



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I55
Title : Crystal structure of tubulin-stathmin-TTL complex
Authors : Prota, A.E.; Bargsten, K.; Zurwerra, D.; Field, J.J.; Diaz, J.F.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2012-11-28
Resolution : 2.20 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

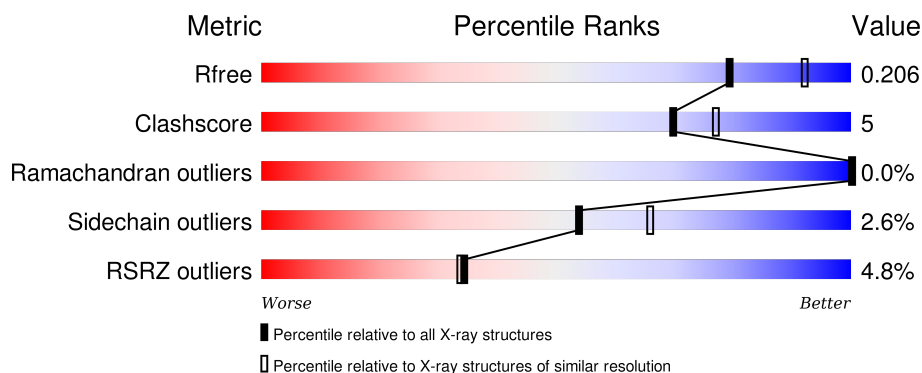
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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>88%</div> <div>9%</div> <div>.</div> </div>
1	C	450	<div> <div>88%</div> <div>8%</div> <div>..</div> </div>
2	B	445	<div> <div>84%</div> <div>11%</div> <div>.</div> </div>
2	D	445	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
3	E	143	<div> <div>2%</div> <div>78%</div> <div>7%</div> <div>13%</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
6	MG	A	502	-	-	-	X
6	MG	C	502	-	-	-	X
6	MG	F	701	-	-	-	X
7	CA	A	505	-	-	-	X
7	CA	B	503	-	-	-	X
7	CA	C	503	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 36041 atoms, of which 17435 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	442	Total	C	H	N	O	S	0	7	0
			6911	2207	3421	591	668	24			
1	C	440	Total	C	H	N	O	S	0	12	0
			6899	2203	3420	586	664	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	8	0
			6685	2131	3295	579	653	27			
2	D	421	Total	C	H	N	O	S	0	5	0
			6533	2087	3213	562	644	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	124	Total	C	H	N	O	S	0	4	0
			2109	643	1067	188	205	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	CLONING ARTIFACT	UNP P63043
E	4	ALA	SER	CLONING ARTIFACT	UNP P63043

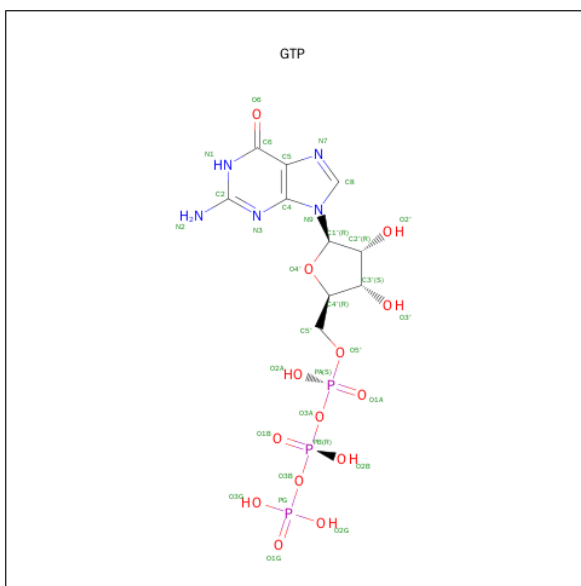
- Molecule 4 is a protein called Tubulin tyrosine ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	353	Total	C	H	N	O	S	0	6	0
			5869	1885	2936	504	528	16			

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	2	Total	Mg	0	0
			2	2		
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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		

