	92	LEU
2	Н	102	ASP
2	Н	106	VAL
2	Н	112	ILE
2	Н	113	CYS
2	Н	114	ASP
2	Н	138	VAL
2	Н	143	LYS
2	Н	149	CYS
2	Н	159	PHE
2	Н	160	VAL
2	Н	162	LYS
2	Н	176	TYR
2	Н	188	LEU
2	Н	199	PRO
2	Н	245	CYS
2	Н	265	ASN
2	Н	266	CYS
2	Н	267	SER
2	Н	271	ASN
2	Н	278	VAL
2	Н	299	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

$1 \qquad A \qquad 40 \qquad HIS$	е
1 A 40 IIIS	



Mol	Chain	Res	Type
1	А	60	GLN
1	А	73	GLN
1	А	135	HIS
1	А	145	ASN
1	А	158	ASN
1	А	286	ASN
1	А	331	GLN
1	А	363	ASN
1	А	401	ASN
1	А	417	GLN
1	В	12	GLN
1	В	40	HIS
1	В	51	GLN
1	В	201	ASN
1	В	286	ASN
1	В	401	ASN
2	Е	67	GLN
2	Е	79	HIS
2	Е	316	GLN
2	Е	339	ASN
1	С	40	HIS
1	С	46	GLN
1	С	67	GLN
1	С	148	GLN
1	С	266	GLN
1	С	304	ASN
1	С	363	ASN
1	С	401	ASN
1	D	12	GLN
1	D	40	HIS
1	D	51	GLN
1	D	135	HIS
1	D	145	ASN
1	D	201	ASN
1	D	276	HIS
1	D	286	ASN
1	D	338	HIS
1	D	401	ASN
2	F	69	GLN
2	G	37	GLN
2	G	67	GLN
2	G	118	GLN



Mol	Chain	Res	Type
2	G	316	GLN
2	Ι	346	HIS
2	J	172	ASN
2	Κ	48	HIS
2	Κ	67	GLN
2	Κ	122	GLN
2	L	48	HIS
2	L	322	ASN
2	L	339	ASN
2	L	346	HIS
2	Н	30	ASN
2	Н	127	HIS
2	Н	221	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)

12 ligands are 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 Ch	Chain	Chain	Dec	Pog Link	Bond lengths			Bond angles		
	Unam	Chain Res		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
4	GTP	L	401	-	26,34,34	1.20	2 (7%)	32,54,54	1.28	3 (9%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	B	ond ang	les
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	GTP	Е	401	-	26,34,34	0.98	1 (3%)	32,54,54	1.47	4 (12%)
4	GTP	J	401	-	26,34,34	1.04	1 (3%)	32,54,54	1.78	5 (15%)
4	GTP	D	501	-	26,34,34	1.06	1 (3%)	32,54,54	1.63	6 (18%)
4	GTP	К	401	2	26,34,34	1.04	1 (3%)	32,54,54	1.54	4 (12%)
4	GTP	В	501	-	26,34,34	1.11	1 (3%)	32,54,54	1.53	5 (15%)
3	GDD	С	501	-	35,42,42	0.98	2 (5%)	46,65,65	1.37	6 (13%)
4	GTP	Н	401	2	26,34,34	0.98	1 (3%)	32,54,54	1.54	5 (15%)
4	GTP	G	401	2	26,34,34	1.02	1 (3%)	32,54,54	1.70	5 (15%)
3	GDD	А	501	-	35,42,42	0.97	1 (2%)	46,65,65	1.37	6 (13%)
4	GTP	F	401	-	26,34,34	1.04	1 (3%)	32,54,54	1.54	4 (12%)
4	GTP	Ι	401	-	26,34,34	1.02	1 (3%)	32,54,54	1.59	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	L	401	-	-	4/18/38/38	0/3/3/3
4	GTP	Е	401	-	-	1/18/38/38	0/3/3/3
4	GTP	J	401	-	-	7/18/38/38	0/3/3/3
4	GTP	D	501	-	-	8/18/38/38	0/3/3/3
4	GTP	К	401	2	-	5/18/38/38	0/3/3/3
4	GTP	В	501	-	-	3/18/38/38	0/3/3/3
3	GDD	С	501	-	-	11/19/59/59	0/4/4/4
4	GTP	Н	401	2	-	8/18/38/38	0/3/3/3
4	GTP	G	401	2	-	6/18/38/38	0/3/3/3
3	GDD	А	501	-	-	6/19/59/59	0/4/4/4
4	GTP	F	401	-	-	5/18/38/38	0/3/3/3
4	GTP	Ι	401	-	-	7/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	L	401	GTP	C5-C6	-3.77	1.39	1.47
3	А	501	GDD	C5-C6	-3.69	1.39	1.47
3	С	501	GDD	C5-C6	-3.57	1.40	1.47



