



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID : 4TUY
Title : Tubulin-Rhizoxin 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 : 2014-06-25
Resolution : 2.10 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

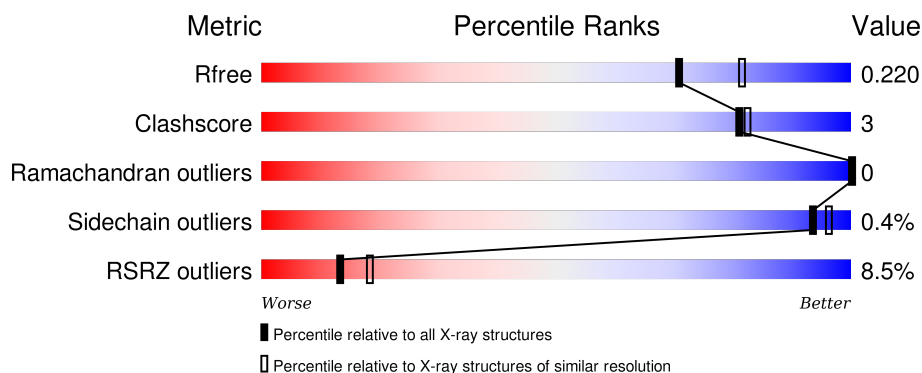
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	C	451	<div> <div>%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
2	B	445	<div> <div>%</div> <div>88%</div> <div>8%</div> <div>5%</div> </div>
2	D	445	<div> <div>8%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
3	E	143	<div> <div>6%</div> <div>80%</div> <div>.</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (32%), green (80%), yellow (7%), and grey (13%). The segments are stacked horizontally, with the red segment starting from the left and the grey segment ending on the right. The percentages are labeled above each segment.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18801 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	438	Total	C	N	O	S	0	12	0
			3475	2210	583	657	25			
1	C	440	Total	C	N	O	S	0	10	0
			3475	2203	585	663	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	8	0
			3372	2121	571	652	28			
2	D	422	Total	C	N	O	S	0	3	0
			3325	2090	563	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1002	619	182	196	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

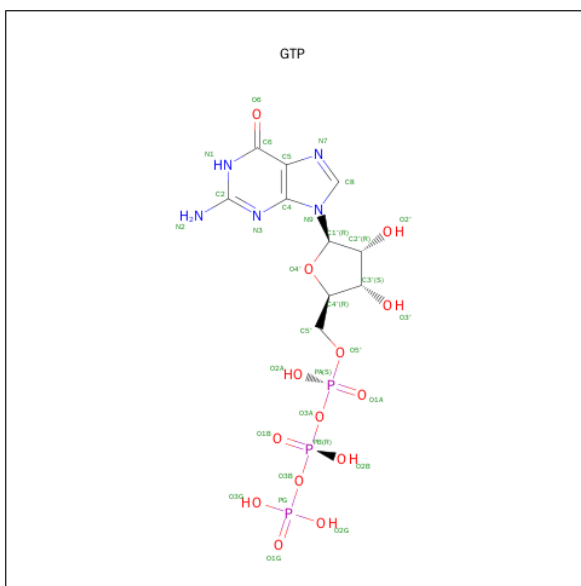
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	335	Total	C	N	O	S	0	0	0
			2749	1768	467	500	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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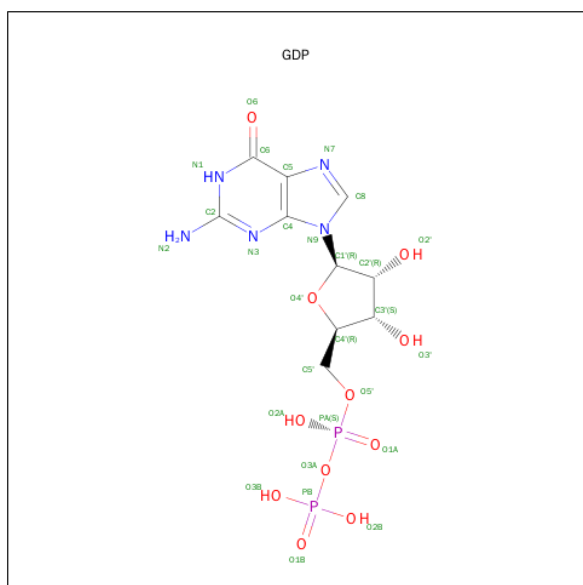
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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		