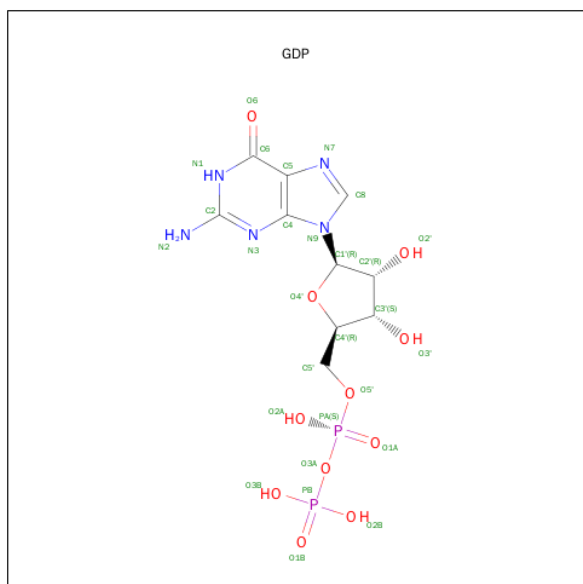
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

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



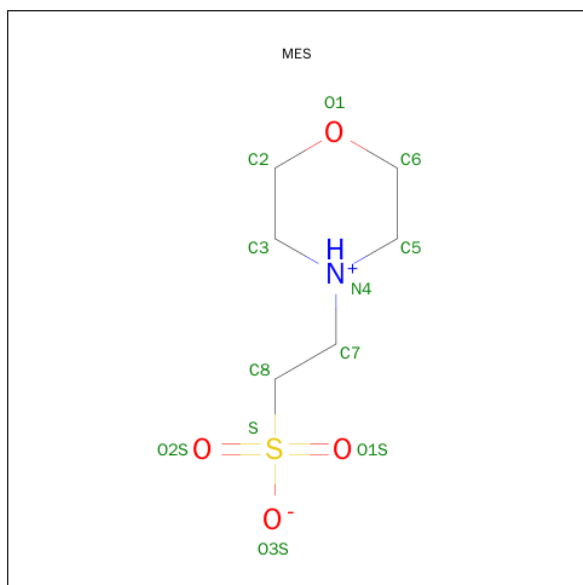
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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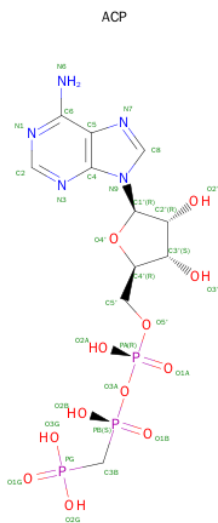
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- 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	H	N	O	S	0	0
			25	6	13	1	4	1		
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 11 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	
11	F	1	Total 48	C 11	H 17	N 5	O 12	P 3	0	0

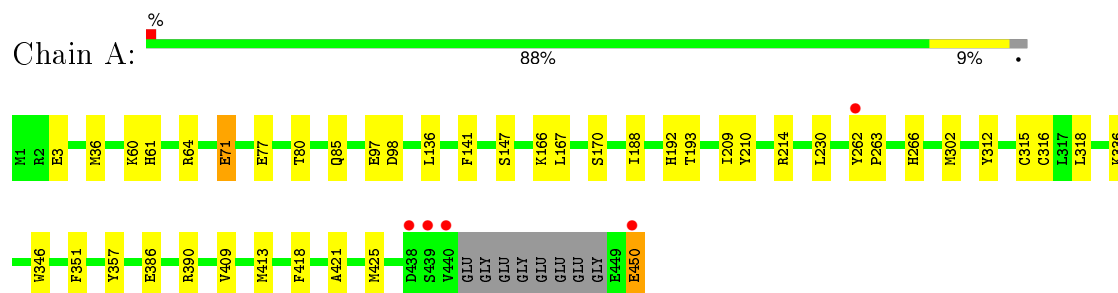
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	169	Total O 169 169	0	0
12	B	157	Total O 157 157	0	0
12	C	280	Total O 280 280	0	0
12	D	80	Total O 80 80	0	0
12	E	35	Total O 35 35	0	0
12	F	44	Total O 44 44	0	0

