



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID : 4TV9
Title : Tubulin-PM060184 complex
Authors : Prota, A.E.; Bargsten, K.; Diaz, J.F.; Marsh, M.; Cuevas, C.; Liniger, M.; Neuhaus, C.; Andreu, J.M.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2014-06-26
Resolution : 2.00 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 (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

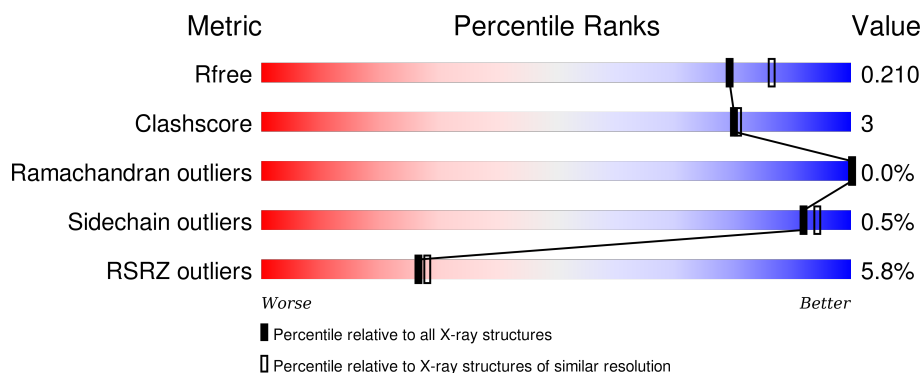
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	451	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	C	451	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
2	B	445	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
2	D	445	<div> <div>3%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
3	E	143	<div> <div>5%</div> <div>80%</div> <div>6%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
8	GOL	B	504	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18487 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	13	0
			3490	2217	587	661	25			
1	C	440	Total	C	N	O	S	0	15	0
			3506	2222	588	672	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	10	0
			3366	2123	566	649	28			
2	D	421	Total	C	N	O	S	0	6	0
			3333	2099	562	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	4	0
			1027	634	184	204	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

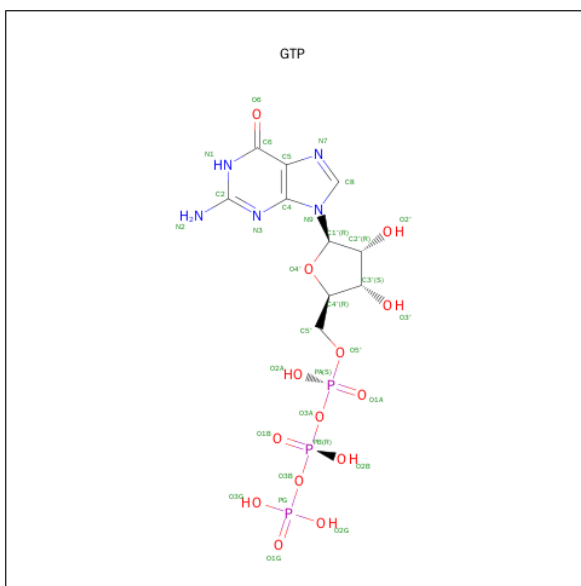
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	7	0
			2796	1805	467	510	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	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	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	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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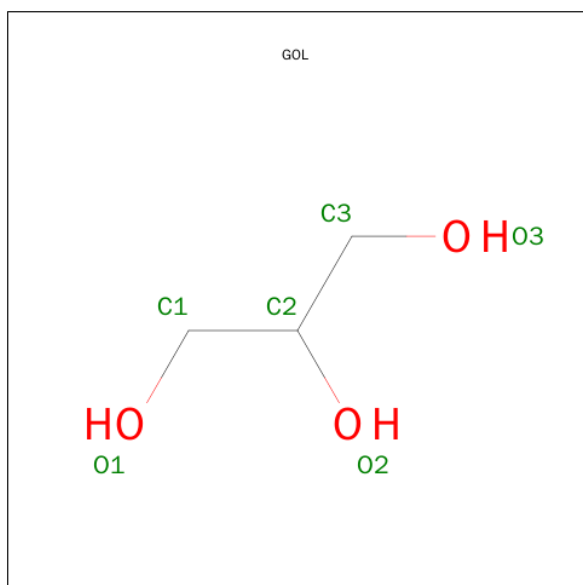
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

