



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:34 am GMT

PDB ID : 5C8Y
Title : Crystal structure of T2R-TTL-Plinabulin complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2015-06-26
Resolution : 2.59 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

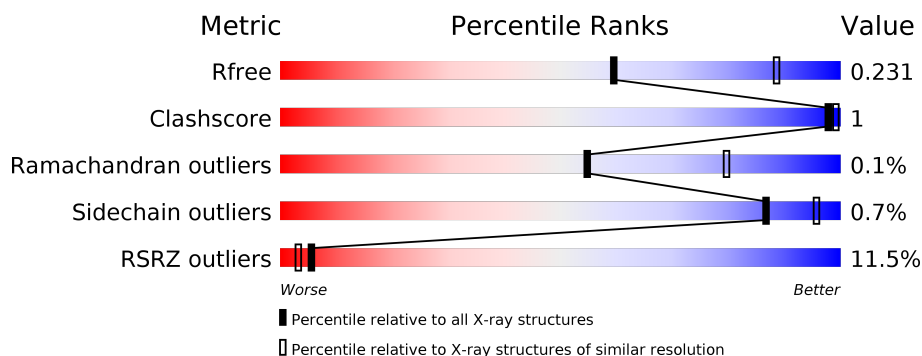
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 ≥ 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	450	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
1	C	450	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	445	<div> <div>7%</div> <div>92%</div> <div>• •</div> </div>
2	D	445	<div> <div>14%</div> <div>92%</div> <div>• 5%</div> </div>
3	E	143	<div> <div>10%</div> <div>84%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>27%</div> <div>83%</div> <div>• 13%</div> </div>

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
6	MG	C	502	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34616 atoms, of which 16867 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 Tubulin alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

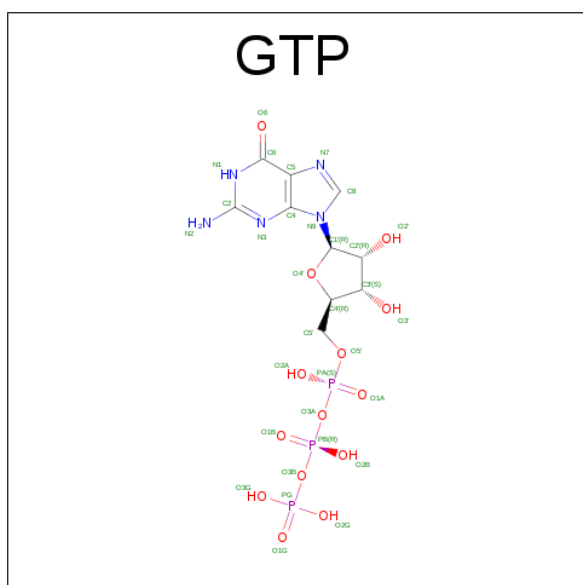
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

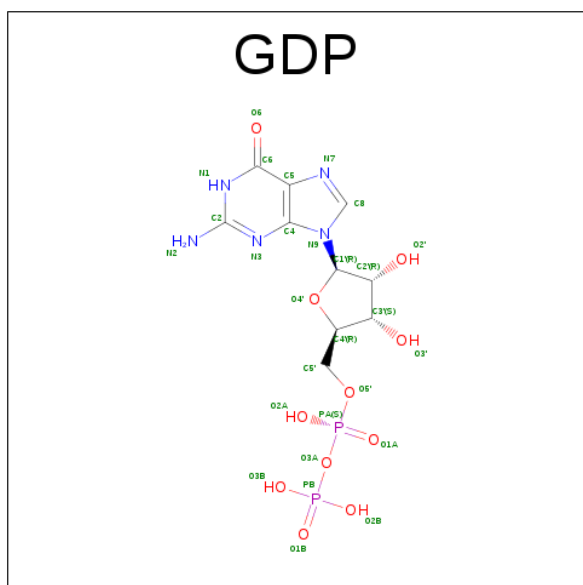
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

