



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:03 AM GMT

PDB ID : 3E22
Title : Tubulin-colchicine-soblidotin:Stathmin-like domain complex
Authors : Cormier, A.; Marchand, M.; Ravelli, R.B.; Knossow, M.; Gigant, B.
Deposited on : 2008-08-05
Resolution : 3.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

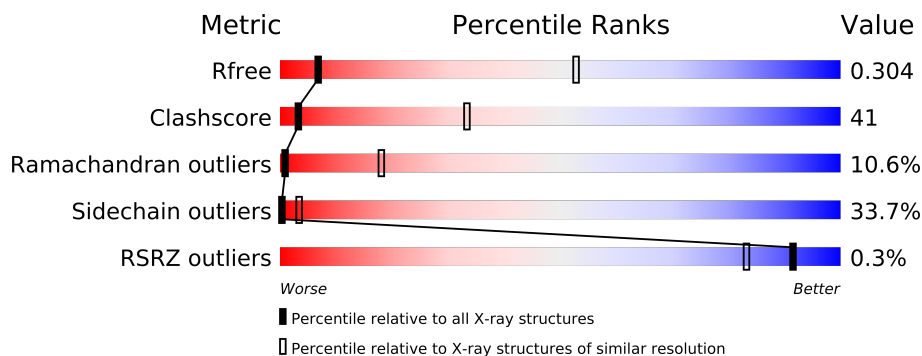
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	449	
1	C	449	
2	B	445	
2	D	445	
3	E	142	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MG	A	601	-	X
7	LOC	B	700	-	X
7	LOC	D	700	-	X
8	TZT	B	800	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14154 atoms, of which 0 are hydrogen and 0 are deuterium.

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-1C chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3290	2089	556	624	21			
1	C	421	Total	C	N	O	S	0	0	0
			3234	2055	547	611	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
A	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
A	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
A	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
C	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
C	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3238	2036	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3246	2041	549	632	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	SEE REMARK 999	UNP Q6B856
B	318	VAL	ILE	SEE REMARK 999	UNP Q6B856
D	203	SER	CYS	SEE REMARK 999	UNP Q6B856
D	318	VAL	ILE	SEE REMARK 999	UNP Q6B856

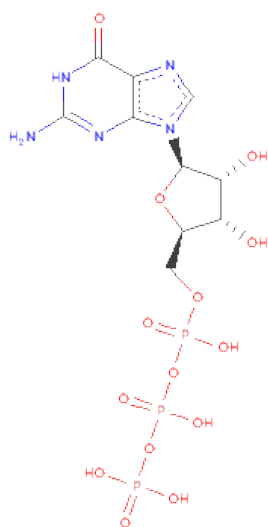
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			916	555	173	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

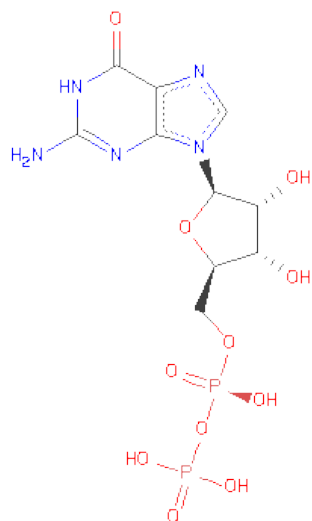


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

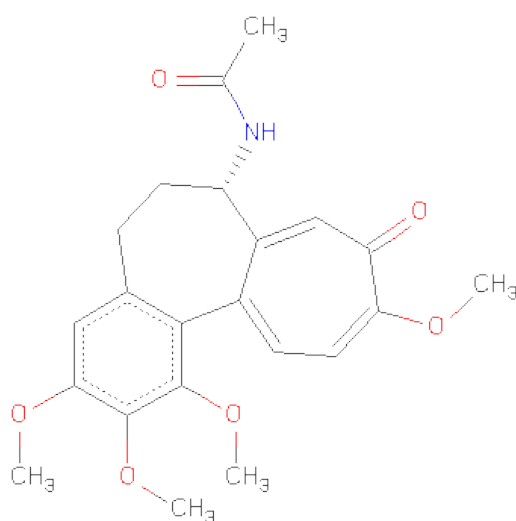
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



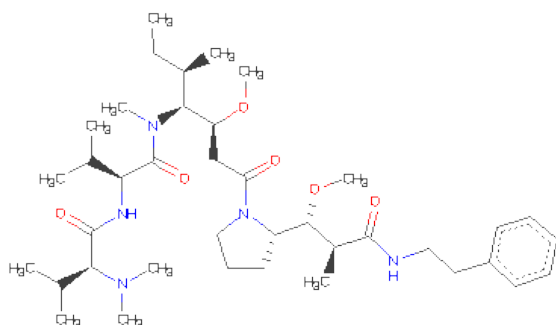
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	28	10	5	11	2	0	0
6	D	1	28	10	5	11	2	0	0

- Molecule 7 is N-[(7S)-1,2,3,10-TETRAMETHOXY-9-OXO-6,7-DIHYDRO-5H-BENZO[D]HEPTALEN-7-YL]ETHANAMIDE (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).