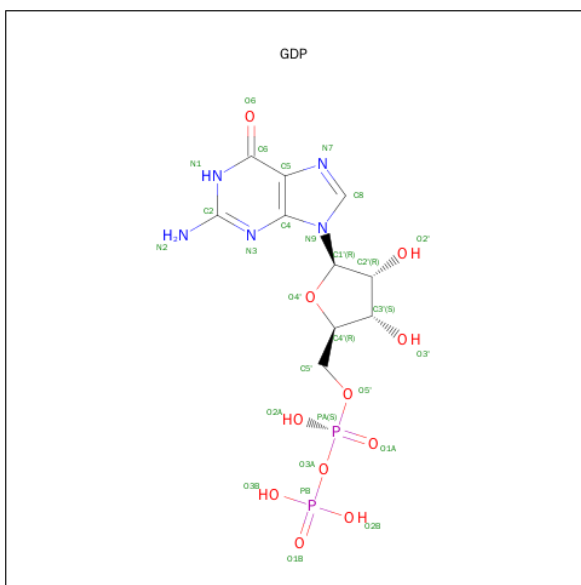
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



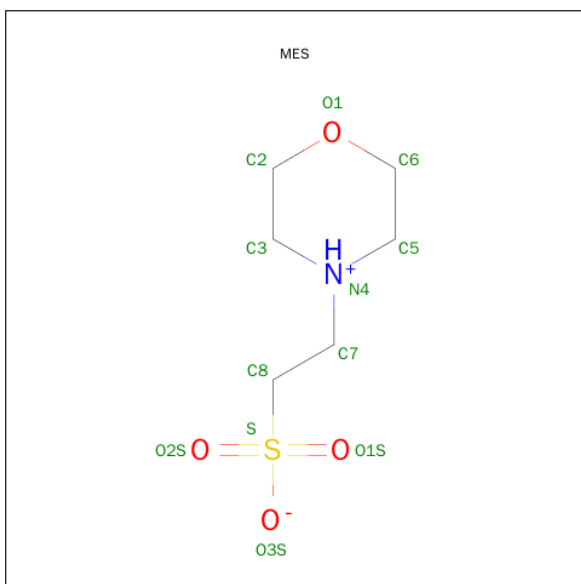
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



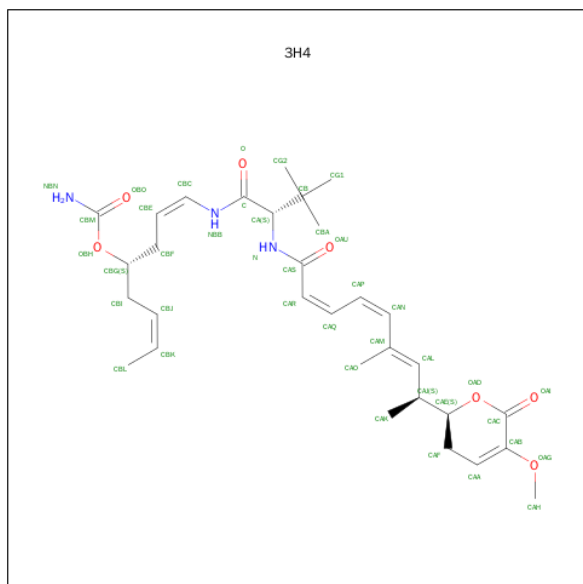
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



