



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:31 am GMT

PDB ID : 5J2T
Title : Tubulin-vinblastine complex
Authors : Waight, A.B.; Bargsten, K.; Doronina, S.; Steinmetz, M.O.; Sussman, D.;
Prota, A.E.
Deposited on : 2016-03-30
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 : 1.7.2 (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

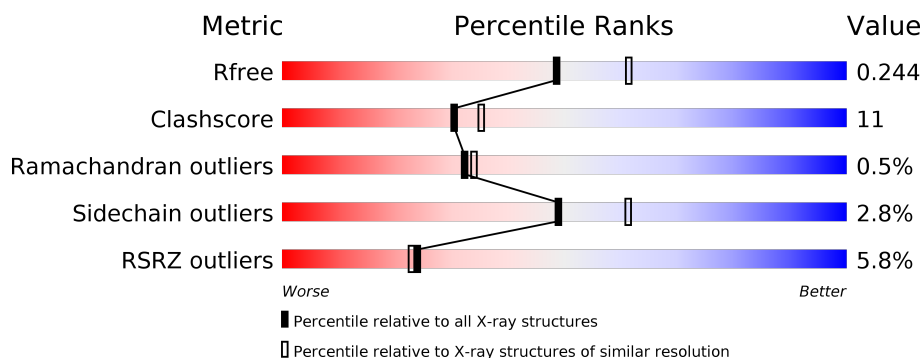
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	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	451	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>80%</div> <div>17%</div> <div>•</div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
2	D	445	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>• 16%</div> </div> </div>
4	F	384	<div> <div>21%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>• 14%</div> </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
10	MES	B	503	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17989 atoms, of which 71 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	9	0
			3469	2202	584	659	24			
1	C	440	Total	C	N	O	S	0	9	0
			3476	2204	585	663	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	0	4	0
			3347	2105	568	646	28			
2	B	428	Total	C	N	O	S	0	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

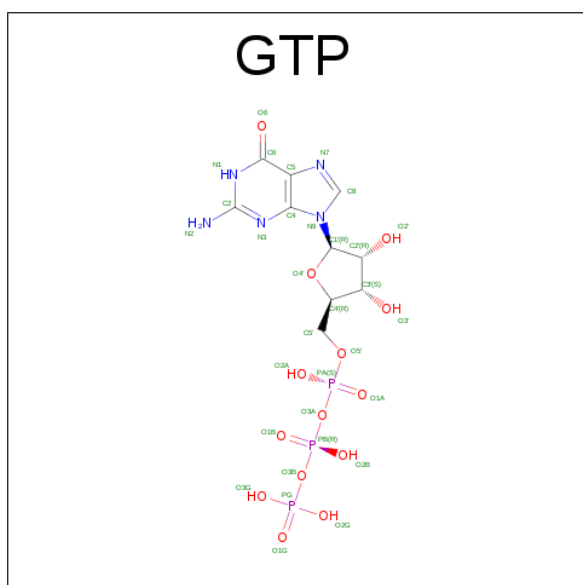
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	6	0
			2740	1771	458	497	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		

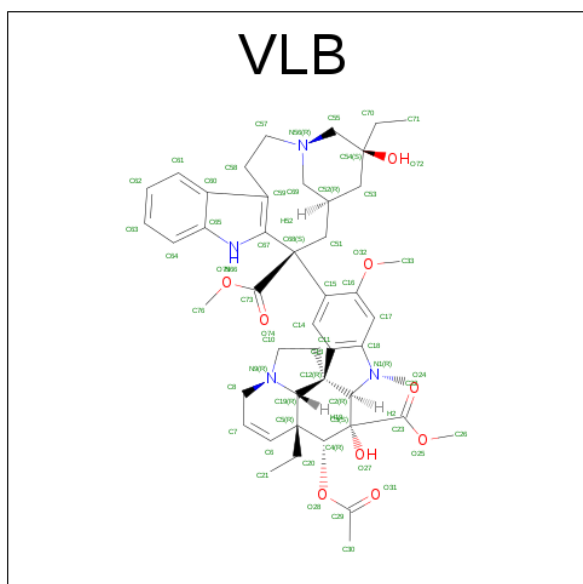
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	C	1	Total	Mg	0	0
			1	1		