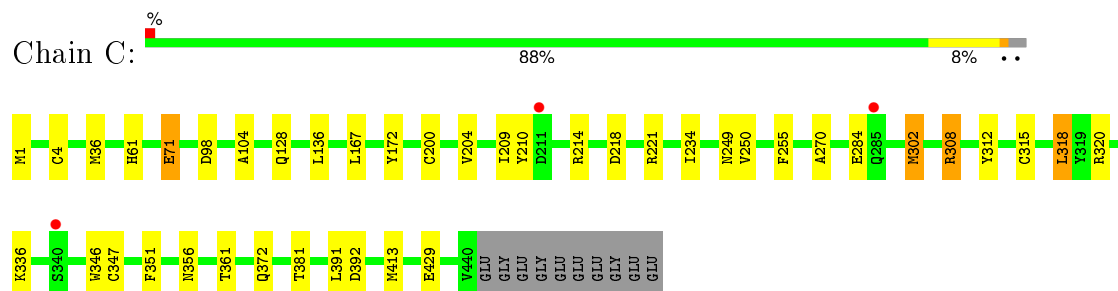
3 Residue-property plots [i](#)

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.

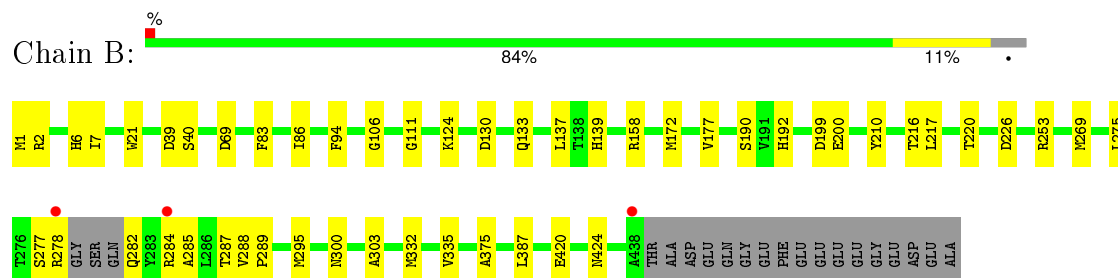
- Molecule 1: Tubulin alpha-1B chain



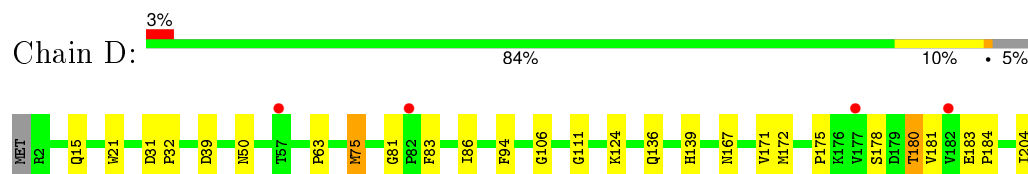
- Molecule 1: Tubulin alpha-1B chain

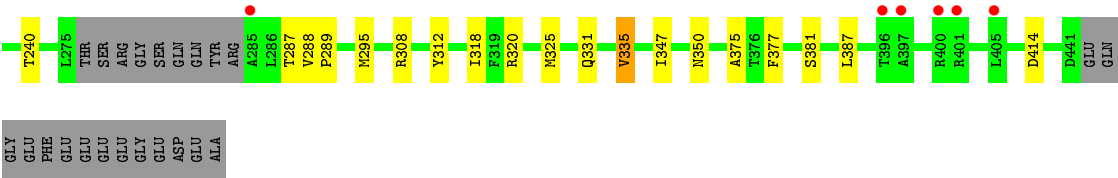


- Molecule 2: Tubulin beta-2B chain

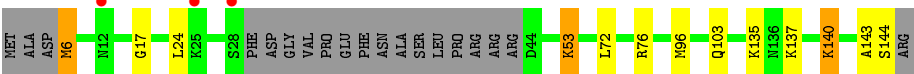
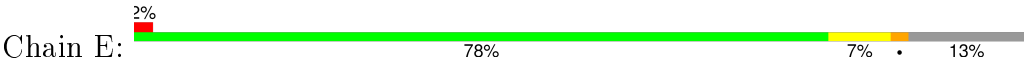