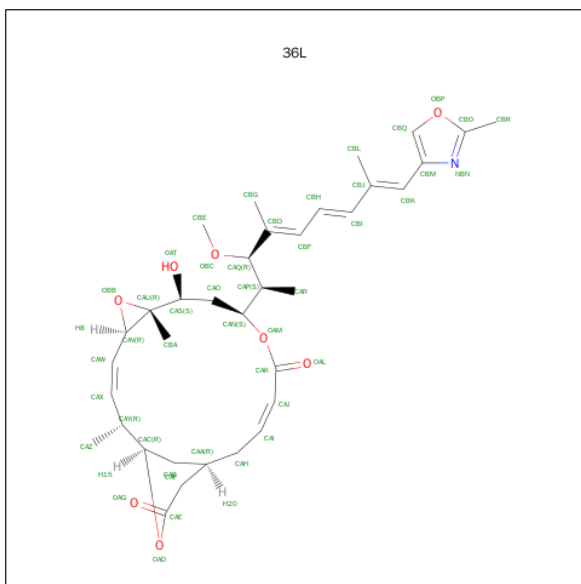
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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

- Molecule 10 is (1R,2R,3E,5R,7R,8S,10S,13E,16R)-8-hydroxy-10-[(2S,3R,4E,6E,8E)-3-methoxy-4,8-dimethyl-9-(2-methyl-1,3-oxazol-4-yl)nona-4,6,8-trien-2-yl]-2,7-dimethyl-6,11,19-trioxatricyclo[14.3.1.0 5,7]icosa-3,13-diene-12,18-dione (three-letter code: 36L) (formula: C₃₅H₄₇NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			44	35	1	8		

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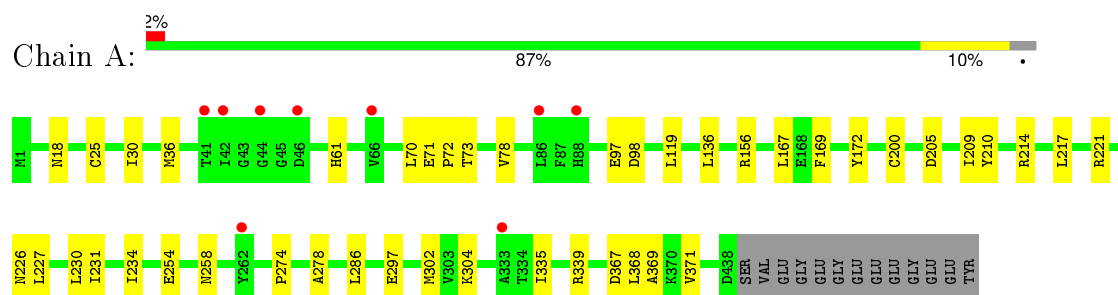
- Molecule 12 is water.

WORLDWIDE
 PDB
PROTEIN DATA BANK

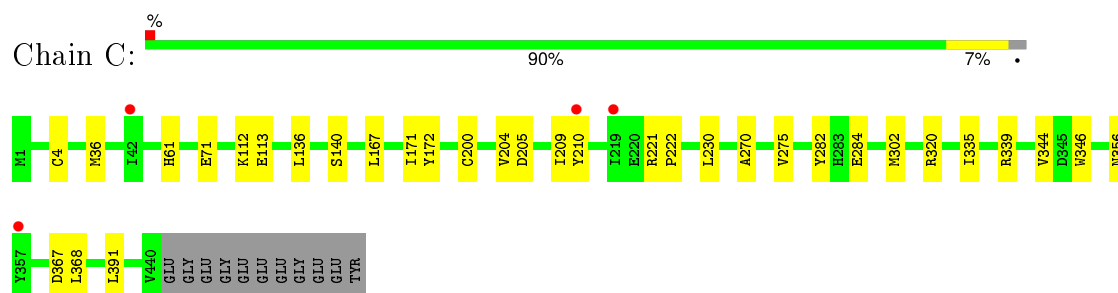
3 Residue-property plots [i](#)

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.

