



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:40 am GMT

PDB ID : 5CB4
Title : Crystal structure of T2R-TTL-Tivantinib complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2015-06-30
Resolution : 2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

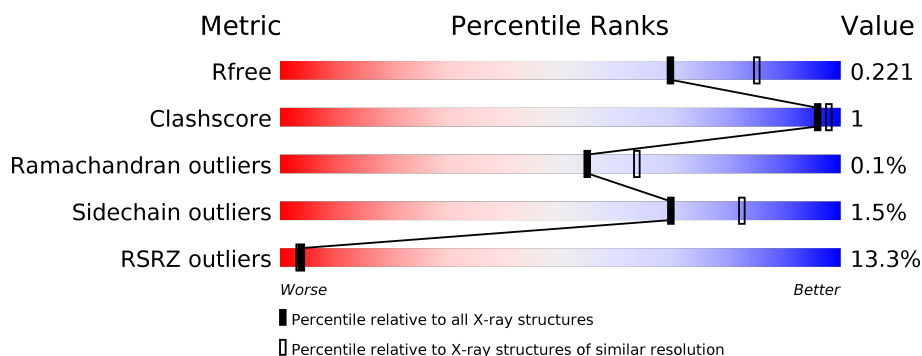
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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>10%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>3%</div> <div>95%</div> <div>• •</div> </div>
2	B	445	<div> <div>9%</div> <div>94%</div> <div>• •</div> </div>
2	D	445	<div> <div>18%</div> <div>89%</div> <div>5% • 5%</div> </div>
3	E	143	<div> <div>13%</div> <div>82%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>24%</div> <div>82%</div> <div>5% 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	A	502	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 35199 atoms, of which 16873 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

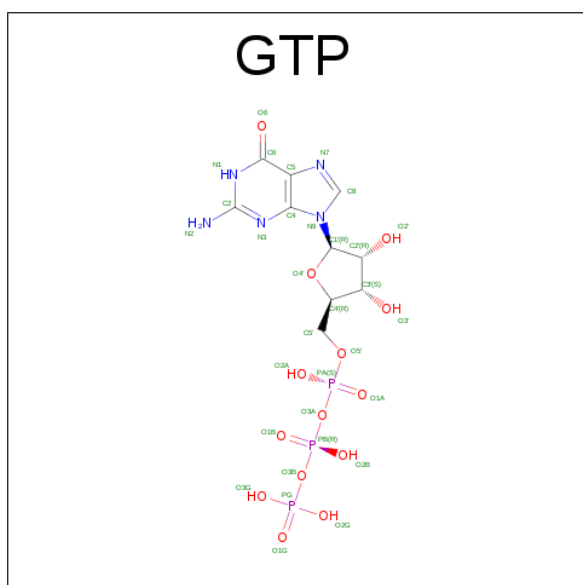
- Molecule 4 is a protein called Uncharacterized protein.

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).

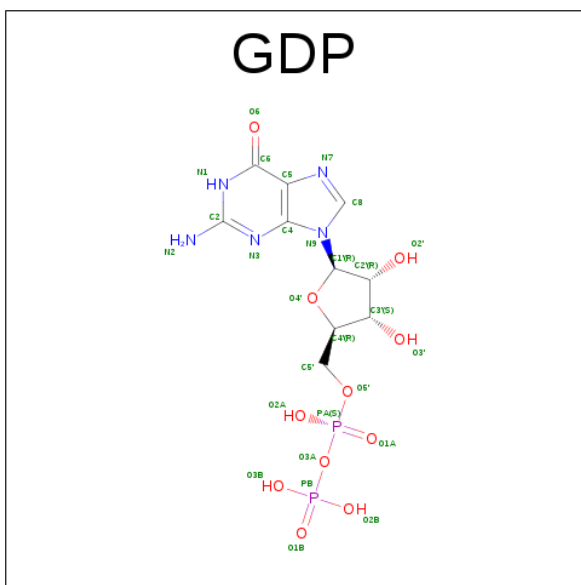
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