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

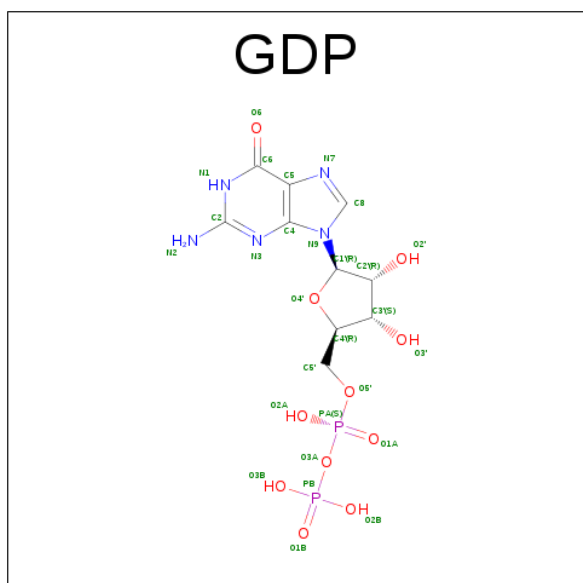
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$).



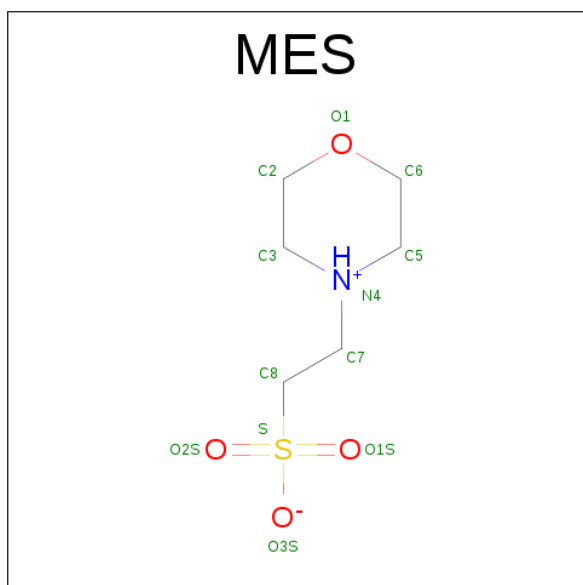
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			117	46	58	4	9		

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



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

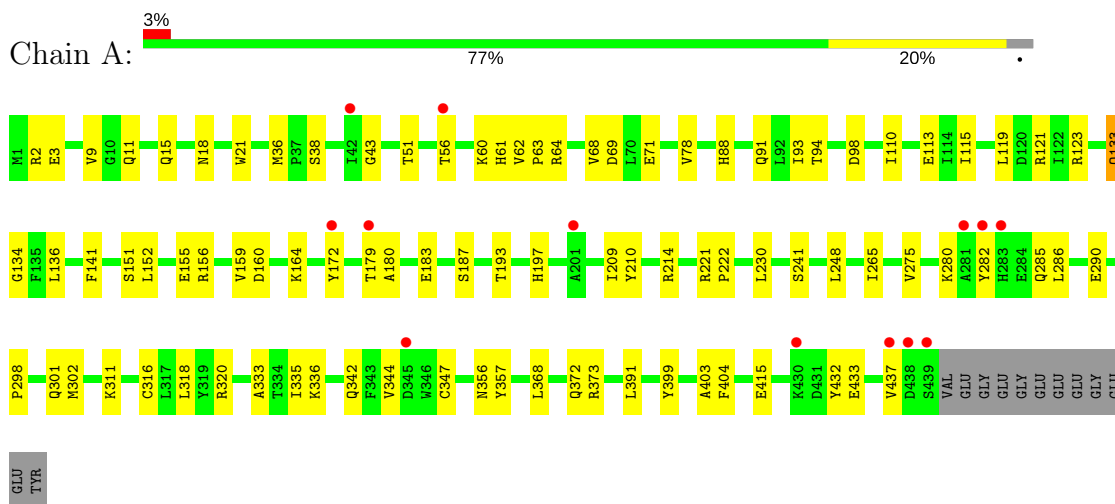
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	59	Total	O	0	0
			59	59		
11	C	124	Total	O	0	0
			124	124		
11	D	26	Total	O	0	0
			26	26		
11	E	10	Total	O	0	0
			10	10		
11	F	31	Total	O	0	0
			31	31		
11	B	80	Total	O	0	0
			80	80		