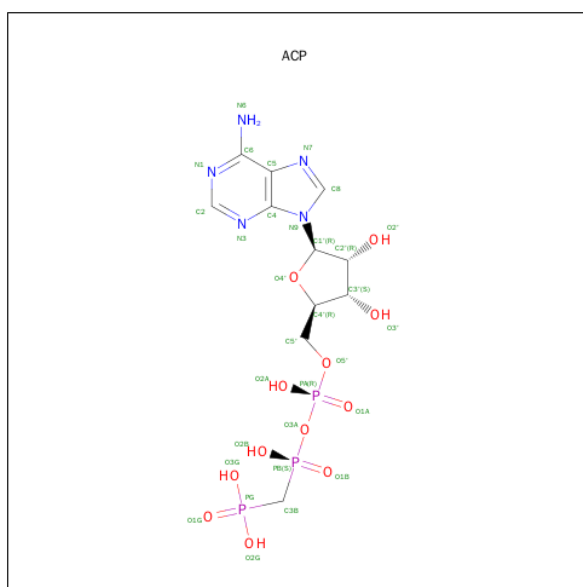
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (1Z,4S,6Z)-1-[(N-{(2Z,4Z,6E,8S)-8-[(2S)-5-methoxy-6-oxo-3,6-dihydro-2H-pyran-2-yl]-6-methylnona-2,4,6-trienoyl}-3-methyl-L-valyl)amino]octa-1,6-dien-4-yl carbamate (three-letter code: 3H4) (formula: C₃₁H₄₅N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			41	31	3	7		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

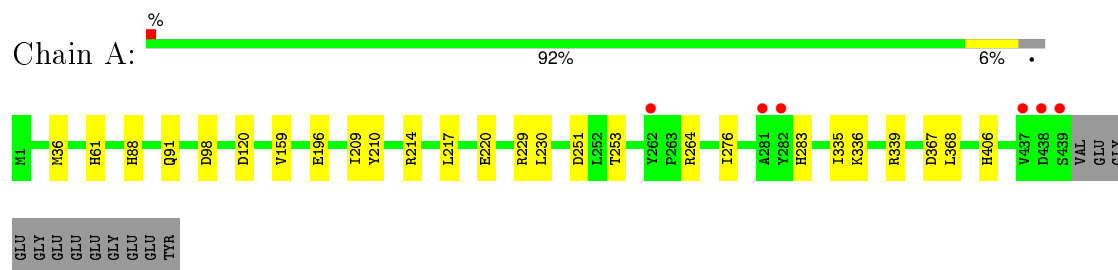
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	143	Total	O	0	0
			143	143		
13	B	134	Total	O	0	0
			134	134		
13	C	245	Total	O	0	0
			245	245		
13	D	119	Total	O	0	0
			119	119		
13	E	42	Total	O	0	0
			42	42		
13	F	63	Total	O	0	0
			63	63		

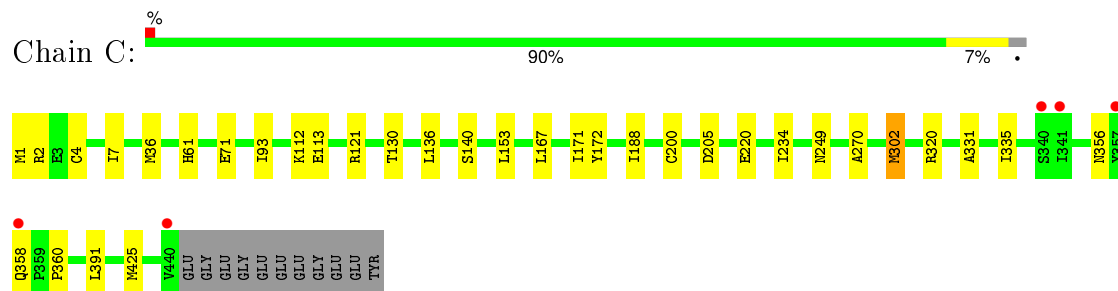
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