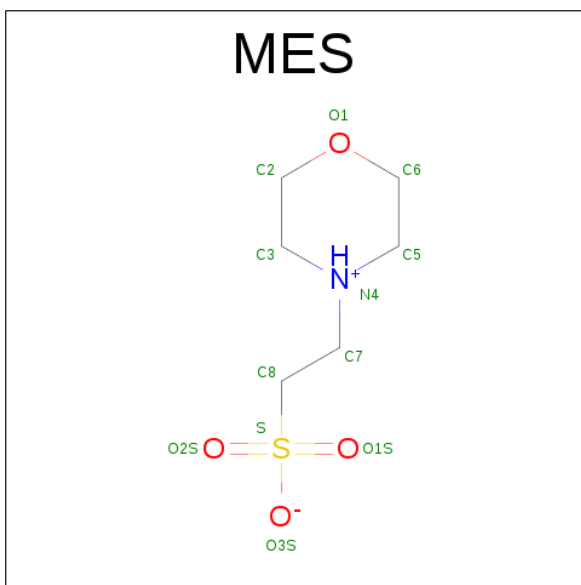
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



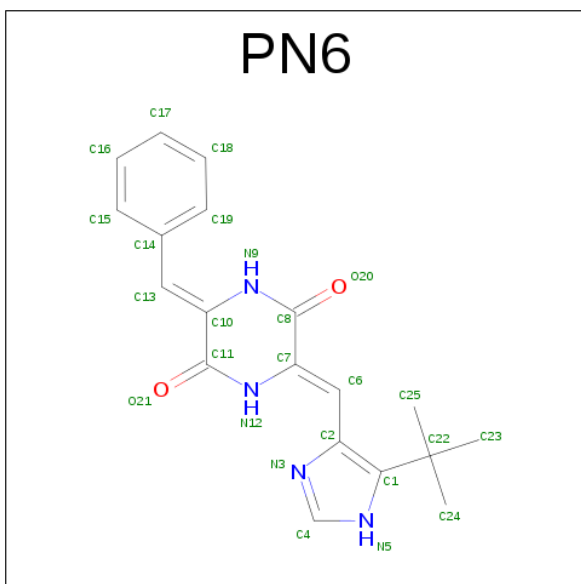
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
8	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is (3Z,6Z)-3-benzylidene-6-[(5-tert-butyl-1H-imidazol-4-yl)methylidene]piperazine-2,5-dione (three-letter code: PN6) (formula: $C_{19}H_{20}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			45	19	20	4	2		
10	D	1	Total	C	H	N	O	0	0
			45	19	20	4	2		

- # ACP
-
- The chemical structure of Adenosine 3'-Phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate group. The structure is labeled with atom names and numbers, and includes stereochemical indicators like wedges and dashes.
- Key features of the structure include:
- Adenine Base:** A purine ring system with atoms labeled N1 through N9 and C2 through C8. The amino group (NH₂) is attached to C6.
 - Ribose Sugar:** A five-membered ring with atoms labeled C1 through C5 and O4. The sugar is in the β-D-ribofuranose form.
 - Triphosphate Group:** Three phosphate groups are attached to the 3' carbon of the ribose sugar. The first phosphate is linked via an oxygen atom (O3'). The second and third phosphates are linked via oxygen atoms (O3A and O3B) to the first and second phosphorus atoms, respectively.
 - Atom Labeling:** Atoms are labeled with their element symbol and a number (e.g., N1, C2, O3, P1, O1A, O1B, O1C).
 - Stereochemistry:** The structure uses wedges and dashes to indicate the three-dimensional arrangement of atoms. For example, the phosphate group at the 3' position is shown with a wedge bond to the ribose sugar.

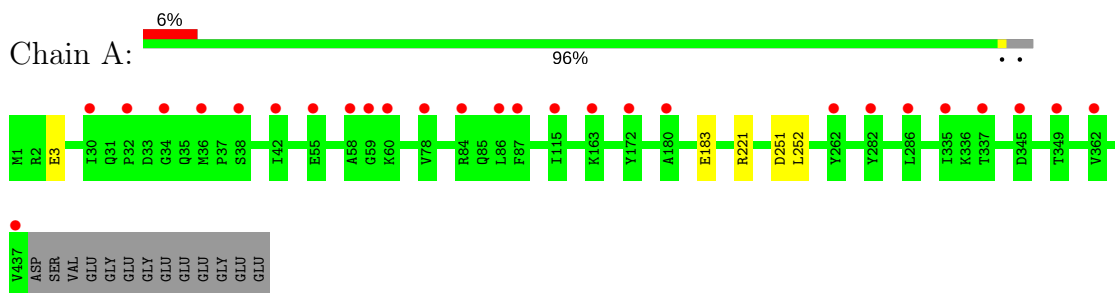
- Molecule 12 is water.