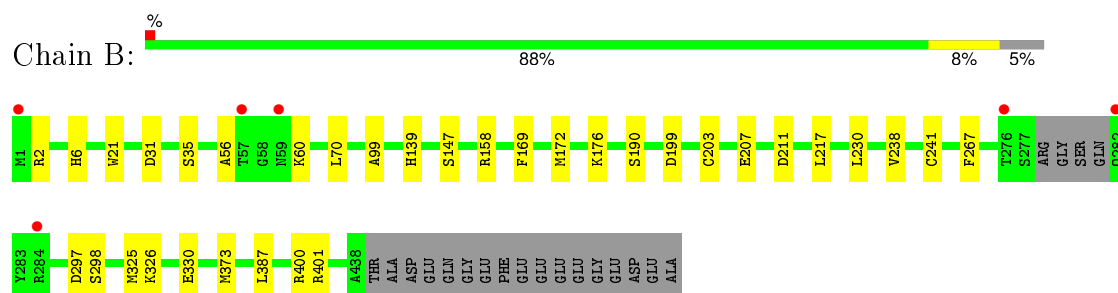
- Molecule 1: Tubulin alpha-1B chain



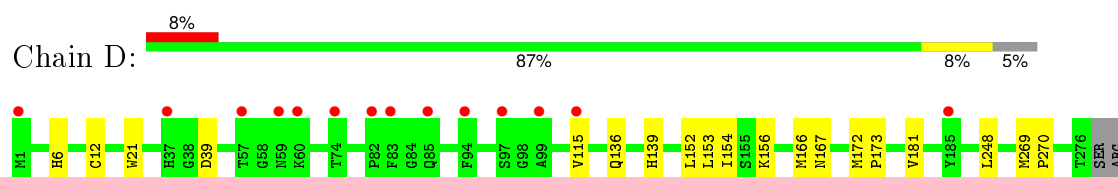
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain

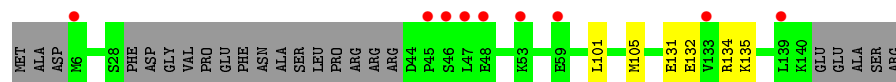
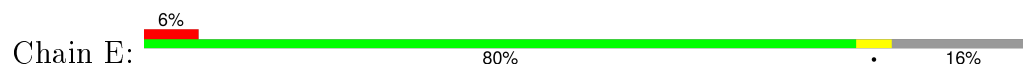


- Molecule 2: Tubulin beta-2B chain

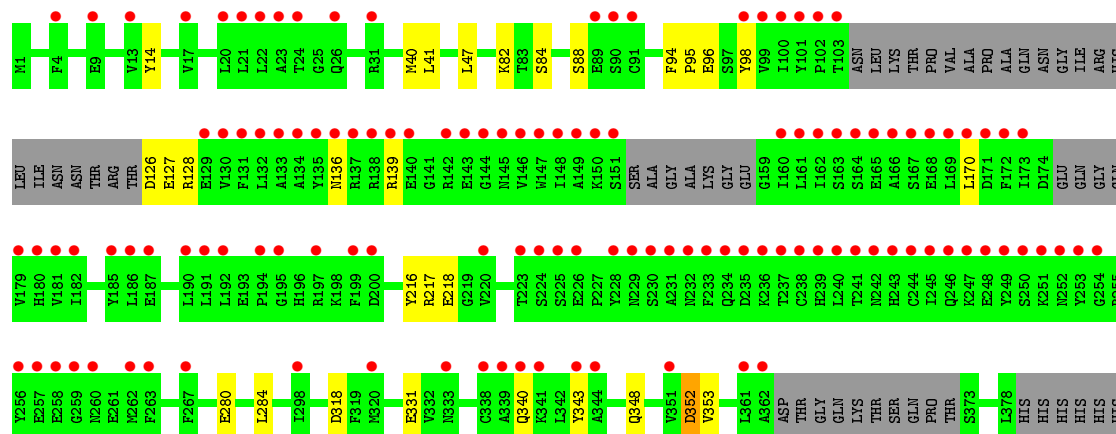
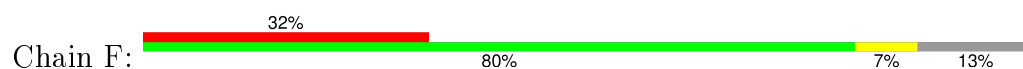




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.31Å 156.92Å 181.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.70 – 2.10 68.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.70-2.10) 100.0 (68.38-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.184 , 0.217 0.192 , 0.220	Depositor DCC
R_{free} test set	8662 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.0	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 173211 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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, MG, CA, 36L, 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	0/3590	0.39	0/4875
1	C	0.23	0/3583	0.39	0/4867
2	B	0.22	0/3467	0.38	0/4695
2	D	0.21	0/3407	0.37	0/4615
3	E	0.21	0/1016	0.32	0/1348
4	F	0.21	0/2810	0.37	0/3794
All	All	0.22	0/17873	0.38	0/24194

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	3475	0	3429	30	0
1	C	3475	0	3410	18	0
2	B	3372	0	3265	21	0
2	D	3325	0	3211	24	0
3	E	1002	0	1026	3	0
4	F	2749	0	2728	16	0
5	A	32	0	12	0	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	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	13	3	0
10	D	44	0	47	10	0
11	F	31	0	14	2	0
12	A	244	0	0	2	0
12	B	226	0	0	2	0
12	C	378	0	0	1	0
12	D	172	0	0	3	0
12	E	74	0	0	0	0
12	F	95	0	0	0	0
All	All	18801	0	17191	113	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 113 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)
10:D:503:36L:H40	10:D:503:36L:H47	1.20	1.13
10:D:503:36L:H40	10:D:503:36L:CBQ	1.91	0.96
2:D:404:PHE:HE1	10:D:503:36L:H41	1.36	0.90
2:D:404:PHE:CE1	10:D:503:36L:H41	2.14	0.82
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82

