

wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 07:16 pm BST

PDB ID : 8B7B

Title: Tubulin - maytansinoid - 6 complex

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Deposited on : 2022-09-29

Resolution : 2.25 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

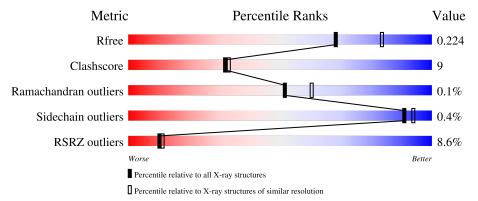
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.25 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 $(\# \mathrm{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\text{Å}))$
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	79%	18%	•
1	С	451	80%	17%	
2	В	445	75%	21%	•
2	D	445	71%	24%	•

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Mol	Chain	Length	Quality of chain						
3	Е	143	71%	15%	·	14%			
4	F	384	68%	17%		15%			



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18322 atoms, of which 8 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 3427	C 2169	N 582	O 653	S 23	0	1	0
1	С	440	Total 3478	C 2200	N 588	O 665	S 25	0	8	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	425	Total 3357	C 2109	- 1	O 647	S 27	0	1	0
2	D	426	Total 3354	C 2104	N 574	O 649	S 27	0	1	0

• Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	Е	123	Total 1029	C 634	N 187	O 203	S 5	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	F	328	Total 2704	C 1738	N 461	O 490	S 15	0	1	0

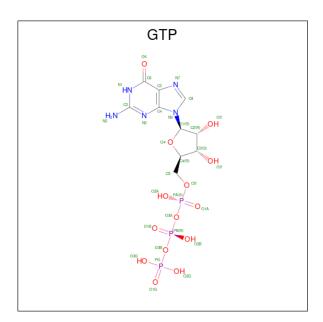
There are 39 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	_	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
5	Λ	1	Total	С	N	О	Р	0	0	
9	A	1	32	10	5	14	3	U	U	
5	C	1	Total	С	N	О	Р	0	0	
3		1	32	10	5	14	3	U		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	В	1	Total Mg 1 1	0	0
6	С	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

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

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

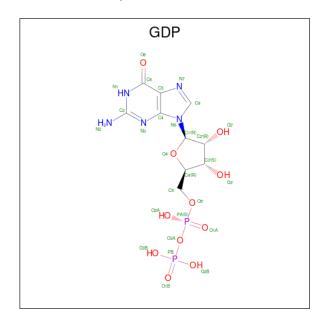
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total Ca 1 1	0	0
7	Е	1	Total Ca 1 1	0	0

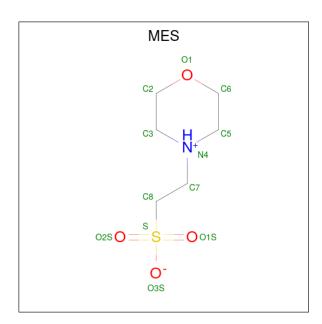
• Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
Q	D	1	Total	С	N	О	Р	0	0
0	Б	1	28	10	5	11	2		
Q	D	1	Total	С	N	О	Р	0	0
8	D	1	28	10	5	11	2	U	

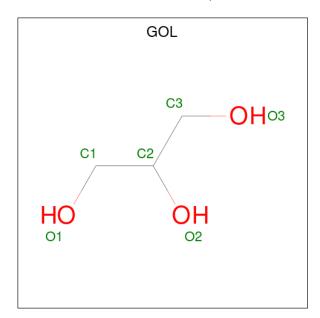
• Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	B	1	Total	С	N	О	S	0	0
	Б	1	12	6	1	4	1	0	0

• Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

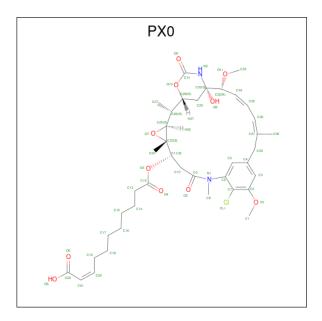


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	С	Н	О	0	0
10		1	14	3	8	3	U	U

• Molecule 11 is ($\{Z\}$)-11-[[(1 $\{R\}$,2 $\{R\}$,3 $\{S\}$,5 $\{S\}$,6 $\{S\}$,16 $\{E\}$,18 $\{E\}$,20 $\{R\}$,21 $\{S\}$)-11-chloranyl-12,20-dimethoxy-2,5,9,16-tetramethyl-21-oxidanyl-8,23-bis(oxidanylidene)-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1^ $\{10,14\}$.0^ $\{3,5\}$]hexacosa-10(26),11,13,16,18-

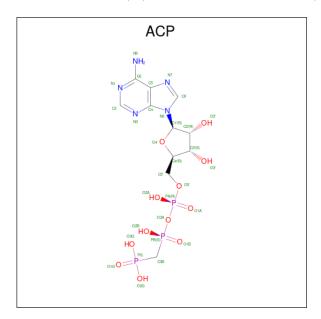


pentaen-6-yl]oxy]-11-oxidanylidene-undec-2-enoic acid (three-letter code: PX0) (formula: $C_{39}H_{53}ClN_2O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		At	$\overline{\text{oms}}$			ZeroOcc	AltConf
11	D	1	Total	С	Cl	N	О	0	0
11	D	1	53	39	1	2	11	U	

• Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf
12	F	1	Total 31		_	 P 3	0	0



• Molecule 13 is water.