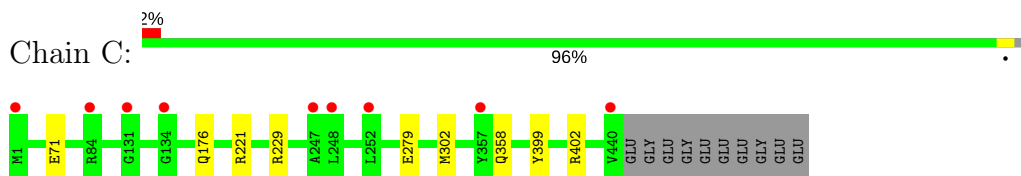
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

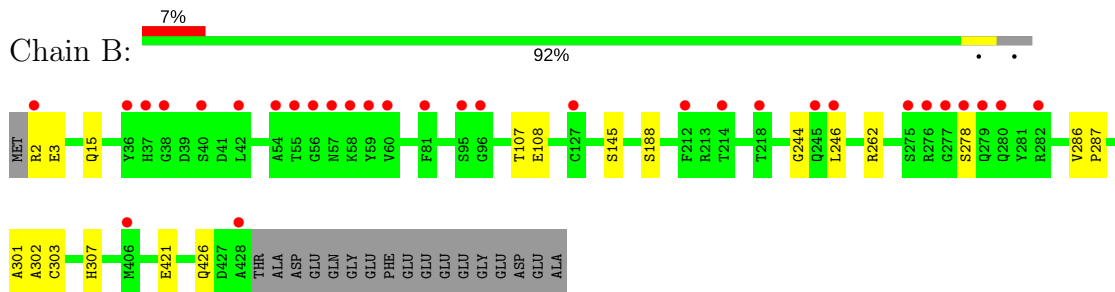
• Molecule 1: Tubulin alpha



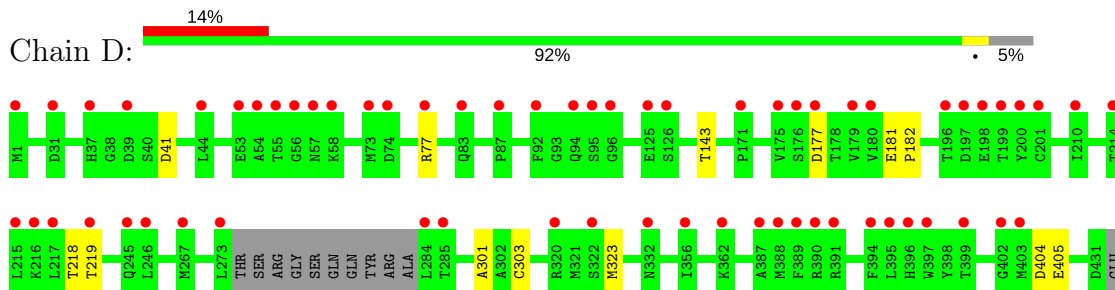
• Molecule 1: Tubulin alpha



• Molecule 2: Tubulin beta

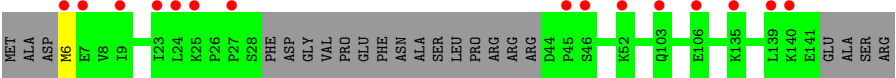
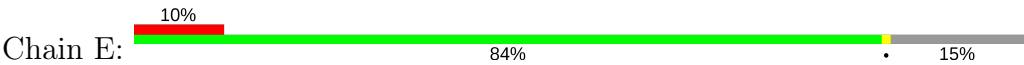


