



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:41 PM GMT

PDB ID : 1UPT  
Title : STRUCTURE OF A COMPLEX OF THE GOLGIN-245 GRIP DOMAIN  
WITH ARL1  
Authors : Panic, B.; Perisic, O.; Veprintsev, D.B.; Williams, R.L.; Munro, S.  
Deposited on : 2003-10-12  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

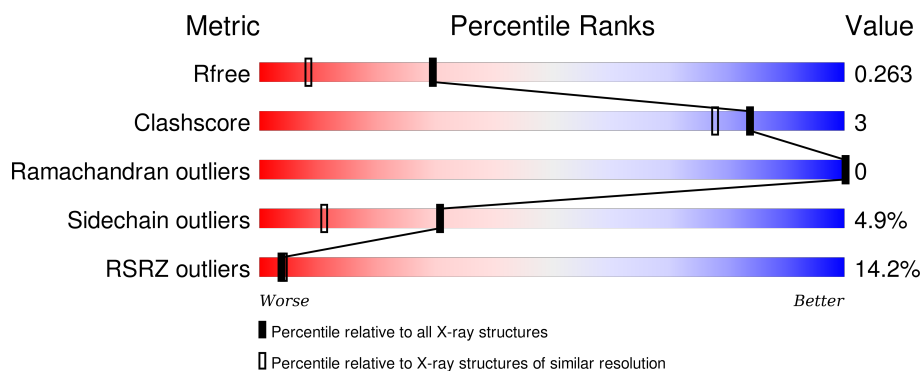
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	<div> <div>13%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	171	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
1	E	171	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	G	171	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	60	<div> <div>18%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	60	<div><div></div><div>7%</div><div>82%</div><div>• •</div><div>13%</div></div>
2	F	60	<div><div></div><div>25%</div><div>78%</div><div>15%</div><div>7%</div></div>
2	H	60	<div><div></div><div>13%</div><div>72%</div><div>13%</div><div>15%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7542 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ADP-RIBOSYLATION FACTOR-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	Se	0	0	0
			1345	854	227	255	2	7			
1	C	163	Total	C	N	O	S	Se	0	0	0
			1291	823	215	245	2	6			
1	E	168	Total	C	N	O	S	Se	0	0	0
			1336	849	225	253	2	7			
1	G	170	Total	C	N	O	S	Se	0	0	0
			1346	854	227	256	2	7			

- Molecule 2 is a protein called GOLGI AUTOANTIGEN, GOLGIN SUBFAMILY A MEMBER 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	58	Total	C	N	O	Se	0	0	0
			487	310	81	92	4			
2	D	52	Total	C	N	O	Se	0	0	0
			434	277	71	82	4			
2	F	56	Total	C	N	O	Se	0	0	0
			475	304	79	88	4			
2	H	51	Total	C	N	O	Se	0	0	0
			426	272	70	81	3			

There are 28 discrepancies between the modelled and reference sequences:

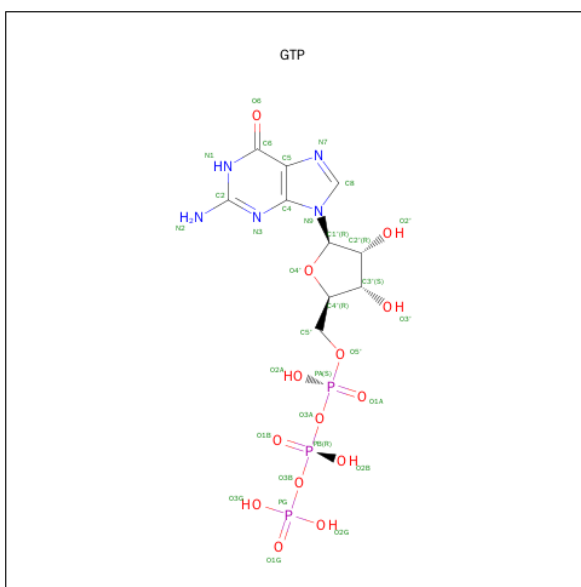
Chain	Residue	Modelled	Actual	Comment	Reference
B	2222	SER	PHE	VARIANT SEE REMARK 99	UNP Q13439
B	2223	TRP	THR	VARIANT SEE REMARK 99	UNP Q13439
B	2224	LEU	SER	VARIANT SEE REMARK 99	UNP Q13439
B	2225	ARG	PRO	VARIANT SEE REMARK 99	UNP Q13439
B	2226	SER	ARG	VARIANT SEE REMARK 99	UNP Q13439
B	2227	SER	SER	VARIANT SEE REMARK 99	UNP Q13439
B	2228	SER	GLY	VARIANT SEE REMARK 99	UNP Q13439
D	2222	SER	PHE	VARIANT SEE REMARK 99	UNP Q13439