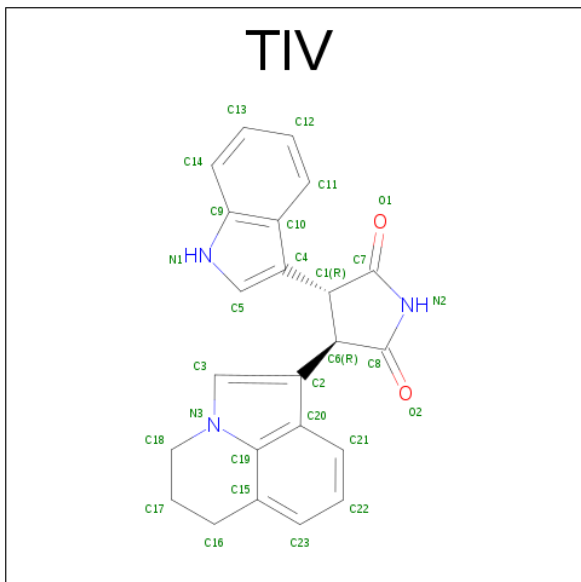


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

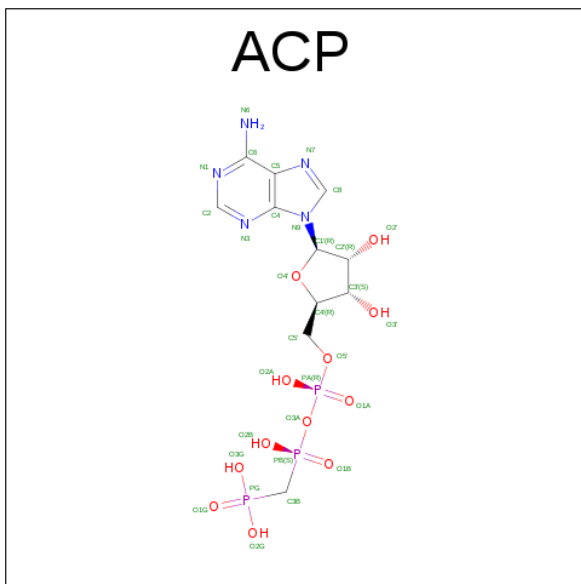


- Molecule 11 is (3R,4R)-3-(5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-1-yl)-4-(1H-indol-3-yl)pyrrolidine-2,5-dione (three-letter code: TIV) (formula: $C_{23}H_{19}N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			47	23	19	3	2		
11	D	1	Total	C	H	N	O	0	0
			47	23	19	3	2		

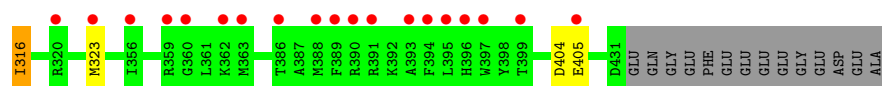
- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



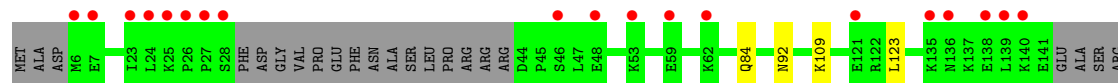
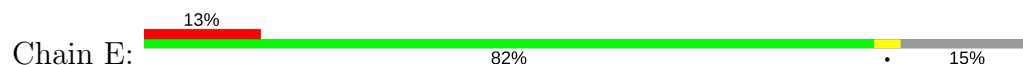
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			35	11	4	5	12	3		

- Molecule 13 is water.