• Molecule 2: Tubulin beta

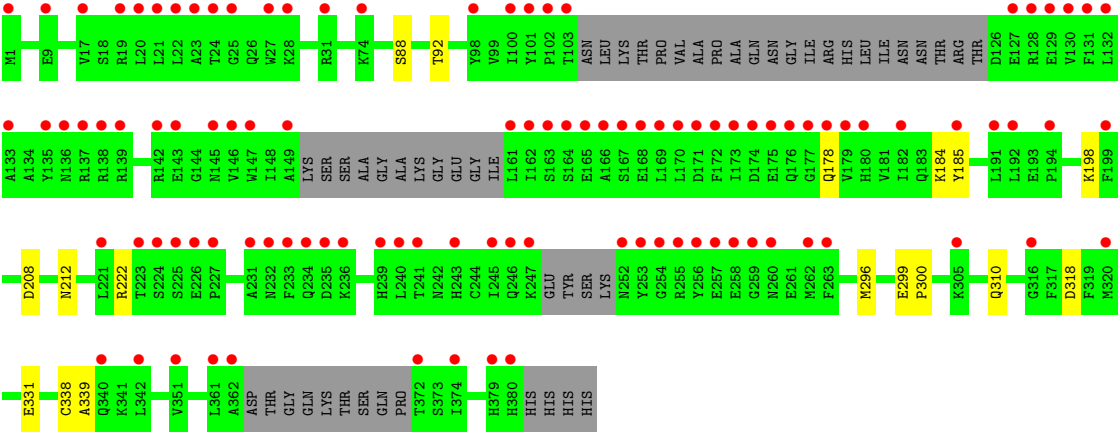
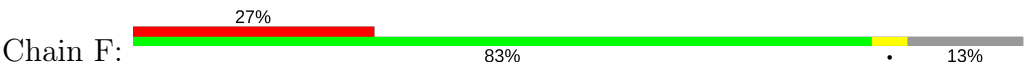


GLN
GLY
GLU
PHE
GLU
GLU
GLU
GLU
GLY
ASP
GLU
ALA

● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.06Å 158.44Å 181.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.59 45.48 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.70-2.59) 98.8 (45.48-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.222 , 0.271 0.223 , 0.231	Depositor DCC
R_{free} test set	4630 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34616	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GDP, MG, CA, PN6, GTP, ACP, MES

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	0.22	0/3494	0.37	0/4743
1	C	0.22	0/3515	0.37	0/4772
2	B	0.22	0/3436	0.38	0/4654
2	D	0.22	0/3382	0.37	0/4581
3	E	0.21	0/1008	0.32	0/1337
4	F	0.22	0/2806	0.36	0/3791
All	All	0.22	0/17641	0.37	0/23878

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	A	3416	3317	3330	3	0
1	C	3437	3335	3348	5	0
2	B	3361	3228	3238	8	0
2	D	3309	3179	3189	6	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	7	0
5	A	32	10	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	1	0
9	B	12	12	12	0	0
10	B	25	20	20	0	0
10	D	25	20	20	1	0
11	F	31	4	14	0	0
12	A	68	0	0	0	0
12	B	49	0	0	1	0
12	C	89	0	0	3	0
12	D	20	0	0	1	0
12	E	13	0	0	1	0
12	F	25	0	0	0	0
All	All	17749	16867	16946	31	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 1.

All (31) 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:B:2:ARG:NH1	12:B:603:HOH:O	2.27	0.67
2:D:77:ARG:NH2	12:D:1201:HOH:O	2.30	0.64
4:F:222:ARG:NH1	4:F:318:ASP:OD1	2.33	0.62
2:B:301:ALA:O	2:B:303:CYS:N	2.32	0.61
2:D:404:ASP:OD1	2:D:405:GLU:N	2.35	0.59
1:C:176:GLN:NE2	12:C:604:HOH:O	2.35	0.58
1:A:251:ASP:OD1	1:A:252:LEU:N	2.37	0.58
2:B:145:SER:HG	2:B:188:SER:HG	1.53	0.56
1:C:229:ARG:NH2	12:C:606:HOH:O	2.38	0.56
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.39	0.56
2:D:143:THR:N	8:D:501:GDP:O2B	2.43	0.51
10:D:502:PN6:N12	10:D:502:PN6:N3	2.49	0.51
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.45	0.49
4:F:178:GLN:OE1	4:F:178:GLN:N	2.45	0.49
1:C:399:TYR:O	1:C:402:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:OE1	1:C:279:GLU:N	2.46	0.46
1:C:71:GLU:O	12:C:601:HOH:O	2.20	0.46
2:D:301:ALA:O	2:D:303:CYS:N	2.48	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.31	0.45
4:F:208:ASP:OD1	4:F:212:ASN:N	2.47	0.44
2:B:307:HIS:O	2:B:426:GLN:NE2	2.51	0.43
1:A:183:GLU:OE2	5:A:501:GTP:O3'	2.20	0.43
3:E:6:MET:N	12:E:204:HOH:O	2.51	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.42
4:F:184:LYS:NZ	4:F:185:TYR:O	2.51	0.42
2:B:107:THR:OG1	2:B:108:GLU:N	2.53	0.41
2:B:3:GLU:OE2	2:B:3:GLU:N	2.53	0.41
2:D:218:THR:O	2:D:219:THR:OG1	2.37	0.41
1:A:3:GLU:N	1:A:3:GLU:OE1	2.54	0.40
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	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	435/450 (97%)	414 (95%)	21 (5%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	408 (96%)	14 (3%)	3 (1%)	25	49
2	D	417/445 (94%)	401 (96%)	16 (4%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2077 (96%)	76 (4%)	3 (0%)	55	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	GLY
2	B	302	ALA
2	B	278	SER