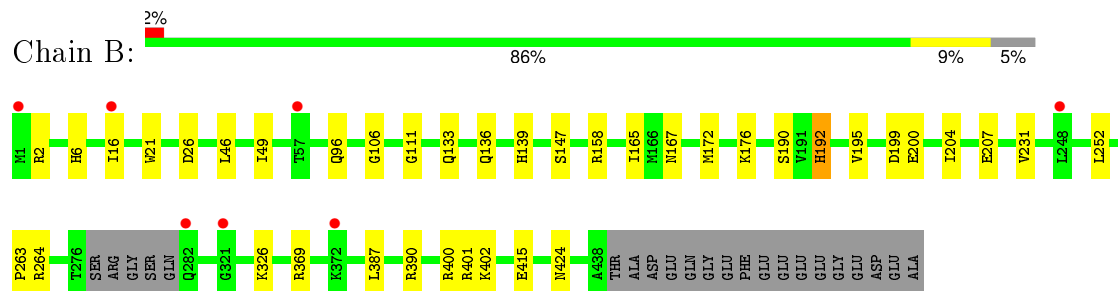
- Molecule 1: Tubulin alpha-1B chain



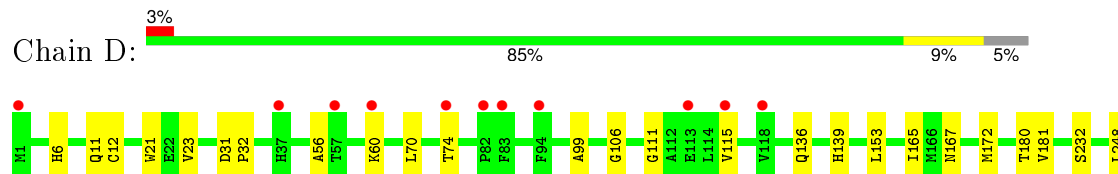
- Molecule 1: Tubulin alpha-1B chain

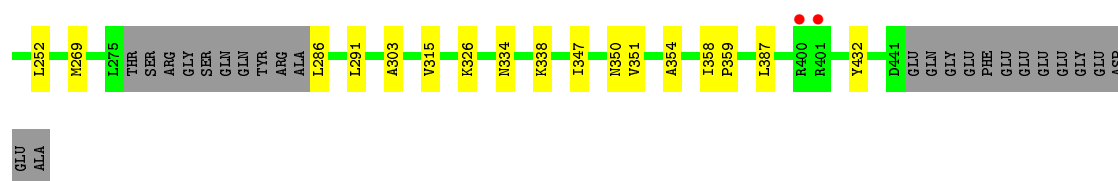


- Molecule 2: Tubulin beta-2B chain

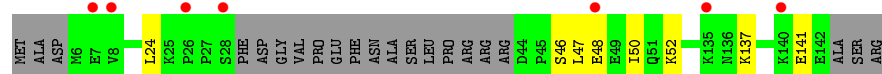
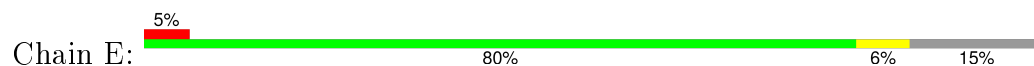


- Molecule 2: Tubulin beta-2B chain

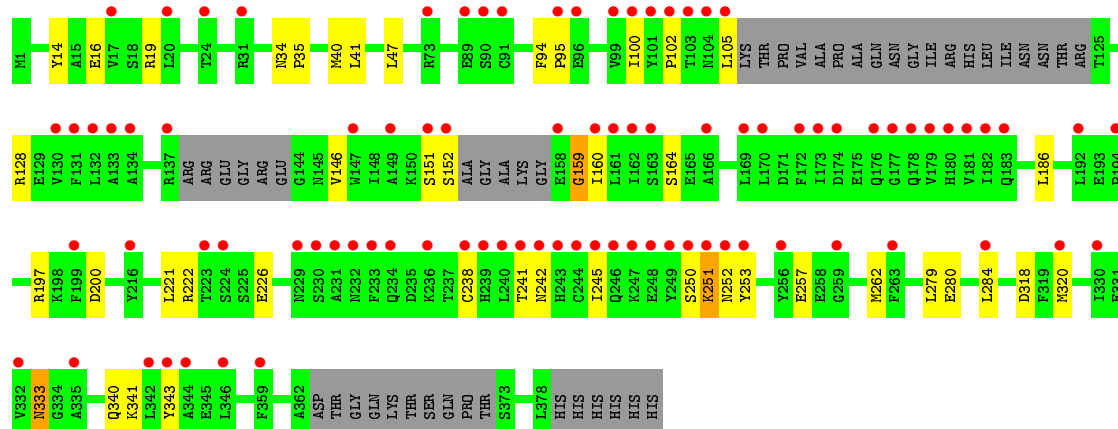
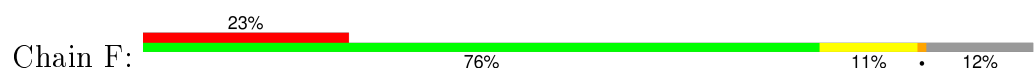