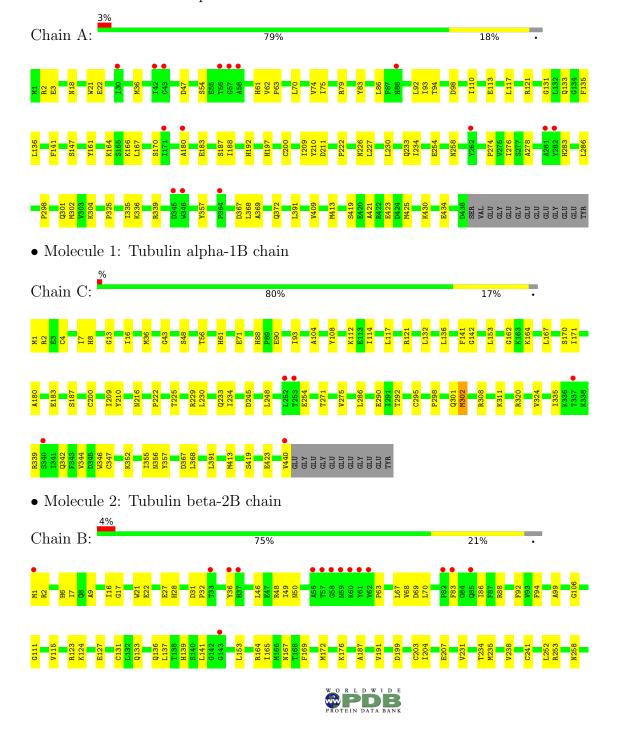
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	123	Total O 123 123	0	0
13	В	187	Total O 187 187	0	0
13	С	280	Total O 280 280	0	0
13	D	83	Total O 83 83	0	0
13	E	26	Total O 26 26	0	0
13	F	34	Total O 34 34	0	0

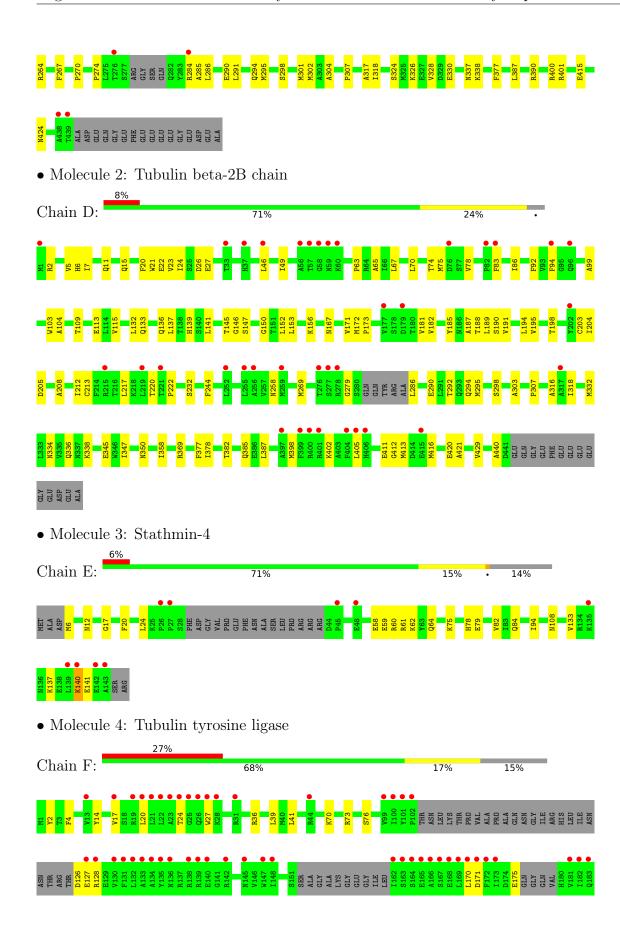


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	104.08Å 155.64Å 181.92Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 - 2.25	Depositor
Resolution (A)	47.83 - 2.25	EDS
% Data completeness	99.3 (47.83-2.25)	Depositor
(in resolution range)	99.3 (47.83-2.25)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.07 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
D D.	0.184 , 0.224	Depositor
R, R_{free}	0.182 , 0.224	DCC
R_{free} test set	6998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 49.2	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18322	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 2.61% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: PX0, MES, GOL, CA, GDP, MG, GTP, ACP

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	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	A	0.25	0/3508	0.47	0/4762		
1	С	0.26	0/3574	0.47	0/4852		
2	В	0.25	0/3431	0.47	0/4646		
2	D	0.24	0/3427	0.46	0/4640		
3	Е	0.24	0/1041	0.41	0/1382		
4	F	0.24	0/2768	0.46	0/3735		
All	All	0.25	0/17749	0.46	0/24017		