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	368/378 (97%)	367 (100%)	1 (0%)	94	98
1	C	371/378 (98%)	368 (99%)	3 (1%)	85	94
2	B	369/383 (96%)	367 (100%)	2 (0%)	91	97
2	D	364/383 (95%)	361 (99%)	3 (1%)	85	94
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	296 (98%)	5 (2%)	66	86
All	All	1882/1991 (94%)	1868 (99%)	14 (1%)	87	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	15	GLN
2	B	246	LEU
1	C	221	ARG
1	C	302	MET
1	C	358	GLN
2	D	41	ASP
2	D	177	ASP
2	D	323	MET
4	F	88	SER
4	F	92	THR
4	F	296	MET
4	F	310	GLN
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
5	GTP	A	501	6	27,34,34	1.07	1 (3%)	24,54,54	1.18	1 (4%)
8	GDP	B	501	6	25,30,30	1.38	4 (16%)	23,47,47	1.36	2 (8%)
9	MES	B	503	-	12,12,12	2.17	1 (8%)	14,16,16	2.22	5 (35%)
10	PN6	B	504	-	21,27,27	1.68	6 (28%)	16,39,39	0.81	0
5	GTP	C	501	6	27,34,34	1.07	1 (3%)	24,54,54	1.15	1 (4%)
8	GDP	D	501	-	25,30,30	1.40	4 (16%)	23,47,47	1.41	3 (13%)
10	PN6	D	502	-	21,27,27	1.77	5 (23%)	16,39,39	0.72	0
11	ACP	F	401	-	27,33,33	1.90	7 (25%)	30,52,52	1.98	7 (23%)