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2223	TRP	THR	VARIANT SEE REMARK 99	UNP Q13439
D	2224	LEU	SER	VARIANT SEE REMARK 99	UNP Q13439
D	2225	ARG	PRO	VARIANT SEE REMARK 99	UNP Q13439
D	2226	SER	ARG	VARIANT SEE REMARK 99	UNP Q13439
D	2227	SER	SER	VARIANT SEE REMARK 99	UNP Q13439
D	2228	SER	GLY	VARIANT SEE REMARK 99	UNP Q13439
F	2222	SER	PHE	VARIANT SEE REMARK 99	UNP Q13439
F	2223	TRP	THR	VARIANT SEE REMARK 99	UNP Q13439
F	2224	LEU	SER	VARIANT SEE REMARK 99	UNP Q13439
F	2225	ARG	PRO	VARIANT SEE REMARK 99	UNP Q13439
F	2226	SER	ARG	VARIANT SEE REMARK 99	UNP Q13439
F	2227	SER	SER	VARIANT SEE REMARK 99	UNP Q13439
F	2228	SER	GLY	VARIANT SEE REMARK 99	UNP Q13439
H	2222	SER	PHE	VARIANT SEE REMARK 99	UNP Q13439
H	2223	TRP	THR	VARIANT SEE REMARK 99	UNP Q13439
H	2224	LEU	SER	VARIANT SEE REMARK 99	UNP Q13439
H	2225	ARG	PRO	VARIANT SEE REMARK 99	UNP Q13439
H	2226	SER	ARG	VARIANT SEE REMARK 99	UNP Q13439
H	2227	SER	SER	VARIANT SEE REMARK 99	UNP Q13439
H	2228	SER	GLY	VARIANT SEE REMARK 99	UNP Q13439

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

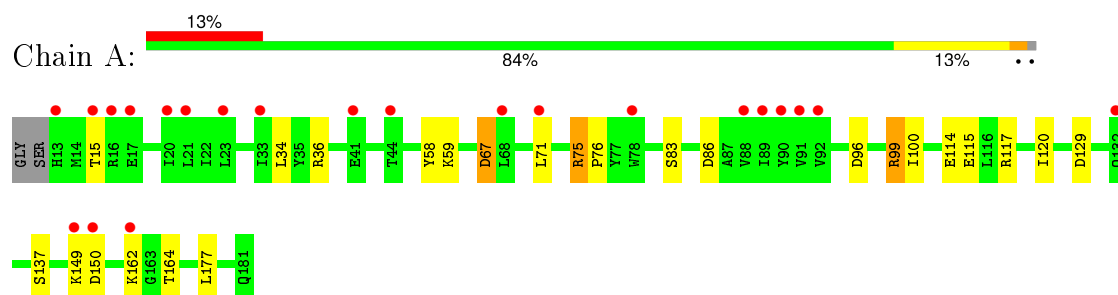
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	15	Total	O	0	0
			15	15		
5	C	34	Total	O	0	0
			34	34		
5	D	5	Total	O	0	0
			5	5		
5	E	96	Total	O	0	0
			96	96		
5	F	8	Total	O	0	0
			8	8		
5	G	54	Total	O	0	0
			54	54		
5	H	8	Total	O	0	0
			8	8		