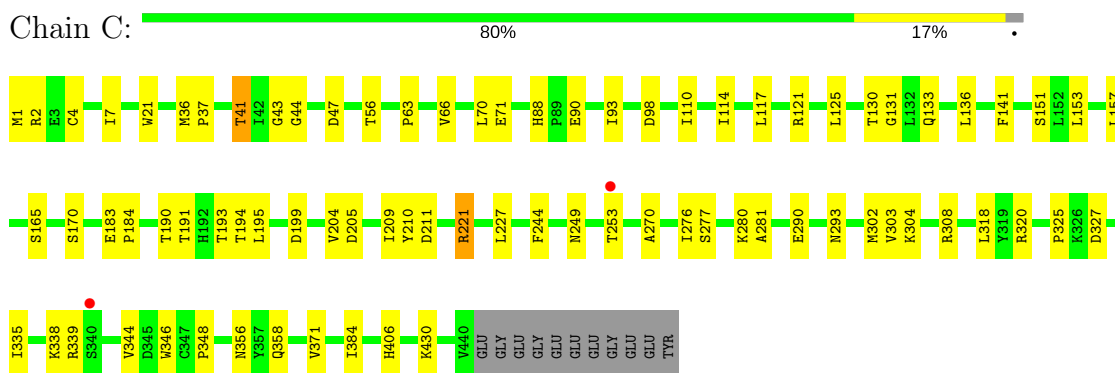
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

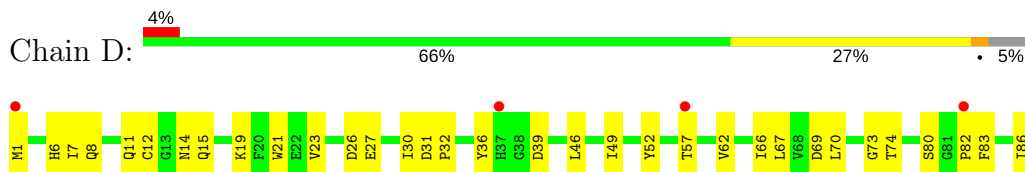
- Molecule 1: Tubulin alpha-1B chain

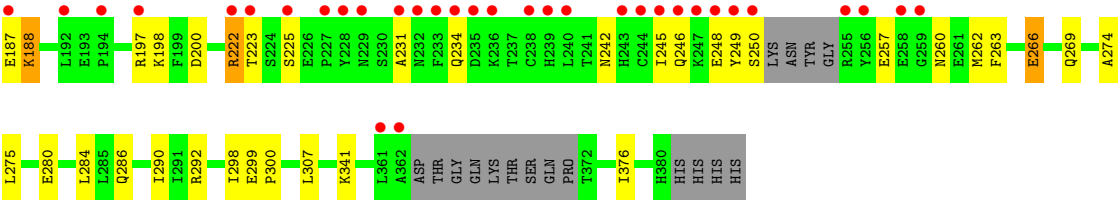


- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.25Å 157.74Å 182.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.20 48.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.17-2.20) 97.8 (48.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.193 , 0.244 0.194 , 0.244	Depositor DCC
R_{free} test set	7493 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17989	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, MG, CA, VLB, GTP, 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	0.42	0/3575	0.53	0/4854
1	C	0.48	0/3581	0.58	0/4863
2	B	0.46	0/3451	0.56	0/4675
2	D	0.36	0/3432	0.50	0/4649
3	E	0.41	0/999	0.45	0/1325
4	F	0.32	0/2819	0.48	0/3812
All	All	0.42	0/17857	0.53	0/24178

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	3469	0	3406	62	1
1	C	3476	0	3409	71	1
2	B	3370	0	3250	71	0
2	D	3347	0	3242	96	0
3	E	991	0	1012	21	0
4	F	2740	0	2734	51	0
5	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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
8	C	59	58	58	5	0
9	B	28	0	12	1	0
9	D	28	0	12	4	0
10	B	12	13	13	1	0
11	A	59	0	0	5	0
11	B	80	0	0	3	0
11	C	124	0	0	5	0
11	D	26	0	0	5	0
11	E	10	0	0	0	0
11	F	31	0	0	1	0
All	All	17918	71	17172	366	1

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 11.