- Molecule 2: Tubulin beta-2B chain

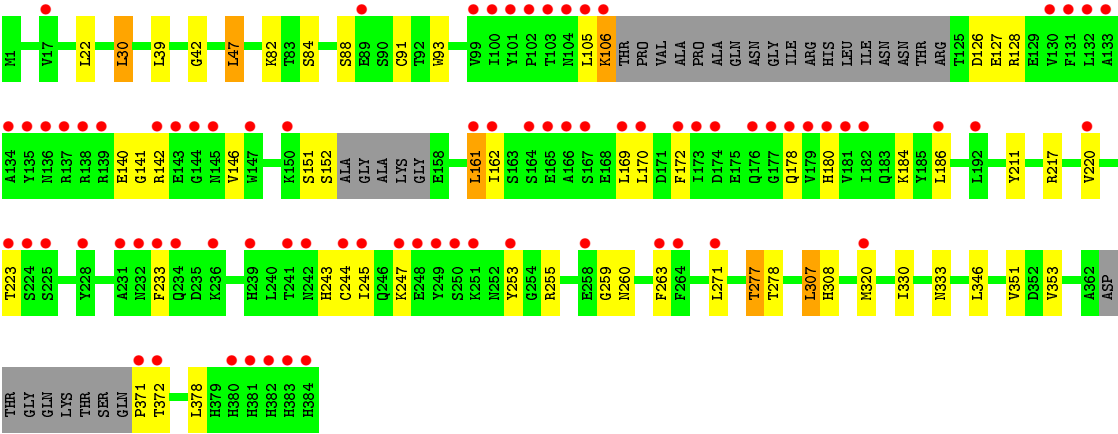
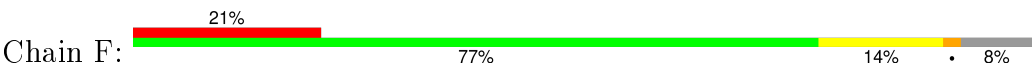




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase, TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.16Å 156.47Å 181.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.84 – 2.20 78.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (71.84-2.20) 99.2 (78.50-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.208 0.168 , 0.206	Depositor DCC
R_{free} test set	7515 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	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 149402 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36041	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, CL, 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	0.41	0/3588	0.58	0/4867
1	C	0.50	0/3595	0.61	1/4881 (0.0%)
2	B	0.44	0/3495	0.55	0/4732
2	D	0.38	0/3407	0.53	0/4616
3	E	0.44	0/1063	0.50	0/1411
4	F	0.33	0/3020	0.52	0/4078
All	All	0.42	0/18168	0.56	1/24585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ARG	NE-CZ-NH1	5.11	122.86	120.30

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	3421	3408	27	0
1	C	3479	3420	3395	29	0
2	B	3390	3295	3275	32	0
2	D	3320	3213	3201	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1042	1067	1062	10	0
4	F	2933	2936	2921	37	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	0	0
10	B	24	26	25	3	0
11	F	31	17	14	6	0
12	A	169	0	0	1	0
12	B	157	0	0	2	0
12	C	280	0	0	5	0
12	D	80	0	0	0	0
12	E	35	0	0	0	0
12	F	44	0	0	1	0
All	All	18606	17435	17349	159	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 5.

The worst 5 of 159 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.14	0.88
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.29	0.72
1:C:308:ARG:NE	12:C:802:HOH:O	2.23	0.71
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.31	0.69
2:B:199:ASP:OD2	10:B:504:MES:H32	1.94	0.68

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	445/450 (99%)	439 (99%)	6 (1%)	0	100	100
1	C	449/450 (100%)	438 (98%)	11 (2%)	0	100	100
2	B	429/445 (96%)	418 (97%)	11 (3%)	0	100	100
2	D	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	52	59
3	E	124/143 (87%)	121 (98%)	3 (2%)	0	100	100
4	F	351/384 (91%)	332 (95%)	19 (5%)	0	100	100
All	All	2219/2317 (96%)	2156 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	81	GLY

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	380/378 (100%)	377 (99%)	3 (1%)	86	93
1	C	382/378 (101%)	375 (98%)	7 (2%)	66	79
2	B	376/383 (98%)	370 (98%)	6 (2%)	70	82
2	D	367/383 (96%)	358 (98%)	9 (2%)	55	67
3	E	115/127 (91%)	109 (95%)	6 (5%)	29	33
4	F	325/342 (95%)	304 (94%)	21 (6%)	21	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1945/1991 (98%)	1893 (97%)	52 (3%)	54 64