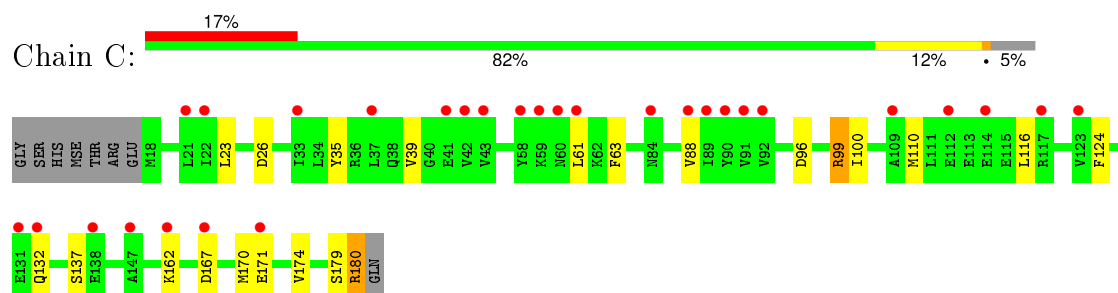
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

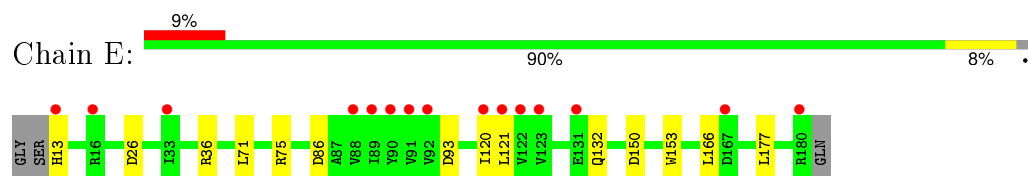
#### • Molecule 1: ADP-RIBOSYLATION FACTOR-LIKE PROTEIN 1



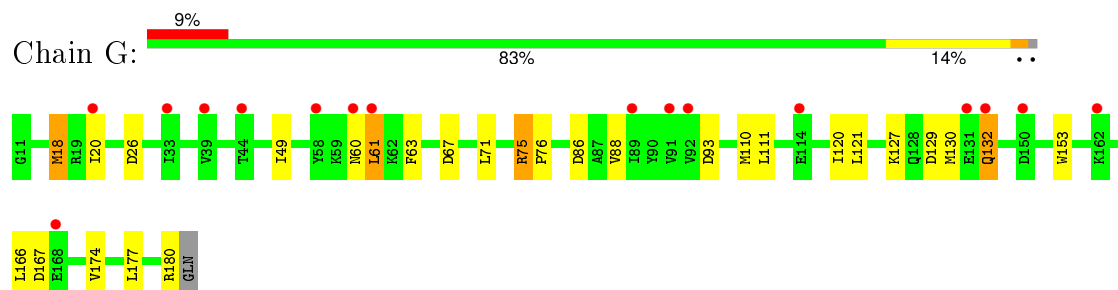
#### • Molecule 1: ADP-RIBOSYLATION FACTOR-LIKE PROTEIN 1



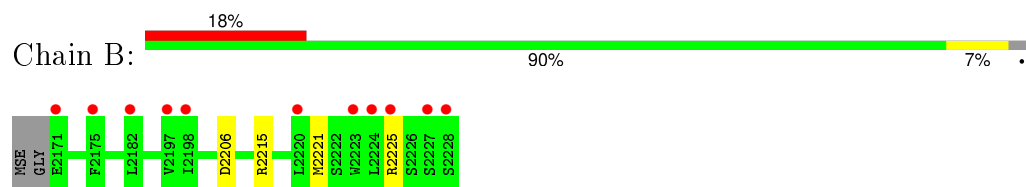
#### • Molecule 1: ADP-RIBOSYLATION FACTOR-LIKE PROTEIN 1