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	448/451 (99%)	437 (98%)	11 (2%)	0	100	100
1	C	448/451 (99%)	441 (98%)	7 (2%)	0	100	100
2	B	428/445 (96%)	420 (98%)	8 (2%)	0	100	100
2	D	421/445 (95%)	414 (98%)	7 (2%)	0	100	100
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
4	F	325/384 (85%)	315 (97%)	10 (3%)	0	100	100
All	All	2188/2319 (94%)	2144 (98%)	44 (2%)	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	381/379 (100%)	381 (100%)	0	100	100
1	C	381/379 (100%)	380 (100%)	1 (0%)	94	97
2	B	375/383 (98%)	373 (100%)	2 (0%)	92	95
2	D	368/383 (96%)	367 (100%)	1 (0%)	94	97
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	302/342 (88%)	299 (99%)	3 (1%)	82	87
All	All	1917/1993 (96%)	1910 (100%)	7 (0%)	93	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	139	HIS
4	F	353	VAL
4	F	217	ARG
2	B	373	MET
4	F	352	ASP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	1.77	6 (17%)
8	GDP	B	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.77	6 (20%)
9	MES	B	503	-	11,12,12	0.59	0	14,16,16	1.19	2 (14%)
5	GTP	C	501	6	25,34,34	1.15	2 (8%)	34,54,54	1.73	6 (17%)
8	GDP	D	501	6	23,30,30	1.16	2 (8%)	30,47,47	1.83	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	36L	D	503	-	40,47,47	1.13	3 (7%)	35,67,67	1.39	8 (22%)
11	ACP	F	401	6	25,33,33	1.40	5 (20%)	31,52,52	1.82	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	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	6	-	0/12/32/32	0/3/3/3
10	36L	D	503	-	-	1/51/73/73	0/0/4/4
11	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)
10	D	503	36L	OBB-CAV	-4.21	1.40	1.45
10	D	503	36L	OBB-CAU	-4.12	1.40	1.45
10	D	503	36L	OAD-CAC	-2.29	1.43	1.46
11	F	401	ACP	PB-O2B	2.01	1.61	1.56
11	F	401	ACP	PG-O3G	2.66	1.61	1.54

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-6.73	123.74	128.89
11	F	401	ACP	PA-O3A-PB	-4.17	121.02	132.73
5	C	501	GTP	C5-C6-N1	-4.12	117.96	123.59
8	D	501	GDP	C5-C6-N1	-4.08	118.01	123.59
5	A	501	GTP	C5-C6-N1	-4.07	118.03	123.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	503	36L	CBJ-CBK-CBM-NBN

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	3	0
8	D	501	GDP	1	0
10	D	503	36L	10	0
11	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	438/451 (97%)	0.32	9 (2%) 67 72	28, 43, 76, 92	0
1	C	440/451 (97%)	0.29	4 (0%) 85 88	22, 34, 57, 106	0
2	B	424/445 (95%)	0.40	6 (1%) 78 82	24, 41, 73, 113	1 (0%)
2	D	422/445 (94%)	0.63	34 (8%) 15 20	31, 52, 83, 108	4 (0%)
3	E	120/143 (83%)	0.78	9 (7%) 17 23	35, 57, 90, 101	0
4	F	335/384 (87%)	1.76	123 (36%) 0 0	35, 68, 128, 158	0
All	All	2179/2319 (93%)	0.64	185 (8%) 13 18	22, 46, 89, 158	5 (0%)

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	10.1
4	F	249	TYR	10.0
4	F	173	ILE	9.6
4	F	172	PHE	8.6
4	F	251	LYS	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
10	36L	D	503	44/44	0.84	0.30	1.60	51,64,73,74	0
5	GTP	C	501	32/32	0.99	0.15	0.44	18,26,29,34	0
5	GTP	A	501	32/32	0.98	0.14	0.39	22,29,34,37	0
8	GDP	B	501	28/28	0.98	0.15	0.31	23,29,34,34	0
8	GDP	D	501	28/28	0.95	0.14	-0.20	37,46,60,60	0
9	MES	B	503	12/12	0.95	0.15	-0.81	43,52,62,64	0
11	ACP	F	401	31/31	0.91	0.16	-1.60	61,71,119,144	0
7	CA	C	503	1/1	0.98	0.04	-2.74	43,43,43,43	0
7	CA	A	503	1/1	0.92	0.06	-3.38	59,59,59,59	0
6	MG	B	502	1/1	1.00	0.15	-	20,20,20,20	0
6	MG	C	502	1/1	0.98	0.14	-	25,25,25,25	0
6	MG	A	502	1/1	0.99	0.11	-	29,29,29,29	0
6	MG	F	402	1/1	0.87	0.06	-	61,61,61,61	0
6	MG	D	502	1/1	0.92	0.08	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.