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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	PN6	B	504	-	-	0/10/14/14	0/3/3/3
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
10	PN6	D	502	-	-	0/10/14/14	0/3/3/3
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.25	1.66	1.77
11	F	401	ACP	PB-O2B	-3.87	1.46	1.56
10	B	504	PN6	C14-C13	-3.48	1.39	1.46
10	D	502	PN6	C14-C13	-3.45	1.39	1.46
11	F	401	ACP	PG-O2G	-3.41	1.46	1.54
11	F	401	ACP	C2'-C1'	-2.85	1.49	1.53
8	B	501	GDP	C2-N3	2.07	1.36	1.33
10	D	502	PN6	C11-N12	2.10	1.39	1.36
11	F	401	ACP	C5-C4	2.12	1.45	1.40
10	B	504	PN6	C7-N12	2.13	1.40	1.36
10	B	504	PN6	C11-N12	2.19	1.39	1.36
8	D	501	GDP	C2-N3	2.26	1.36	1.33
11	F	401	ACP	PG-O3G	2.32	1.60	1.54
10	B	504	PN6	C10-N9	2.47	1.40	1.36
8	B	501	GDP	C2-N2	2.59	1.36	1.32
8	D	501	GDP	C2-N2	2.60	1.36	1.32
8	B	501	GDP	C5-C4	2.92	1.47	1.40
8	D	501	GDP	C5-C4	2.97	1.47	1.40
10	D	502	PN6	C10-N9	3.02	1.41	1.36
10	D	502	PN6	C22-C1	3.12	1.57	1.52
10	B	504	PN6	C22-C1	3.19	1.57	1.52
11	F	401	ACP	PB-O1B	3.38	1.60	1.51
10	B	504	PN6	C8-N9	3.40	1.41	1.36
8	D	501	GDP	C6-C5	4.02	1.48	1.41
8	B	501	GDP	C6-C5	4.05	1.48	1.41
10	D	502	PN6	C8-N9	4.08	1.42	1.36
5	C	501	GTP	C2-N3	4.10	1.38	1.33
5	A	501	GTP	C2-N3	4.10	1.38	1.33
11	F	401	ACP	PG-O1G	5.21	1.61	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-6.11	123.54	128.86
11	F	401	ACP	PA-O3A-PB	-5.01	116.24	132.39
11	F	401	ACP	C4-C5-N7	-3.44	106.08	109.41
8	B	501	GDP	C4-C5-N7	-2.79	106.71	109.41
8	D	501	GDP	C4-C5-N7	-2.70	106.80	109.41
11	F	401	ACP	O2'-C2'-C1'	-2.44	103.99	111.61
11	F	401	ACP	O2'-C2'-C3'	-2.42	104.09	111.83
11	F	401	ACP	C2-N1-C6	2.03	122.32	118.77
8	D	501	GDP	C2'-C3'-C4'	2.03	106.58	102.62
11	F	401	ACP	O1B-PB-C3B	2.24	114.50	108.97
9	B	503	MES	O2S-S-C8	2.43	108.88	106.79
9	B	503	MES	C7-N4-C5	2.61	117.94	111.26
9	B	503	MES	O3S-S-C8	2.88	109.60	106.06
9	B	503	MES	O1S-S-C8	4.11	110.33	106.79
5	C	501	GTP	C2-N3-C4	4.26	120.14	115.16
5	A	501	GTP	C2-N3-C4	4.38	120.27	115.16
9	B	503	MES	C5-N4-C3	4.64	119.38	108.87
8	B	501	GDP	C2-N3-C4	4.68	120.62	115.16
8	D	501	GDP	C2-N3-C4	4.84	120.81	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	D	501	GDP	1	0
10	D	502	PN6	1	0