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	401	GTP	C5-C6	-3.39	1.40	1.47
4	В	501	GTP	C5-C6	-3.38	1.40	1.47
4	J	401	GTP	C5-C6	-3.28	1.40	1.47
4	F	401	GTP	C5-C6	-3.22	1.40	1.47
4	Κ	401	GTP	C5-C6	-3.21	1.40	1.47
4	D	501	GTP	C5-C6	-3.21	1.40	1.47
4	Е	401	GTP	C5-C6	-3.16	1.41	1.47
4	L	401	GTP	C6-N1	-3.11	1.33	1.37
4	Н	401	GTP	C5-C6	-3.06	1.41	1.47
4	I	401	GTP	C5-C6	-2.93	1.41	1.47
3	С	501	GDD	C6-N1	-2.02	1.34	1.37

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Ι	401	GTP	C2-N1-C6	-5.32	115.31	125.10
4	В	501	GTP	C2-N1-C6	-5.26	115.41	125.10
4	G	401	GTP	C2-N1-C6	-5.17	115.58	125.10
4	D	501	GTP	C2-N1-C6	-5.10	115.71	125.10
4	J	401	GTP	C2-N1-C6	-5.10	115.71	125.10
4	F	401	GTP	C2-N1-C6	-5.09	115.72	125.10
4	Κ	401	GTP	C2-N1-C6	-5.07	115.77	125.10
4	Е	401	GTP	C2-N1-C6	-5.02	115.85	125.10
4	Н	401	GTP	C2-N1-C6	-4.98	115.93	125.10
3	А	501	GDD	C2-N1-C6	-4.80	116.27	125.10
4	J	401	GTP	C5-C6-N1	4.39	121.70	113.95
3	С	501	GDD	C2-N1-C6	-4.35	117.09	125.10
4	J	401	GTP	O4'-C1'-C2'	-4.23	100.75	106.93
4	G	401	GTP	C5-C6-N1	4.22	121.40	113.95
4	L	401	GTP	C2-N1-C6	-4.03	117.67	125.10
4	F	401	GTP	C5-C6-N1	3.91	120.86	113.95
4	Κ	401	GTP	C5-C6-N1	3.90	120.84	113.95
4	В	501	GTP	C5-C6-N1	3.84	120.73	113.95
4	Н	401	GTP	C5-C6-N1	3.81	120.68	113.95
4	Ι	401	GTP	C5-C6-N1	3.69	120.47	113.95
4	D	501	GTP	C5-C6-N1	3.65	120.40	113.95
4	Е	401	GTP	C5-C6-N1	3.55	120.22	113.95
3	А	501	GDD	C5-C6-N1	3.49	120.11	113.95
3	С	501	GDD	C5-C6-N1	3.46	120.06	113.95
4	J	401	GTP	O6-C6-C5	-3.24	118.05	124.37
4	L	401	GTP	C5-C6-N1	3.13	119.48	113.95
4	G	401	GTP	O6-C6-C5	-3.04	118.43	124.37