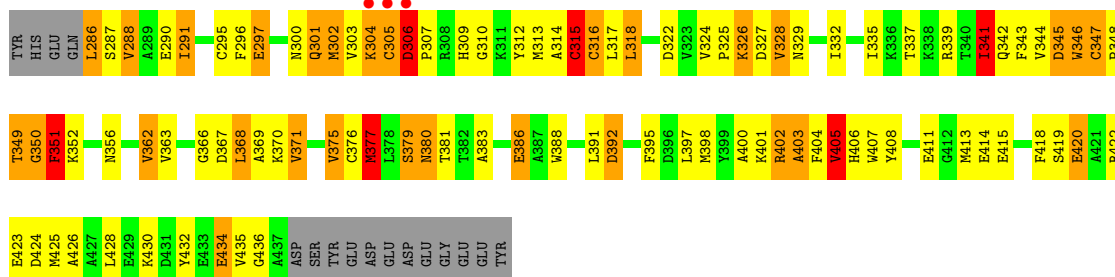


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is SOBLIDOTIN (three-letter code: TZT) (formula: $C_{39}H_{67}N_5O_6$).

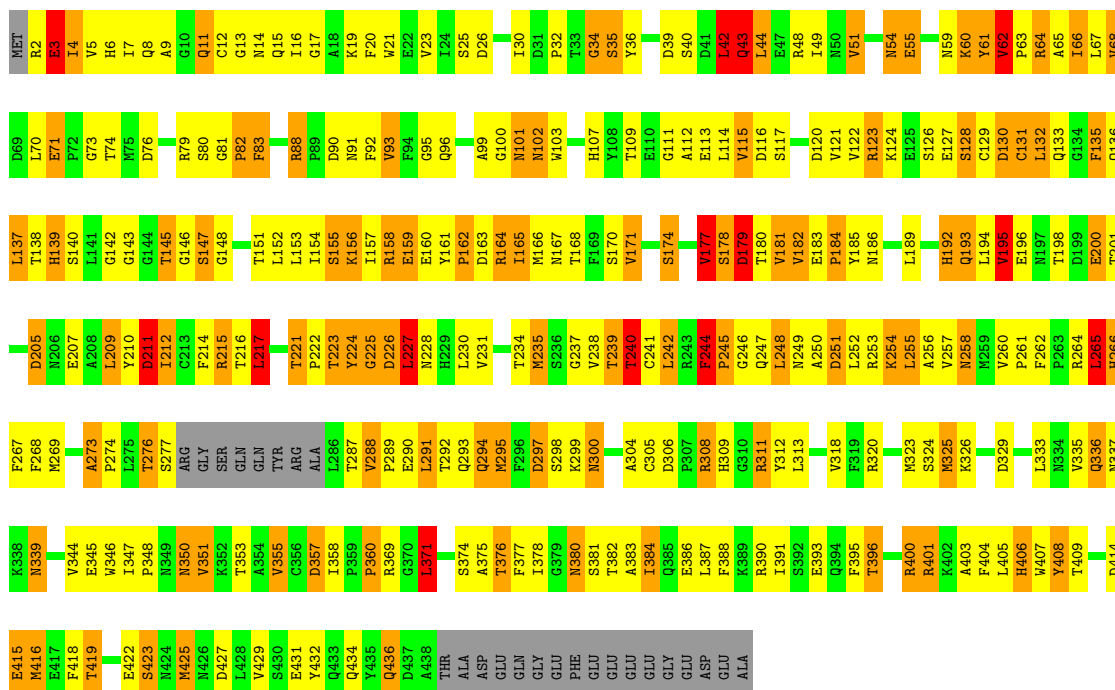


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			50	39	5	6		



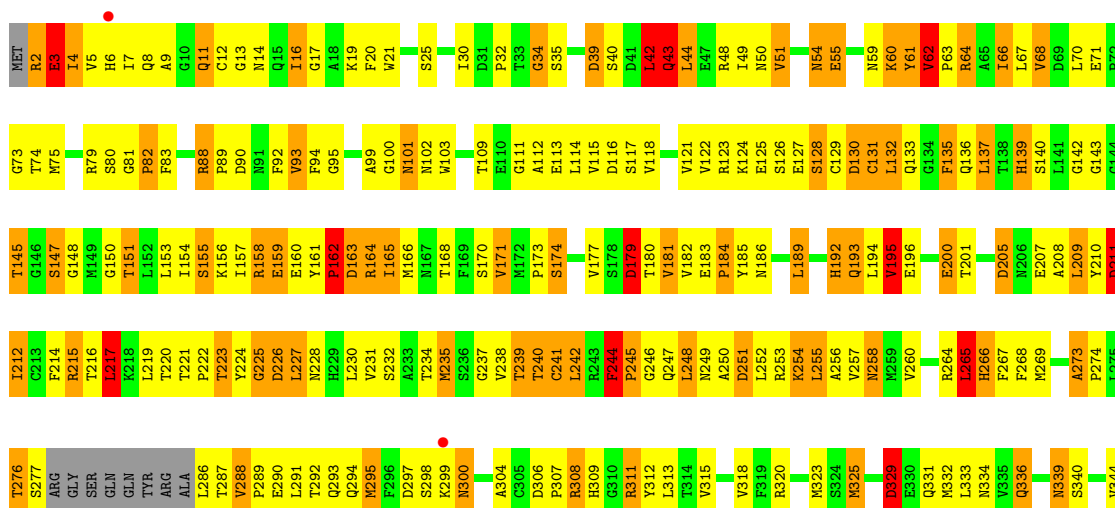
• Molecule 2: Tubulin beta-2B chain

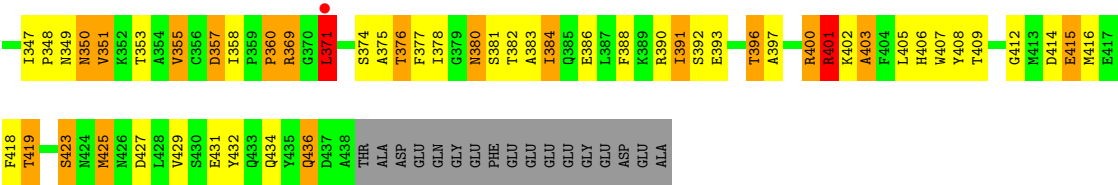
Chain B:



• Molecule 2: Tubulin beta-2B chain

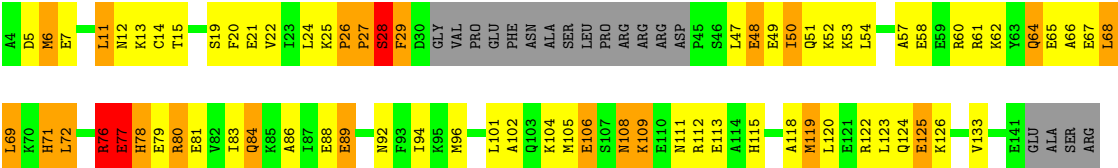
Chain D:





● Molecule 3: Stathmin-4

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	324.09Å 324.09Å 53.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 19.91 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.80) 97.6 (19.91-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.82Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.295 0.247 , 0.304	Depositor DCC
R_{free} test set	1598 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	140.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 105.9	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31414 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14154	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, LOC, MG, GDP, TZT

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	0.95	1/3367 (0.0%)	1.09	19/4579 (0.4%)
1	C	0.67	1/3308 (0.0%)	0.96	15/4498 (0.3%)