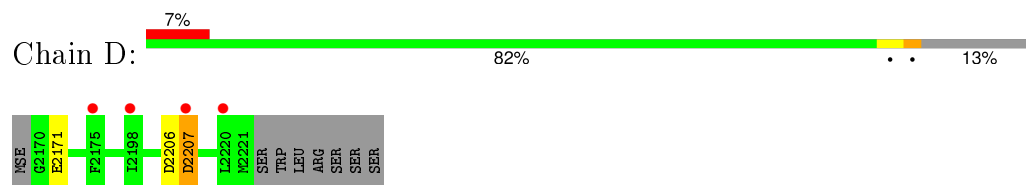
#### • Molecule 1: ADP-RIBOSYLATION FACTOR-LIKE PROTEIN 1



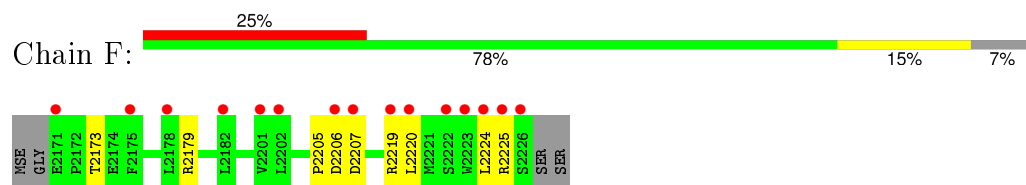
- Molecule 2: GOLGI AUTOANTIGEN, GOLGIN SUBFAMILY A MEMBER 4



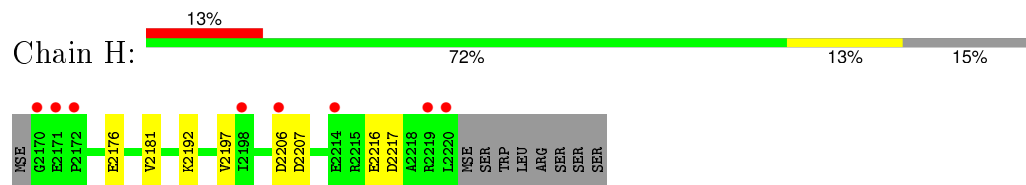
- Molecule 2: GOLGI AUTOANTIGEN, GOLGIN SUBFAMILY A MEMBER 4