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	401	GTP	C8-N7-C5	2.88	108.48	102.99
4	K	401	GTP	C8-N7-C5	2.88	108.47	102.99
4	D	501	GTP	C8-N7-C5	2.87	108.47	102.99
3	А	501	GDD	C8-N7-C5	2.80	108.33	102.99
3	С	501	GDD	C8-N7-C5	2.80	108.32	102.99
4	Н	401	GTP	C8-N7-C5	2.76	108.25	102.99
4	G	401	GTP	C8-N7-C5	2.74	108.21	102.99
4	В	501	GTP	O6-C6-C5	-2.72	119.06	124.37
4	Ι	401	GTP	C8-N7-C5	2.69	108.11	102.99
3	А	501	GDD	O6-C6-C5	-2.68	119.14	124.37
4	G	401	GTP	O2'-C2'-C3'	-2.67	103.20	111.82
4	Е	401	GTP	C8-N7-C5	2.63	108.00	102.99
4	L	401	GTP	C8-N7-C5	2.62	107.97	102.99
3	С	501	GDD	O6-C6-C5	-2.52	119.45	124.37
4	Н	401	GTP	O6-C6-C5	-2.52	119.45	124.37
4	D	501	GTP	O6-C6-C5	-2.49	119.50	124.37
4	Ι	401	GTP	O6-C6-C5	-2.49	119.51	124.37
3	С	501	GDD	C61-C51-C41	-2.44	107.30	113.00
4	K	401	GTP	O6-C6-C5	-2.39	119.69	124.37
4	F	401	GTP	O6-C6-C5	-2.39	119.71	124.37
4	Е	401	GTP	O6-C6-C5	-2.38	119.71	124.37
3	А	501	GDD	N2-C2-N3	-2.35	115.16	119.74
3	С	501	GDD	N2-C2-N3	-2.27	115.32	119.74
4	Ι	401	GTP	N1-C2-N3	2.26	127.54	123.32
4	J	401	GTP	C8-N7-C5	2.25	107.29	102.99
3	А	501	GDD	O31-C31-C21	-2.23	105.20	110.35
4	В	501	GTP	C8-N7-C5	2.16	107.11	102.99
4	D	501	GTP	O4'-C1'-C2'	2.13	110.04	106.93
4	H	401	GTP	C3'-C2'-C1'	2.09	104.13	100.98
4	В	501	GTP	N1-C2-N3	2.03	127.12	123.32
4	D	501	GTP	N1-C2-N3	2.03	127.11	123.32
4	Ι	401	GTP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	501	GDD	O4'-C4'-C5'-O5'
3	С	501	GDD	C5'-O5'-PA-O2A
3	С	501	GDD	C5'-O5'-PA-O3A
3	С	501	GDD	C11-O1B-PB-O3A
4	В	501	GTP	O4'-C4'-C5'-O5'