The worst 5 of 366 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:1:MET:HE3	1:C:131:GLY:HA3	1.34	1.06
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.46	0.94
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.50	0.90
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.54	0.90
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.54	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:OE1	1:C:308:ARG:NH1[3_555]	2.16	0.04

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	446/451 (99%)	427 (96%)	18 (4%)	1 (0%)	51	58
1	C	447/451 (99%)	433 (97%)	13 (3%)	1 (0%)	51	58
2	B	428/445 (96%)	416 (97%)	11 (3%)	1 (0%)	51	58
2	D	424/445 (95%)	405 (96%)	16 (4%)	3 (1%)	25	24
3	E	116/143 (81%)	114 (98%)	1 (1%)	1 (1%)	20	18
4	F	325/384 (85%)	302 (93%)	19 (6%)	4 (1%)	15	12
All	All	2186/2319 (94%)	2097 (96%)	78 (4%)	11 (0%)	32	34

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	181	VAL
2	D	404	PHE
4	F	231	ALA
1	C	41	THR
4	F	249	TYR

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	379/379 (100%)	374 (99%)	5 (1%)	73	85
1	C	380/379 (100%)	375 (99%)	5 (1%)	73	85
2	B	369/383 (96%)	357 (97%)	12 (3%)	43	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	370/383 (97%)	357 (96%)	13 (4%)	41	51
3	E	108/127 (85%)	97 (90%)	11 (10%)	8	8
4	F	305/342 (89%)	298 (98%)	7 (2%)	56	69
All	All	1911/1993 (96%)	1858 (97%)	53 (3%)	49	61

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	10	GLU
3	E	68	LEU
2	B	139	HIS
3	E	44	ASP
3	E	59	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	HIS
4	F	260	ASN

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	-	27,34,34	1.01	1 (3%)	27,54,54	1.65	5 (18%)
9	GDP	B	501	6	25,30,30	1.03	3 (12%)	26,47,47	1.98	7 (26%)
10	MES	B	503	-	12,12,12	2.60	1 (8%)	16,16,16	1.79	5 (31%)
5	GTP	C	501	6	27,34,34	0.95	1 (3%)	27,54,54	2.00	5 (18%)
8	VLB	C	503	-	65,67,67	2.42	13 (20%)	72,108,108	2.38	20 (27%)
9	GDP	D	501	-	25,30,30	1.15	2 (8%)	26,47,47	2.03	6 (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	-	-	0/18/38/38	0/3/3/3
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
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	VLB	C	503	-	-	0/38/131/131	0/7/9/9
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-8.70	1.64	1.77
8	C	503	VLB	C61-C60	-2.36	1.37	1.42
8	C	503	VLB	C51-C68	2.01	1.58	1.56
5	C	501	GTP	C6-N1	2.04	1.36	1.33
9	B	501	GDP	O4'-C1'	2.04	1.44	1.41

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.47	119.48	127.46
5	A	501	GTP	N3-C2-N1	-4.46	120.95	127.46
9	B	501	GDP	C6-C5-C4	-4.12	116.75	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C6-N1	-4.10	117.64	123.48
5	C	501	GTP	C5-C6-N1	-3.92	117.91	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	3	0
9	B	501	GDP	1	0
10	B	503	MES	1	0
5	C	501	GTP	1	0
8	C	503	VLB	5	0
9	D	501	GDP	4	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%)	0.03	13 (2%) 51 48	41, 63, 97, 155	0
1	C	440/451 (97%)	-0.15	2 (0%) 90 90	35, 50, 83, 105	0
2	B	428/445 (96%)	-0.02	9 (2%) 64 61	34, 52, 90, 141	2 (0%)
2	D	424/445 (95%)	0.17	19 (4%) 34 32	46, 75, 112, 162	6 (1%)
3	E	120/143 (83%)	0.02	4 (3%) 47 44	47, 78, 107, 121	0
4	F	331/384 (86%)	0.84	80 (24%) 1 1	47, 84, 152, 186	0
All	All	2182/2319 (94%)	0.13	127 (5%) 24 23	34, 64, 114, 186	8 (0%)

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	8.2
2	D	1	MET	7.4
4	F	233	PHE	7.3
4	F	161	LEU	6.7
4	F	232	ASN	6.3

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	MES	B	503	12/12	0.77	0.18	2.17	53,75,130,134	0
9	GDP	B	501	28/28	0.99	0.19	0.55	32,39,45,47	0
5	GTP	A	501	32/32	0.98	0.19	0.07	41,47,53,64	0
5	GTP	C	501	32/32	0.97	0.16	0.03	32,41,49,67	0
9	GDP	D	501	28/28	0.94	0.11	-0.13	54,69,83,97	0
8	VLB	C	503	59/59	0.96	0.10	-0.79	30,48,64,84	0
7	CA	A	503	1/1	0.90	0.05	-1.68	96,96,96,96	0
6	MG	C	502	1/1	0.90	0.21	-	42,42,42,42	0
6	MG	B	502	1/1	0.92	0.55	-	85,85,85,85	0
6	MG	A	502	1/1	0.97	0.12	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.