- Molecule 2: GOLGI AUTOANTIGEN, GOLGIN SUBFAMILY A MEMBER 4



- Molecule 2: GOLGI AUTOANTIGEN, GOLGIN SUBFAMILY A MEMBER 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.50 Å   89.71 Å   72.53 Å 90.00°   110.69°   90.00°	Depositor
Resolution (Å)	67.42 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (67.42-1.70) 98.3 (19.95-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.221 , 0.252 0.236 , 0.263	Depositor DCC
$R_{free}$ test set	3196 reflections (3.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.8	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 93675 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.6731e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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, 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	A	0.64	0/1359	0.87	5/1824 (0.3%)
1	C	0.56	0/1306	0.84	4/1757 (0.2%)
1	E	0.68	0/1350	0.84	5/1812 (0.3%)
1	G	0.61	0/1360	0.83	5/1825 (0.3%)
2	B	0.61	0/491	0.81	1/651 (0.2%)
2	D	0.61	0/436	0.81	2/576 (0.3%)
2	F	0.61	0/479	0.85	3/635 (0.5%)
2	H	0.62	0/429	0.83	3/569 (0.5%)
All	All	0.62	0/7210	0.84	28/9649 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	G	75	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	75	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	86	ASP	CB-CG-OD2	7.09	124.68	118.30
1	E	86	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	99	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	129	ASP	CB-CG-OD2	6.78	124.40	118.30
1	C	167	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	150	ASP	CB-CG-OD2	6.13	123.82	118.30
2	H	2207	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	150	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	99	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	E	75	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	G	167	ASP	CB-CG-OD2	5.80	123.52	118.30
1	G	129	ASP	CB-CG-OD2	5.77	123.49	118.30
2	H	2217	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	26	ASP	CB-CG-OD2	5.58	123.32	118.30
2	F	2207	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	86	ASP	CB-CG-OD2	5.49	123.24	118.30
2	B	2206	ASP	CB-CG-OD2	5.37	123.14	118.30
2	D	2207	ASP	CB-CG-OD2	5.33	123.10	118.30
2	D	2206	ASP	CB-CG-OD2	5.27	123.05	118.30
2	F	2206	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	26	ASP	CB-CG-OD2	5.14	122.93	118.30
2	H	2206	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	93	ASP	CB-CG-OD1	5.03	122.83	118.30
2	F	2179	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	26	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1345	0	1367	8	0
1	C	1291	0	1317	12	0
1	E	1336	0	1359	3	0
1	G	1346	0	1367	17	0
2	B	487	0	494	0	0
2	D	434	0	443	0	0
2	F	475	0	484	0	0
2	H	426	0	434	3	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	G	32	0	12	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	0	0	0
5	C	34	0	0	0	0
5	D	5	0	0	0	0
5	E	96	0	0	0	0
5	F	8	0	0	0	0
5	G	54	0	0	0	0