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Mol	Chain	Res	Type	Atoms
4	D	501	GTP	C5'-O5'-PA-O3A
4	G	401	GTP	PB-O3B-PG-O3G
4	G	401	GTP	C5'-O5'-PA-O1A
4	G	401	GTP	C5'-O5'-PA-O2A
4	Ι	401	GTP	PB-O3A-PA-O5'
4	Ι	401	GTP	C5'-O5'-PA-O3A
4	Ι	401	GTP	C5'-O5'-PA-O1A
4	Ι	401	GTP	C5'-O5'-PA-O2A
4	J	401	GTP	PB-O3B-PG-O2G
4	J	401	GTP	PB-O3B-PG-O3G
4	J	401	GTP	C5'-O5'-PA-O1A
4	J	401	GTP	C5'-O5'-PA-O2A
4	L	401	GTP	C5'-O5'-PA-O1A
4	L	401	GTP	C5'-O5'-PA-O2A
4	Н	401	GTP	C5'-O5'-PA-O1A
4	Н	401	GTP	O4'-C4'-C5'-O5'
4	Н	401	GTP	C3'-C4'-C5'-O5'
3	С	501	GDD	C3'-C4'-C5'-O5'
4	F	401	GTP	O4'-C4'-C5'-O5'
4	K	401	GTP	O4'-C4'-C5'-O5'
3	A	501	GDD	C3'-C4'-C5'-O5'
3	А	501	GDD	O4'-C4'-C5'-O5'
4	В	501	GTP	C3'-C4'-C5'-O5'
4	Ι	401	GTP	O4'-C4'-C5'-O5'
4	Ι	401	GTP	C3'-C4'-C5'-O5'
3	А	501	GDD	C41-C51-C61-O6A
4	D	501	GTP	C3'-C4'-C5'-O5'
4	F	401	GTP	C3'-C4'-C5'-O5'
4	K	401	GTP	C3'-C4'-C5'-O5'
4	D	501	GTP	O4'-C4'-C5'-O5'
3	С	501	GDD	O51-C51-C61-O6A
3	А	501	GDD	O51-C51-C61-O6A
4	J	401	GTP	C4'-C5'-O5'-PA
4	Н	401	GTP	C4'-C5'-O5'-PA
3	А	501	GDD	PB-O3A-PA-O5'
3	С	501	GDD	C11-O1B-PB-O3B
4	Н	401	GTP	PA-O3A-PB-O1B
3	С	501	GDD	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
4	Е	401	GTP	O4'-C4'-C5'-O5'
4	L	401	GTP	PB-O3B-PG-O1G
3	С	501	GDD	051-C11-O1B-PB

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Mol	Chain	Res	Type	Atoms
3	С	501	GDD	PA-O3A-PB-O2B
4	Н	401	GTP	PB-O3A-PA-O1A
4	D	501	GTP	PB-O3B-PG-O1G
4	F	401	GTP	PB-O3B-PG-O1G
4	K	401	GTP	PB-O3B-PG-O1G
4	J	401	GTP	PB-O3A-PA-O1A
4	G	401	GTP	PB-O3B-PG-O1G
4	В	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O3G
4	F	401	GTP	PB-O3B-PG-O2G
4	F	401	GTP	PB-O3B-PG-O3G
4	G	401	GTP	PB-O3B-PG-O2G
4	K	401	GTP	PB-O3B-PG-O2G
4	K	401	GTP	PB-O3B-PG-O3G
4	G	401	GTP	C5'-O5'-PA-O3A
4	J	401	GTP	C5'-O5'-PA-O3A
4	L	401	GTP	C5'-O5'-PA-O3A
4	Н	401	GTP	C5'-O5'-PA-O3A
3	С	501	GDD	PA-O3A-PB-O3B
4	D	501	GTP	PA-O3A-PB-O1B
4	Ι	401	GTP	PG-O3B-PB-O2B
4	Н	401	GTP	PA-O3A-PB-O2B
3	А	501	GDD	C5'-O5'-PA-O2A

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There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	401	GTP	5	0
4	Е	401	GTP	1	0
4	J	401	GTP	2	0
4	D	501	GTP	1	0
4	Н	401	GTP	1	0
4	G	401	GTP	2	0
3	А	501	GDD	1	0
4	F	401	GTP	16	0
4	Ι	401	GTP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and 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-30600. 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: 120

Y Index: 120



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: 117

Y Index: 127

Z Index: 116

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



The images above show the 3D surface view of the map at the recommended contour level 0.0389. 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 (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 144  $\rm nm^3;$  this corresponds to an approximate mass of 130 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 0.333  ${\rm \AA^{-1}}$ 



# 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-30600 and PDB model 7D73. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0389 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 (0.0389).



### 9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.



### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0389) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.5717	0.5150	<b>—</b> 10
А	0.8621	0.6130	1.0
В	0.8511	0.6100	
С	0.8400	0.6100	
D	0.8428	0.6100	
E	0.3494	0.4360	
F	0.4648	0.4670	
G	0.4348	0.4770	
Н	0.4233	0.4620	
I	0.3871	0.4490	0.0
J	0.4251	0.4810	<0.0
K	0.4625	0.4650	
L	0.3641	0.4490	