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 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, 95th 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 ²)	Q<0.9
1	A	437/450 (97%)	0.79	27 (6%)	21 16	27, 49, 78, 145	0
1	C	440/450 (97%)	0.26	9 (2%)	65 59	21, 37, 66, 90	0
2	B	427/445 (95%)	0.65	31 (7%)	16 11	23, 47, 88, 121	0
2	D	421/445 (94%)	1.01	63 (14%)	3 1	33, 65, 102, 124	0
3	E	121/143 (84%)	1.04	15 (12%)	4 2	30, 67, 100, 127	0
4	F	334/384 (86%)	1.62	105 (31%)	0 0	38, 76, 126, 153	0
All	All	2180/2317 (94%)	0.84	250 (11%)	5 3	21, 54, 102, 153	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	8.6
4	F	233	PHE	8.1
4	F	234	GLN	8.1
4	F	161	LEU	7.6
4	F	169	LEU	7.3
2	D	394	PHE	7.2
4	F	132	LEU	6.9
2	D	1	MET	6.6
2	D	55	THR	6.5
4	F	173	ILE	6.5
4	F	142	ARG	6.2
4	F	135	TYR	5.8
4	F	167	SER	5.8
4	F	103	THR	5.8
4	F	245	ILE	5.8
4	F	232	ASN	5.7
4	F	100	ILE	5.7
4	F	253	TYR	5.6
4	F	170	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	94	GLN	5.1
2	B	279	GLN	4.9
4	F	178	GLN	4.9
4	F	194	PRO	4.9
2	D	390	ARG	4.9
4	F	172	PHE	4.8
4	F	225	SER	4.8
4	F	372	THR	4.7
4	F	162	ILE	4.7
4	F	256	TYR	4.6
4	F	180	HIS	4.4
2	D	397	TRP	4.4
2	D	37	HIS	4.4
4	F	31	ARG	4.4
2	D	92	PHE	4.4
4	F	168	GLU	4.4
4	F	139	ARG	4.3
4	F	182	ILE	4.3
4	F	130	VAL	4.2
2	D	391	ARG	4.2
2	B	280	GLN	4.2
4	F	361	LEU	4.2
4	F	227	PRO	4.2
4	F	240	LEU	4.2
4	F	101	TYR	4.2
2	B	37	HIS	4.0
4	F	98	TYR	4.0
2	D	389	PHE	4.0
2	D	216	LYS	4.0
2	D	54	ALA	4.0
2	B	245	GLN	4.0
2	D	180	VAL	3.9
4	F	255	ARG	3.9
1	A	86	LEU	3.8
3	E	139	LEU	3.8
2	D	396	HIS	3.8
4	F	252	ASN	3.7
2	D	285	THR	3.7
4	F	25	GLY	3.7
2	D	56	GLY	3.7
3	E	27	PRO	3.7
2	B	282	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	177	ASP	3.7
4	F	231	ALA	3.6
4	F	246	GLN	3.6
2	D	356	ILE	3.6
4	F	235	ASP	3.6
2	B	55	THR	3.6
4	F	128	ARG	3.5
4	F	137	ARG	3.5
4	F	223	THR	3.5
4	F	175	GLU	3.5
3	E	24	LEU	3.5
4	F	27	TRP	3.5
4	F	236	LYS	3.5
4	F	243	HIS	3.5
4	F	254	GLY	3.5
4	F	133	ALA	3.4
2	D	53	GLU	3.4
4	F	176	GLN	3.4
2	B	276	ARG	3.4
2	D	219	THR	3.4
2	D	245	GLN	3.4
2	B	95	SER	3.4
1	C	247	ALA	3.3
4	F	179	VAL	3.3
4	F	199	PHE	3.3
4	F	258	GLU	3.3
1	A	34	GLY	3.3
2	D	214	THR	3.3
2	B	277	GLY	3.3
3	E	6	MET	3.3
4	F	136	ASN	3.3
3	E	135	LYS	3.3
4	F	145	ASN	3.2
2	D	87	PRO	3.2
2	D	96	GLY	3.2
2	D	217	LEU	3.2
2	D	320	ARG	3.2
4	F	171	ASP	3.2
4	F	129	GLU	3.2
1	A	42	ILE	3.2
2	D	322	SER	3.2
2	B	278	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	200	TYR	3.1
2	D	362	LYS	3.0
2	D	215	LEU	3.0
4	F	22	LEU	3.0
4	F	165	GLU	3.0
4	F	247	LYS	3.0
3	E	7	GLU	3.0
2	D	395	LEU	3.0
2	D	74	ASP	2.9
2	D	95	SER	2.9
4	F	20	LEU	2.9
4	F	138	ARG	2.9
1	A	437	VAL	2.9
4	F	17	VAL	2.9
4	F	380	HIS	2.9
2	D	73	MET	2.9
4	F	163	SER	2.9
2	D	388	MET	2.9
2	B	218	THR	2.9
2	B	96	GLY	2.9
1	C	357	TYR	2.9
1	A	59	GLY	2.8
4	F	191	LEU	2.8
2	D	176	SER	2.8
1	C	440	VAL	2.8