5	H	8	0	0	1	0
All	All	7542	0	7313	43	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 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:VAL:HG21	1:G:110:MSE:HE3	1.68	0.74
1:C:170:MSE:HE2	1:C:170:MSE:HA	1.71	0.72
1:C:96:ASP:OD2	1:C:99:ARG:HD3	1.90	0.71
1:C:124:PHE:HZ	1:C:170:MSE:HE3	1.58	0.67
1:G:61:LEU:HD12	1:G:174:VAL:HG13	1.79	0.64
1:A:96:ASP:OD2	1:A:99:ARG:HD3	1.97	0.64
1:G:88:VAL:HG21	1:G:110:MSE:CE	2.32	0.59
1:G:61:LEU:HD13	1:G:63:PHE:CZ	2.39	0.57
1:C:179:SER:O	1:C:180:ARG:HB2	2.06	0.55
1:C:88:VAL:HG21	1:C:110:MSE:CE	2.36	0.54
1:G:110:MSE:HE2	1:G:111:LEU:HD21	1.93	0.51
1:G:18:MSE:HE3	1:G:61:LEU:HD21	1.95	0.49
1:A:83:SER:OG	1:A:115:GLU:OE2	2.31	0.49
1:G:88:VAL:HG11	1:G:110:MSE:HE1	1.94	0.48
2:H:2176:GLU:HG2	5:H:2001:HOH:O	2.12	0.48
1:C:110:MSE:HE2	1:C:116:LEU:HD13	1.95	0.47
1:G:120:ILE:HD12	1:G:177:LEU:HD23	1.96	0.47
1:C:88:VAL:HG21	1:C:110:MSE:HE2	1.96	0.47
1:C:63:PHE:CZ	1:C:174:VAL:HG22	2.50	0.46
1:C:35:TYR:O	1:C:39:VAL:HG22	2.15	0.46
1:G:121:LEU:O	1:G:153:TRP:HA	2.15	0.46
1:A:59:LYS:HB3	5:A:2006:HOH:O	2.14	0.46
1:C:23:LEU:HD12	1:C:110:MSE:HE1	1.97	0.46
1:G:130:MSE:HB3	1:G:132:GLN:HE21	1.80	0.46
1:E:120:ILE:HD12	1:E:177:LEU:HD23	1.98	0.46
1:E:120:ILE:HD12	1:E:177:LEU:CD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:N	1:A:76:PRO:CD	2.79	0.45
1:E:121:LEU:O	1:E:153:TRP:HA	2.17	0.45
1:C:88:VAL:HG21	1:C:110:MSE:HE1	1.99	0.44
1:G:49:ILE:CD1	1:G:71:LEU:HD12	2.48	0.44
1:A:120:ILE:HD12	1:A:177:LEU:HD23	2.00	0.43
1:C:124:PHE:CZ	1:C:170:MSE:HE3	2.46	0.42
1:G:75:ARG:N	1:G:76:PRO:CD	2.82	0.42
1:G:93:ASP:OD1	1:G:127:LYS:HD2	2.19	0.42
1:G:127:LYS:HG2	3:G:1181:GTP:C6	2.53	0.42
1:G:20:ILE:CD1	1:G:63:PHE:CD1	3.03	0.42
1:A:58:TYR:CE2	1:A:59:LYS:HG3	2.55	0.41
2:H:2181:VAL:HG21	2:H:2197:VAL:HG11	2.01	0.41
2:H:2192:LYS:HA	2:H:2216:GLU:HG2	2.03	0.41
1:G:120:ILE:HD12	1:G:177:LEU:CD2	2.51	0.40
1:G:61:LEU:HD13	1:G:63:PHE:HZ	1.87	0.40
1:A:162:LYS:HG2	1:A:164:THR:HG23	2.03	0.40
1:A:34:LEU:HD22	1:A:67:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	C	161/171 (94%)	159 (99%)	2 (1%)	0	100	100
1	E	166/171 (97%)	165 (99%)	1 (1%)	0	100	100
1	G	168/171 (98%)	167 (99%)	1 (1%)	0	100	100
2	B	56/60 (93%)	56 (100%)	0	0	100	100
2	D	50/60 (83%)	50 (100%)	0	0	100	100
2	F	54/60 (90%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	49/60 (82%)	48 (98%)	1 (2%)	0	100	100
All	All	871/924 (94%)	862 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/142 (104%)	139 (94%)	9 (6%)	23	7
1	C	142/142 (100%)	135 (95%)	7 (5%)	31	11
1	E	147/142 (104%)	142 (97%)	5 (3%)	44	21
1	G	148/142 (104%)	141 (95%)	7 (5%)	32	12
2	B	55/51 (108%)	52 (94%)	3 (6%)	27	9
2	D	48/51 (94%)	46 (96%)	2 (4%)	36	14
2	F	53/51 (104%)	47 (89%)	6 (11%)	7	1
2	H	47/51 (92%)	47 (100%)	0	100	100
All	All	788/772 (102%)	749 (95%)	39 (5%)	31	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	36	ARG
1	A	67	ASP
1	A	71	LEU
1	A	100	ILE
1	A	114	GLU
1	A	117	ARG
1	A	137	SER
1	A	149	LYS
2	B	2215	ARG