2	B	0.76	0/3310	0.99	11/4495 (0.2%)
2	D	0.61	0/3318	0.92	13/4505 (0.3%)
3	E	0.72	0/924	0.90	0/1239
All	All	0.76	2/14227 (0.0%)	0.99	58/19316 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLU	CD-OE1	5.64	1.31	1.25
1	C	436	GLY	C-O	-5.23	1.15	1.23

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	CA-CB-CG	7.48	132.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	7.28	124.86	118.30
1	A	33	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	76	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	47	ASP	CB-CG-OD2	6.64	124.28	118.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
1	A	265	ILE	Peptide
2	B	162	PRO	Peptide
2	B	244	PHE	Peptide
2	B	265	LEU	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3149	276	0
1	C	3234	0	3102	267	0
2	B	3238	0	3049	290	0
2	D	3246	0	3067	253	0
3	E	916	0	799	62	0
4	A	32	0	12	4	0
4	C	32	0	12	6	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	4	0
6	D	28	0	12	1	0
7	B	29	0	23	3	0
7	D	29	0	23	3	0
8	B	50	0	67	30	0
All	All	14154	0	13327	1115	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 1115 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.77	1.14
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.81	1.10
1:C:273:ALA:HB1	1:C:274:PRO:HD3	1.23	1.10
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.20	1.09
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.53	1.07