• Molecule 3: Stathmin-4



• 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	104.20Å 157.29Å 180.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.04 – 2.00 78.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.04-2.00) 99.9 (78.64-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.180 , 0.208 0.188 , 0.210	Depositor DCC
R_{free} test set	9968 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 199377 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18487	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, 0.375 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: GDP, GOL, MG, 3H4, CA, 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	0/3607	0.40	0/4897
1	C	0.24	0/3626	0.42	0/4926
2	B	0.23	0/3470	0.39	0/4699
2	D	0.22	0/3424	0.38	0/4640
3	E	0.21	0/1047	0.32	0/1390
4	F	0.21	0/2878	0.38	0/3890
All	All	0.23	0/18052	0.39	0/24442

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	3490	0	3444	16	0
1	C	3506	0	3439	20	0
2	B	3366	0	3273	26	0
2	D	3333	0	3233	26	0
3	E	1027	0	1050	5	0
4	F	2796	0	2799	27	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	13	5	0
11	D	41	0	45	10	0
12	F	31	0	14	2	0
13	A	143	0	0	2	0
13	B	134	0	0	1	0
13	C	245	0	0	0	0
13	D	119	0	0	1	0
13	E	42	0	0	0	0
13	F	63	0	0	3	0
All	All	18487	0	17374	120	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.

The worst 5 of 120 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)
11:D:503:3H4:CAQ	11:D:503:3H4:H13	1.80	1.09
11:D:503:3H4:H18	11:D:503:3H4:CAO	1.91	1.00
11:D:503:3H4:H18	11:D:503:3H4:H13	0.95	0.92
2:D:181:VAL:HG12	11:D:503:3H4:CAQ	2.17	0.74
2:B:264:ARG:NH2	2:B:424:ASN:OD1	2.26	0.69

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 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	450/451 (100%)	442 (98%)	8 (2%)	0	100	100
1	C	453/451 (100%)	446 (98%)	7 (2%)	0	100	100
2	B	429/445 (96%)	421 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	8 (2%)	0	100	100
3	E	122/143 (85%)	121 (99%)	1 (1%)	0	100	100
4	F	335/384 (87%)	320 (96%)	14 (4%)	1 (0%)	46	41
All	All	2212/2319 (95%)	2165 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	159	GLY

5.3.2 Protein sidechains [i](#)

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	383/379 (101%)	382 (100%)	1 (0%)	94	96
1	C	386/379 (102%)	384 (100%)	2 (0%)	92	94
2	B	375/383 (98%)	373 (100%)	2 (0%)	92	94
2	D	370/383 (97%)	369 (100%)	1 (0%)	94	96
3	E	114/127 (90%)	114 (100%)	0	100	100
4	F	312/342 (91%)	309 (99%)	3 (1%)	82	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1940/1993 (97%)	1931 (100%)	9 (0%)	92 94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	302	MET
4	F	333	ASN
4	F	251	LYS
2	B	192	HIS
2	D	139	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	180	HIS
4	F	252	ASN
4	F	183	GLN
2	B	167	ASN
4	F	243	HIS