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Mol	Chain	Res	Type
2	B	2221	MSE
2	B	2225	ARG
1	C	61	LEU
1	C	100	ILE
1	C	132	GLN
1	C	137	SER
1	C	162	LYS
1	C	171	GLU
1	C	180	ARG
2	D	2171	GLU
2	D	2207	ASP
1	E	13	HIS
1	E	36	ARG
1	E	71	LEU
1	E	132	GLN
1	E	166	LEU
2	F	2173	THR
2	F	2205	PRO
2	F	2219	ARG
2	F	2220	LEU
2	F	2224	LEU
2	F	2225	ARG
1	G	18	MSE
1	G	60	ASN
1	G	61	LEU
1	G	67	ASP
1	G	132	GLN
1	G	166	LEU
1	G	180	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	GTP	A	1182	4	25,34,34	1.10	1 (4%)	34,54,54	1.82	7 (20%)
3	GTP	C	1181	4	25,34,34	0.97	1 (4%)	34,54,54	1.64	7 (20%)
3	GTP	E	1181	4	25,34,34	0.97	1 (4%)	34,54,54	1.72	6 (17%)
3	GTP	G	1181	4	25,34,34	1.00	1 (4%)	34,54,54	1.60	7 (20%)

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
3	GTP	A	1182	4	-	0/18/38/38	0/3/3/3
3	GTP	C	1181	4	-	0/18/38/38	0/3/3/3
3	GTP	E	1181	4	-	0/18/38/38	0/3/3/3
3	GTP	G	1181	4	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1181	GTP	C6-N1	2.17	1.37	1.33
3	E	1181	GTP	C6-N1	2.33	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1182	GTP	C6-N1	2.97	1.38	1.33
3	C	1181	GTP	C6-N1	3.19	1.39	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1181	GTP	N3-C2-N1	-5.39	119.23	127.44
3	A	1182	GTP	N3-C2-N1	-4.82	120.11	127.44
3	G	1181	GTP	N3-C2-N1	-4.80	120.13	127.44
3	C	1181	GTP	N3-C2-N1	-4.61	120.42	127.44
3	A	1182	GTP	C5-C6-N1	-3.54	118.75	123.59
3	G	1181	GTP	C5-C6-N1	-3.11	119.34	123.59
3	E	1181	GTP	C5-C6-N1	-2.98	119.52	123.59
3	C	1181	GTP	C5-C6-N1	-2.80	119.76	123.59
3	A	1182	GTP	PA-O3A-PB	-2.79	124.88	132.73
3	C	1181	GTP	PB-O3B-PG	-2.75	123.45	132.67
3	E	1181	GTP	C1'-N9-C4	-2.68	122.90	126.94
3	C	1181	GTP	C1'-N9-C4	-2.63	122.98	126.94
3	G	1181	GTP	PB-O3B-PG	-2.42	124.55	132.67
3	E	1181	GTP	C6-C5-C4	-2.29	118.16	120.90
3	C	1181	GTP	C6-C5-C4	-2.26	118.19	120.90
3	E	1181	GTP	O3A-PA-O5'	-2.21	97.08	102.94
3	G	1181	GTP	C1'-N9-C4	-2.20	123.61	126.94
3	G	1181	GTP	C6-C5-C4	-2.01	118.49	120.90
3	C	1181	GTP	N2-C2-N1	2.01	120.53	117.20
3	G	1181	GTP	O2B-PB-O3B	2.04	114.37	105.09
3	A	1182	GTP	O2B-PB-O3B	2.54	116.63	105.09
3	A	1182	GTP	O2G-PG-O1G	2.81	119.61	110.58
3	C	1181	GTP	C6-N1-C2	2.92	119.99	115.94
3	A	1182	GTP	N2-C2-N3	2.98	123.51	117.80
3	G	1181	GTP	C6-N1-C2	3.69	121.06	115.94
3	E	1181	GTP	C6-N1-C2	4.06	121.58	115.94
3	A	1182	GTP	C6-N1-C2	4.29	121.89	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1181	GTP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	162/171 (94%)	0.88	22 (13%) 4 5	17, 29, 42, 68	0
1	C	157/171 (91%)	1.12	29 (18%) 2 2	23, 37, 51, 61	0
1	E	161/171 (94%)	0.60	15 (9%) 11 12	14, 23, 36, 61	0
1	G	163/171 (95%)	0.77	16 (9%) 10 10	17, 27, 46, 53	0
2	B	54/60 (90%)	1.31	11 (20%) 1 1	19, 30, 73, 75	0
2	D	48/60 (80%)	0.72	4 (8%) 14 16	24, 32, 43, 62	0