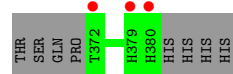
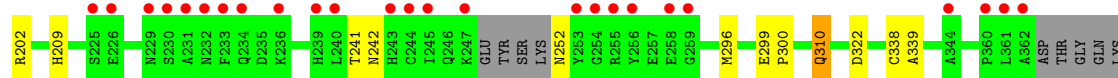
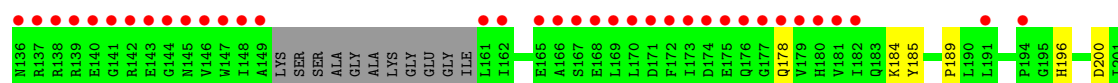
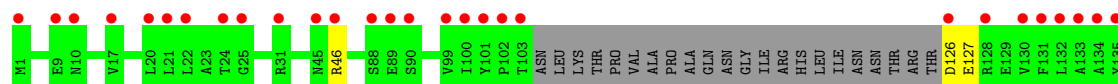
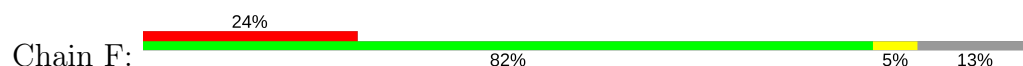
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	185	Total	O	0	0
			185	185		
13	B	164	Total	O	0	0
			164	164		
13	C	273	Total	O	0	0
			273	273		
13	D	92	Total	O	0	0
			92	92		
13	E	31	Total	O	0	0
			31	31		
13	F	84	Total	O	0	0
			84	84		



• 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)	39.82 – 2.19 39.82 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.82-2.19) 99.3 (39.82-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.207 , 0.232 0.208 , 0.221	Depositor DCC
R_{free} test set	7565 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35199	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, GOL, MG, TIV, GTP, ACP, MES, CA

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	0.23	0/3494	0.40	0/4743
1	C	0.23	0/3515	0.40	0/4772
2	B	0.23	0/3436	0.39	0/4654
2	D	0.23	0/3382	0.39	0/4581
3	E	0.22	0/1008	0.35	0/1337
4	F	0.22	0/2806	0.38	0/3791
All	All	0.23	0/17641	0.39	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	7	0
1	C	3437	3335	3348	6	0
2	B	3361	3228	3238	4	0
2	D	3309	3179	3189	12	0
3	E	1000	1014	1018	3	0
4	F	2744	2698	2709	13	0
5	A	32	10	12	0	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	A	6	8	8	0	0
9	B	28	10	12	0	0
9	D	28	10	12	1	0
10	B	12	12	12	0	0
11	B	28	19	19	0	0
11	D	28	19	19	1	0
12	F	31	4	14	2	0
13	A	185	0	0	2	0
13	B	164	0	0	0	0
13	C	273	0	0	3	0
13	D	92	0	0	1	0
13	E	31	0	0	2	0
13	F	84	0	0	3	0
All	All	18326	16873	16952	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 1.

The worst 5 of 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)
4:F:196:HIS:NE2	13:F:502:HOH:O	2.30	0.65
2:B:145:SER:OG	2:B:188:SER:OG	2.16	0.62
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.34	0.61
4:F:126:ASP:N	13:F:510:HOH:O	2.34	0.59
4:F:252:ASN:N	13:F:508:HOH:O	2.35	0.58

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%)	422 (97%)	12 (3%)	1 (0%)	51	58
1	C	438/450 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	9 (2%)	1 (0%)	51	58
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2100 (97%)	54 (2%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	SER
1	A	89	PRO

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%)	362 (98%)	6 (2%)	68	81
1	C	371/378 (98%)	364 (98%)	7 (2%)	62	76
2	B	369/383 (96%)	365 (99%)	4 (1%)	78	88
2	D	364/383 (95%)	357 (98%)	7 (2%)	62	76
3	E	109/127 (86%)	108 (99%)	1 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	301/342 (88%)	298 (99%)	3 (1%)	80	89
All	All	1882/1991 (94%)	1854 (98%)	28 (2%)	70	82

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	GLU
1	C	347	CYS
4	F	242	ASN
1	C	245	ASP
1	C	251	ASP