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 16 ligands modelled in this entry, 7 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	25,34,34	1.14	2 (8%)	34,54,54	1.73	6 (17%)
8	GOL	A	504	-	5,5,5	0.33	0	5,5,5	0.31	0
9	GDP	B	501	6	23,30,30	1.13	2 (8%)	30,47,47	1.77	5 (16%)
10	MES	B	503	-	11,12,12	0.57	0	14,16,16	1.28	2 (14%)
8	GOL	B	504	-	5,5,5	0.36	0	5,5,5	0.21	0
5	GTP	C	501	6	25,34,34	1.14	2 (8%)	34,54,54	1.69	6 (17%)
9	GDP	D	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.80	6 (20%)
11	3H4	D	503	-	38,41,41	0.93	2 (5%)	42,54,54	1.51	7 (16%)
12	ACP	F	401	6	25,33,33	1.65	6 (24%)	31,52,52	1.81	4 (12%)

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
8	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
11	3H4	D	503	-	-	0/45/59/59	0/1/1/1
12	ACP	F	401	6	-	0/15/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O2B	-3.23	1.48	1.56
11	D	503	3H4	OAD-CAE	-2.42	1.43	1.46
11	D	503	3H4	C-NBB	2.47	1.37	1.34
12	F	401	ACP	PG-O2G	2.66	1.61	1.54
12	F	401	ACP	PG-O3G	2.67	1.61	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	F	401	ACP	N3-C2-N1	-6.71	123.75	128.89
11	D	503	3H4	CAF-CAE-CAJ	-5.28	109.19	116.61
12	F	401	ACP	PA-O3A-PB	-4.23	120.84	132.73
5	C	501	GTP	C5-C6-N1	-4.13	117.94	123.59
5	A	501	GTP	C5-C6-N1	-4.13	117.94	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	A	504	GOL	1	0
10	B	503	MES	5	0
9	D	501	GDP	1	0
11	D	503	3H4	10	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	439/451 (97%)	0.25	6 (1%) 78 78	35, 56, 91, 137	0
1	C	440/451 (97%)	0.44	5 (1%) 82 83	30, 43, 68, 115	0
2	B	423/445 (95%)	0.43	7 (1%) 73 73	33, 53, 90, 139	2 (0%)
2	D	421/445 (94%)	0.34	13 (3%) 52 53	37, 60, 90, 114	5 (1%)
3	E	122/143 (85%)	0.64	7 (5%) 27 29	40, 69, 108, 124	0
4	F	338/384 (88%)	1.39	88 (26%) 1 1	45, 78, 145, 175	0
All	All	2183/2319 (94%)	0.54	126 (5%) 26 28	30, 56, 104, 175	7 (0%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	8.5
1	A	439	SER	7.3
4	F	177	GLY	6.7
4	F	232	ASN	6.5
4	F	248	GLU	6.5

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 ⓘ

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
8	GOL	B	504	6/6	0.84	0.23	3.69	80,81,82,84	0
10	MES	B	503	12/12	0.90	0.17	1.89	63,73,86,91	0
11	3H4	D	503	41/41	0.91	0.17	1.00	55,73,81,83	0
5	GTP	C	501	32/32	0.98	0.15	0.62	28,34,36,38	0
9	GDP	D	501	28/28	0.94	0.15	0.60	48,57,65,71	0
8	GOL	A	504	6/6	0.84	0.13	0.54	67,85,89,92	0
5	GTP	A	501	32/32	0.98	0.14	0.42	31,40,43,57	0
7	CA	C	503	1/1	0.99	0.12	-0.24	56,56,56,56	0
9	GDP	B	501	28/28	0.99	0.15	-0.33	30,36,40,42	0
12	ACP	F	401	31/31	0.92	0.17	-1.11	69,82,127,162	0
7	CA	A	503	1/1	0.96	0.08	-2.28	72,72,72,72	0
6	MG	B	502	1/1	0.99	0.18	-	30,30,30,30	0
6	MG	A	502	1/1	0.92	0.10	-	38,38,38,38	0
6	MG	D	502	1/1	0.91	0.07	-	52,52,52,52	0
6	MG	C	502	1/1	0.94	0.10	-	34,34,34,34	0
6	MG	F	402	1/1	0.61	0.09	-	74,74,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.