1	A	163	LYS	2.8
1	A	180	ALA	2.8
1	A	262	TYR	2.8
1	A	345	ASP	2.8
4	F	1	MET	2.8
4	F	226	GLU	2.8
3	E	106	GLU	2.7
2	D	171	PRO	2.7
2	B	275	SER	2.7
4	F	305	LYS	2.7
4	F	21	LEU	2.7
2	B	127	CYS	2.7
4	F	379	HIS	2.7
4	F	146	VAL	2.7
3	E	9	ILE	2.7
4	F	24	THR	2.7
2	B	56	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	57	ASN	2.7
4	F	149	ALA	2.7
4	F	362	ALA	2.7
4	F	147	TRP	2.6
2	B	81	PHE	2.6
4	F	102	PRO	2.6
4	F	19	ARG	2.6
2	B	54	ALA	2.6
4	F	260	ASN	2.6
3	E	25	LYS	2.6
2	D	57	ASN	2.6
2	D	387	ALA	2.6
1	A	60	LYS	2.6
2	D	197	ASP	2.6
3	E	46	SER	2.6
2	D	179	VAL	2.6
1	C	248	LEU	2.6
2	B	246	LEU	2.6
2	D	58	LYS	2.6
3	E	103	GLN	2.5
2	B	2	ARG	2.5
2	D	126	SER	2.5
4	F	143	GLU	2.5
2	B	38	GLY	2.5
4	F	131	PHE	2.5
2	D	199	THR	2.5
4	F	166	ALA	2.5
2	D	175	VAL	2.5
2	B	406	MET	2.5
4	F	23	ALA	2.5
2	D	201	CYS	2.4
4	F	177	GLY	2.4
4	F	316	GLY	2.4
4	F	221	LEU	2.4
1	A	335	ILE	2.4
2	B	428	ALA	2.4
2	B	58	LYS	2.4
4	F	340	GLN	2.4
1	A	349	THR	2.4
1	A	38	SER	2.4
1	A	78	VAL	2.4
1	C	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	267	MET	2.4
3	E	23	ILE	2.4
4	F	320	MET	2.4
2	D	198	GLU	2.4
4	F	263	PHE	2.4
4	F	192	LEU	2.4
4	F	74	LYS	2.3
2	B	59	TYR	2.3
2	D	284	LEU	2.3
1	C	84	ARG	2.3
2	D	332	ASN	2.3
4	F	185	TYR	2.3
2	B	36	TYR	2.3
2	D	210	ILE	2.3
4	F	164	SER	2.3
2	D	196	THR	2.3
2	D	83	GLN	2.3
2	D	399	THR	2.3
4	F	241	THR	2.3
2	D	273	LEU	2.3
4	F	28	LYS	2.2
4	F	174	ASP	2.2
1	A	115	ILE	2.2
2	B	212	PHE	2.2
1	C	134	GLY	2.2
3	E	140	LYS	2.2
2	B	42	LEU	2.2
2	D	125	GLU	2.2
4	F	127	GLU	2.2
4	F	259	GLY	2.2
4	F	351	VAL	2.2
1	A	30	ILE	2.2
2	D	402	GLY	2.2
1	C	131	GLY	2.2
2	B	40	SER	2.2
1	A	362	VAL	2.2
4	F	9	GLU	2.2
4	F	224	SER	2.2
4	F	374	ILE	2.1
1	A	172	TYR	2.1
2	D	403	MET	2.1
1	A	55	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	39	ASP	2.1
1	A	32	PRO	2.1
4	F	257	GLU	2.1
1	A	286	LEU	2.1
2	D	77	ARG	2.1
2	B	214	THR	2.1
4	F	262	MET	2.1
1	A	84	ARG	2.1
3	E	45	PRO	2.0
1	A	87	PHE	2.0
1	A	36	MET	2.0
2	D	31	ASP	2.0
1	A	58	ALA	2.0
1	A	337	THR	2.0
2	B	60	VAL	2.0
2	D	44	LEU	2.0
4	F	342	LEU	2.0
4	F	239	HIS	2.0
1	C	252	LEU	2.0
2	D	246	LEU	2.0
3	E	52	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
6	MG	C	502	1/1	0.96	0.32	4.99	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	PN6	D	502	25/25	0.87	0.33	1.78	41,77,120,145	0
8	GDP	B	501	28/28	0.94	0.24	1.67	18,38,62,71	0
10	PN6	B	504	25/25	0.95	0.25	0.97	30,51,79,97	0
5	GTP	C	501	32/32	0.97	0.21	0.68	16,32,53,91	0
6	MG	A	502	1/1	0.95	0.23	0.39	26,26,26,26	0
5	GTP	A	501	32/32	0.96	0.24	0.33	13,35,46,79	0
9	MES	B	503	12/12	0.90	0.19	0.04	38,57,82,89	0
8	GDP	D	501	28/28	0.90	0.19	-0.55	35,64,100,112	0
11	ACP	F	401	31/31	0.88	0.20	-1.26	72,107,155,168	0
7	CA	C	503	1/1	0.98	0.11	-1.49	55,55,55,55	0
7	CA	A	503	1/1	0.82	0.10	-1.75	76,76,76,76	0
6	MG	B	502	1/1	0.95	0.33	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.