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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	1.08	1 (3%)	24,54,54	1.23	1 (4%)
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.28	0
9	GDP	B	501	6	25,30,30	1.38	4 (16%)	23,47,47	1.24	3 (13%)
10	MES	B	503	-	12,12,12	2.12	1 (8%)	14,16,16	2.80	6 (42%)
11	TIV	B	504	-	26,33,33	2.17	5 (19%)	31,50,50	2.18	7 (22%)
5	GTP	C	501	6	27,34,34	1.06	1 (3%)	24,54,54	1.18	1 (4%)
9	GDP	D	501	-	25,30,30	1.38	5 (20%)	23,47,47	1.27	2 (8%)
11	TIV	D	502	-	26,33,33	1.82	4 (15%)	31,50,50	2.20	8 (25%)
12	ACP	F	401	-	27,33,33	1.70	7 (25%)	30,52,52	1.78	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	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	TIV	B	504	-	-	0/0/30/30	0/5/6/6
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
11	TIV	D	502	-	-	0/0/30/30	0/5/6/6
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.08	1.66	1.77
12	F	401	ACP	PB-O2B	-4.59	1.45	1.56
12	F	401	ACP	C2'-C1'	-3.20	1.48	1.53
12	F	401	ACP	C4-N3	-2.52	1.31	1.35
9	B	501	GDP	C6-N1	-2.24	1.33	1.36

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	TIV	C16-C15-C19	-5.96	112.00	119.59
11	D	502	TIV	C7-N2-C8	-5.77	109.55	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	N3-C2-N1	-5.64	123.95	128.86
11	B	504	TIV	C7-N2-C8	-5.63	109.66	113.91
11	D	502	TIV	C16-C15-C19	-5.60	112.47	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
11	D	502	TIV	1	0
12	F	401	ACP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.71	46 (10%) 7 6	26, 42, 66, 96	0
1	C	440/450 (97%)	0.18	14 (3%) 48 46	20, 34, 54, 70	0
2	B	427/445 (95%)	0.56	40 (9%) 9 8	24, 42, 71, 121	0
2	D	421/445 (94%)	1.00	80 (19%) 1 1	27, 54, 88, 108	0
3	E	121/143 (84%)	0.83	19 (15%) 2 2	32, 56, 84, 98	0
4	F	334/384 (86%)	1.47	92 (27%) 1 0	33, 64, 119, 142	0
All	All	2180/2317 (94%)	0.75	291 (13%) 4 3	20, 46, 89, 142	0

The worst 5 of 291 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	11.8
4	F	161	LEU	9.4
4	F	138	ARG	8.7
4	F	169	LEU	8.6
2	D	55	THR	7.4

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, 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	A	502	1/1	0.90	0.21	2.06	35,35,35,35	0
6	MG	C	502	1/1	0.98	0.17	1.58	26,26,26,26	0
11	TIV	D	502	28/28	0.88	0.19	1.29	28,48,63,70	0
5	GTP	C	501	32/32	0.97	0.18	1.14	20,29,38,44	0
11	TIV	B	504	28/28	0.97	0.19	0.87	23,35,44,53	0
9	GDP	B	501	28/28	0.95	0.19	0.59	25,32,41,49	0
8	GOL	A	504	6/6	0.92	0.15	0.48	39,56,65,78	0
5	GTP	A	501	32/32	0.97	0.19	0.23	23,32,41,52	0
9	GDP	D	501	28/28	0.94	0.16	-0.51	42,54,73,87	0
10	MES	B	503	12/12	0.95	0.14	-0.55	44,56,63,72	0
12	ACP	F	401	31/31	0.90	0.17	-0.85	70,84,103,107	0
7	CA	A	503	1/1	0.90	0.07	-1.96	56,56,56,56	0
7	CA	C	503	1/1	0.97	0.04	-2.46	44,44,44,44	0
6	MG	B	502	1/1	0.99	0.22	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.