2	F	52/60 (86%)	1.52	15 (28%) 1 0	19, 33, 83, 87	0
2	H	48/60 (80%)	1.01	8 (16%) 2 2	21, 31, 52, 57	0
All	All	845/924 (91%)	0.92	120 (14%) 4 4	14, 29, 51, 87	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2226	SER	12.8
1	C	60	ASN	8.0
2	H	2170	GLY	7.9
2	D	2220	LEU	6.5
2	H	2220	LEU	6.3
1	A	16	ARG	6.0
1	G	60	ASN	5.9
2	F	2223	TRP	5.6
1	C	58	TYR	5.1
2	B	2224	LEU	5.0
2	F	2220	LEU	5.0
1	C	147	ALA	4.9
2	F	2225	ARG	4.8
2	B	2228	SER	4.8
2	F	2206	ASP	4.3
2	B	2227	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	15	THR	4.2
1	G	131	GLU	4.0
2	F	2224	LEU	4.0
1	E	13	HIS	4.0
1	A	13	HIS	4.0
1	E	16	ARG	4.0
1	C	43	VAL	3.9
1	C	41	GLU	3.9
1	C	61	LEU	3.9
2	B	2175	PHE	3.7
1	A	91	VAL	3.7
1	C	91	VAL	3.6
1	A	88	VAL	3.6
1	C	84	ASN	3.5
2	F	2222	SER	3.4
2	D	2175	PHE	3.4
1	E	123	VAL	3.4
1	C	90	TYR	3.4
1	C	59	LYS	3.4
1	C	42	VAL	3.3
1	E	91	VAL	3.3
1	C	89	ILE	3.3
1	C	167	ASP	3.2
1	G	44	THR	3.2
2	B	2225	ARG	3.2
1	A	71	LEU	3.1
1	A	23	LEU	3.1
1	G	58	TYR	3.1
1	C	112	GLU	3.1
1	G	61	LEU	3.1
1	A	20	ILE	3.1
1	G	91	VAL	3.0
1	C	162	LYS	3.0
2	H	2219	ARG	3.0
1	C	123	VAL	2.9
2	B	2223	TRP	2.9
1	A	149	LYS	2.9
1	C	117	ARG	2.9
1	C	22	ILE	2.9
2	B	2197	VAL	2.9
2	F	2171	GLU	2.8
1	C	33	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	2220	LEU	2.8
1	A	89	ILE	2.8
1	E	89	ILE	2.7
1	E	120	ILE	2.7
1	E	88	VAL	2.7
2	F	2219	ARG	2.7
1	A	17	GLU	2.7
1	A	33	ILE	2.7
1	A	21	LEU	2.7
1	C	171	GLU	2.7
1	E	167	ASP	2.6
1	G	33	ILE	2.6
1	A	92	VAL	2.6
2	H	2198	ILE	2.5
1	A	90	TYR	2.5
1	C	131	GLU	2.5
1	E	180	ARG	2.5
2	H	2206	ASP	2.5
1	E	92	VAL	2.4
2	F	2201	VAL	2.4
2	H	2172	PRO	2.4
1	C	21	LEU	2.4
1	G	114	GLU	2.4
1	E	121	LEU	2.3
2	F	2178	LEU	2.3
1	G	89	ILE	2.3
2	B	2198	ILE	2.3
1	A	44	THR	2.3
1	G	150	ASP	2.3
1	E	90	TYR	2.3
1	C	132	GLN	2.3
2	H	2214	GLU	2.3
1	G	162	LYS	2.2
1	G	132	GLN	2.2
1	C	92	VAL	2.2
2	F	2202	LEU	2.2
1	A	162	LYS	2.2
1	C	109	ALA	2.2
1	E	33	ILE	2.2
2	D	2207	ASP	2.2
2	F	2182	LEU	2.2
1	E	131	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	2171	GLU	2.2
1	C	88	VAL	2.2
1	E	122	VAL	2.2
1	C	114	GLU	2.1
1	A	78	TRP	2.1
1	A	41	GLU	2.1
1	G	168	GLU	2.1
1	C	37	LEU	2.1
1	G	39	VAL	2.1
1	G	92	VAL	2.1
2	F	2175	PHE	2.1
1	A	150	ASP	2.1
1	C	138	GLU	2.1
2	F	2207	ASP	2.1
1	A	132	GLN	2.0
1	G	20	ILE	2.1
2	H	2171	GLU	2.0
1	A	68	LEU	2.0
2	B	2182	LEU	2.0
2	D	2198	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	E	1182	1/1	0.98	0.12	0.67	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GTP	C	1181	32/32	0.96	0.10	-0.76	19,28,36,38	0
3	GTP	E	1181	32/32	0.98	0.08	-0.82	13,18,22,24	0
3	GTP	A	1182	32/32	0.96	0.09	-1.16	19,26,30,34	0
3	GTP	G	1181	32/32	0.98	0.08	-1.55	17,27,33,33	0
4	MG	C	1182	1/1	0.96	0.04	-1.75	21,21,21,21	0
4	MG	G	1182	1/1	0.99	0.08	-2.07	19,19,19,19	0
4	MG	A	1183	1/1	0.97	0.04	-3.92	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.