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	335	VAL
3	E	135	LYS
4	F	346	LEU
2	D	414	ASP
3	E	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	283	HIS
1	A	301	GLN
1	C	197	HIS
4	F	379	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 19 ligands modelled in this entry, 12 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	1.02	1 (4%)	32,54,54	1.20	5 (15%)
9	GDP	B	501	6	23,30,30	1.60	6 (26%)	28,47,47	1.89	3 (10%)
10	MES	B	504	-	12,12,12	1.90	1 (8%)	16,16,16	1.50	2 (12%)
10	MES	B	505	-	12,12,12	2.01	1 (8%)	16,16,16	1.46	2 (12%)
5	GTP	C	501	6	25,34,34	0.95	1 (4%)	32,54,54	1.08	4 (12%)
9	GDP	D	600	6	23,30,30	1.32	3 (13%)	28,47,47	1.55	4 (14%)
11	ACP	F	703	6	25,33,33	1.65	6 (24%)	31,52,52	2.75	7 (22%)

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
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	1/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	600	6	-	0/12/32/32	0/3/3/3
11	ACP	F	703	6	-	0/15/38/38	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-5.98	1.67	1.78
10	B	504	MES	C8-S	-5.77	1.67	1.78
11	F	703	ACP	C2'-C3'	-3.05	1.45	1.53
9	B	501	GDP	C6-N1	-2.89	1.32	1.36
11	F	703	ACP	O3'-C3'	-2.28	1.37	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	703	ACP	N3-C2-N1	-8.77	122.18	128.89
11	F	703	ACP	O4'-C1'-N9	-6.70	94.06	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C1'-N9-C4	-3.96	120.96	126.94
11	F	703	ACP	PA-O3A-PB	-3.92	121.72	132.73
5	C	501	GTP	C4-C5-N7	-3.19	106.55	109.48

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	505	MES	C2-C3-C5-C6-N4-O1

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	3	0
11	F	703	ACP	6	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	442/450 (98%)	0.03	5 (1%) 82 82	29, 46, 79, 143	0
1	C	440/450 (97%)	0.27	3 (0%) 89 88	23, 35, 66, 116	1 (0%)
2	B	425/445 (95%)	0.16	3 (0%) 89 88	23, 43, 79, 128	2 (0%)
2	D	421/445 (94%)	0.21	13 (3%) 52 51	29, 56, 91, 150	7 (1%)
3	E	124/143 (86%)	0.25	3 (2%) 62 61	32, 62, 107, 141	0
4	F	353/384 (91%)	1.07	79 (22%) 1 1	39, 72, 148, 175	0
All	All	2205/2317 (95%)	0.32	106 (4%) 34 34	23, 49, 104, 175	10 (0%)

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	9.4
4	F	173	ILE	8.4
1	A	440	VAL	8.0
4	F	130	VAL	6.6
4	F	134	ALA	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 [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	0.93	0.24	8.24	38,38,38,38	0
6	MG	C	502	1/1	0.95	0.22	7.52	33,33,33,33	0
7	CA	A	505	1/1	0.90	0.24	4.87	95,95,95,95	0
7	CA	B	503	1/1	0.94	0.26	4.84	91,91,91,91	0
7	CA	C	503	1/1	0.96	0.23	4.79	55,55,55,55	0
6	MG	F	701	1/1	0.93	0.37	3.78	93,93,93,93	0
9	GDP	B	501	28/28	0.99	0.19	1.58	19,30,41,42	0
5	GTP	A	501	32/32	0.99	0.16	1.29	24,33,40,45	0
5	GTP	C	501	32/32	0.99	0.16	1.15	22,27,34,37	0
7	CA	A	503	1/1	0.96	0.14	0.86	60,60,60,60	0
10	MES	B	505	12/12	0.97	0.14	0.33	71,86,102,102	0
10	MES	B	504	12/12	0.98	0.14	0.03	48,64,83,93	0
9	GDP	D	600	28/28	0.97	0.13	-0.47	41,54,75,77	0
11	ACP	F	703	31/31	0.91	0.16	-1.06	58,94,138,143	0
6	MG	B	506	1/1	0.89	0.32	-	60,60,60,60	0
6	MG	F	702	1/1	0.97	0.16	-	94,94,94,94	0
8	CL	A	504	1/1	0.91	0.15	-	67,67,67,67	0
6	MG	D	601	1/1	0.82	0.16	-	64,64,64,64	0
6	MG	B	502	1/1	0.98	0.28	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.