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	423/449 (94%)	295 (70%)	85 (20%)	43 (10%)	1	20
1	C	415/449 (92%)	300 (72%)	73 (18%)	42 (10%)	1	20
2	B	415/445 (93%)	289 (70%)	81 (20%)	45 (11%)	1	18
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	1	18
3	E	120/142 (84%)	71 (59%)	35 (29%)	14 (12%)	1	15
All	All	1788/1930 (93%)	1252 (70%)	347 (19%)	189 (11%)	1	18

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	SER
1	A	49	PHE
1	A	62	VAL
1	A	72	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	346/378 (92%)	230 (66%)	116 (34%)	0	4
1	C	340/378 (90%)	234 (69%)	106 (31%)	0	5
2	B	347/383 (91%)	229 (66%)	118 (34%)	0	3
2	D	349/383 (91%)	227 (65%)	122 (35%)	0	3
3	E	80/126 (64%)	49 (61%)	31 (39%)	0	1
All	All	1462/1648 (89%)	969 (66%)	493 (34%)	0	3

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	408	TYR
1	C	206	ASN
2	D	419	THR
2	B	425	MET
1	C	102	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	350	ASN
1	C	101	ASN
2	D	380	ASN
2	B	380	ASN
1	C	28	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 9 ligands modelled in this entry, 2 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$
4	GTP	A	600	-	34,34,34	1.02	3 (8%)	51,54,54	2.33	8 (15%)
6	GDP	B	600	-	30,30,30	0.98	1 (3%)	44,47,47	2.90	12 (27%)
7	LOC	B	700	-	30,31,31	3.78	6 (20%)	39,44,44	7.16	16 (41%)
8	TZT	B	800	-	51,51,51	1.83	9 (17%)	70,70,70	3.02	24 (34%)
4	GTP	C	600	-	34,34,34	0.99	2 (5%)	51,54,54	1.68	10 (19%)
6	GDP	D	600	-	30,30,30	1.04	1 (3%)	44,47,47	1.95	10 (22%)
7	LOC	D	700	-	30,31,31	3.48	6 (20%)	39,44,44	7.05	19 (48%)

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
4	GTP	A	600	-	-	0/22/38/38	0/1/3/3
6	GDP	B	600	-	-	0/16/32/32	0/1/3/3
7	LOC	B	700	-	-	0/10/25/25	0/0/3/3
8	TZT	B	800	-	-	0/72/82/82	0/2/2/2
4	GTP	C	600	-	-	0/22/38/38	0/1/3/3
6	GDP	D	600	-	-	0/16/32/32	0/1/3/3
7	LOC	D	700	-	-	0/10/25/25	0/0/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	LOC	C20-C21	-12.87	1.20	1.40
7	D	700	LOC	C20-C21	-11.15	1.22	1.40
7	B	700	LOC	C19-C17	-9.93	1.21	1.39
7	D	700	LOC	C19-C17	-9.65	1.22	1.39
7	B	700	LOC	C19-C20	-9.35	1.13	1.40

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	LOC	C20-C21-C22	32.19	126.29	113.34
7	D	700	LOC	C20-C21-C22	31.49	126.01	113.34
7	D	700	LOC	C19-C20-C21	17.98	149.27	129.32
7	B	700	LOC	C19-C20-C21	17.73	148.99	129.32
6	B	600	GDP	C6-C5-N7	14.59	136.10	134.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	427/449 (95%)	-0.29	0 100 100	91, 95, 97, 103	0
1	C	421/449 (93%)	-0.08	3 (0%) 84 67	94, 95, 96, 98	1 (0%)
2	B	419/445 (94%)	-0.20	0 100 100	94, 95, 96, 97	0
2	D	419/445 (94%)	-0.06	3 (0%) 84 67	94, 95, 96, 96	0
3	E	124/142 (87%)	-0.14	0 100 100	91, 95, 97, 99	0
All	All	1810/1930 (93%)	-0.16	6 (0%) 91 83	91, 95, 96, 103	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	CYS	3.4
2	D	299	LYS	3.0
1	C	306	ASP	2.8
2	D	6	HIS	2.7
1	C	304	LYS	2.5

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	A	601	1/1	0.30	3.04	93,93,93,93	0
8	TZT	B	800	50/50	0.35	2.43	92,94,102,102	0
7	LOC	B	700	29/29	0.28	2.41	95,95,95,95	0
7	LOC	D	700	29/29	0.32	2.05	94,95,95,95	0
6	GDP	B	600	28/28	0.22	0.42	94,95,95,96	0
4	GTP	C	600	32/32	0.21	-0.11	94,95,95,95	0
4	GTP	A	600	32/32	0.16	-0.18	94,95,95,96	0
6	GDP	D	600	28/28	0.22	-0.47	95,95,95,95	0
5	MG	C	601	1/1	0.21	-0.82	96,96,96,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.