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	3427	0	3339	52	0
1	С	3478	0	3392	57	0
2	В	3357	0	3239	73	0
2	D	3354	0	3234	76	0
3	Е	1029	0	1041	18	0
4	F	2704	0	2675	42	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	32	0	12	0	0
6	A	1	0	0	0	0
6	В	1	0	0	0	0
6	С	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	В	2	0	0	0	0
7	С	1	0	0	0	0
7	Е	1	0	0	0	0
8	В	28	0	12	0	0
8	D	28	0	12	2	0
9	В	12	0	12	5	0
10	С	6	8	8	0	0
11	D	53	0	0	0	0
12	F	31	0	14	0	0
13	A	123	0	0	2	0
13	В	187	0	0	11	0
13	С	280	0	0	3	0
13	D	83	0	0	2	0
13	E	26	0	0	3	0
13	F	34	0	0	1	0
All	All	18314	8	17002	309	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 9.

The worst 5 of 309 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.46	0.97
2:B:294:GLN:NE2	13:B:603:HOH:O	2.17	0.78
2:B:83:PHE:O	2:B:86:ILE:HG22	1.84	0.77
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.18	0.74
2:B:415:GLU:OE1	13:B:601:HOH:O	2.06	0.73

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	437/451 (97%)	427 (98%)	10 (2%)	0	100	100	
1	\mathbf{C}	446/451 (99%)	437 (98%)	9 (2%)	0	100	100	
2	В	422/445 (95%)	412 (98%)	10 (2%)	0	100	100	
2	D	423/445 (95%)	410 (97%)	12 (3%)	1 (0%)	47	55	
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100	
4	F	317/384 (83%)	303 (96%)	13 (4%)	1 (0%)	41	46	
All	All	2166/2319 (93%)	2109 (97%)	55 (2%)	2 (0%)	51	60	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
4	F	186	LEU	
2	D	279	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	370/379~(98%)	369 (100%)	1 (0%)	92	95	
1	С	379/379 (100%)	376 (99%)	3 (1%)	81	88	
2	В	$369/383 \ (96\%)$	368 (100%)	1 (0%)	92	95	
2	D	369/383~(96%)	368 (100%)	1 (0%)	92	95	
3	Е	112/127 (88%)	110 (98%)	2 (2%)	59	68	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
4	F	297/342 (87%)	297 (100%)	0	100	100	
All	All	1896/1993 (95%)	1888 (100%)	8 (0%)	91	94	

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Ε	140	LYS
3	Е	59	GLU
1	С	302	MET
1	С	71	GLU
2	D	139	HIS

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

Mol	Chain	Res	Type
2	В	294	GLN
2	В	424	ASN
1	С	11	GLN
2	D	50	ASN
2	D	247	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	Вс	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	В	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.09	3 (10%)
8	GDP	D	501	6	24,30,30	0.96	1 (4%)	30,47,47	1.24	4 (13%)
12	ACP	F	401	6	27,33,33	0.82	1 (3%)	32,52,52	1.36	2 (6%)
9	MES	В	504	-	12,12,12	2.14	1 (8%)	14,16,16	2.08	5 (35%)
11	PX0	D	503	-	54,56,56	0.77	2 (3%)	62,80,80	0.94	5 (8%)
5	GTP	С	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.33	5 (15%)
10	GOL	С	504	-	5,5,5	0.78	0	5,5,5	1.03	0
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.33	5 (15%)

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
8	GDP	В	501	6	-	3/12/32/32	0/3/3/3
8	GDP	D	501	6	-	1/12/32/32	0/3/3/3
12	ACP	F	401	6	-	3/15/38/38	0/3/3/3
9	MES	В	504	-	-	3/6/14/14	0/1/1/1
11	PX0	D	503	-	-	11/57/84/84	0/2/4/4
5	GTP	С	501	6	-	8/18/38/38	0/3/3/3
10	GOL	С	504	-	-	2/4/4/4	-
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
9	В	504	MES	C8-S	-7.14	1.67	1.77
5	A	501	GTP	C5-C6	-4.01	1.39	1.47
5	С	501	GTP	C5-C6	-4.00	1.39	1.47
11	D	503	PX0	C35-C36	-3.39	1.33	1.43
12	F	401	ACP	PB-O3A	3.16	1.61	1.58



The worst	5	of 2	9	bond	angle	outliers	are	listed	below:
TITO HOLDO	$\overline{}$	O	•	OILG	WII DIO	Cathere	COL C	IID CCC	CIO III.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
12	F	401	ACP	PB-O3A-PA	-6.94	110.55	132.56
9	В	504	MES	O1S-S-C8	4.15	111.91	106.92
9	В	504	MES	C5-N4-C3	3.78	117.33	108.83
8	D	501	GDP	PA-O3A-PB	-3.77	119.90	132.83
5	С	501	GTP	C8-N7-C5	3.10	108.90	102.99

There are no chirality outliers.

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5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	С	501	GTP	C5'-O5'-PA-O1A
5	С	501	GTP	C5'-O5'-PA-O2A
8	В	501	GDP	C5'-O5'-PA-O1A

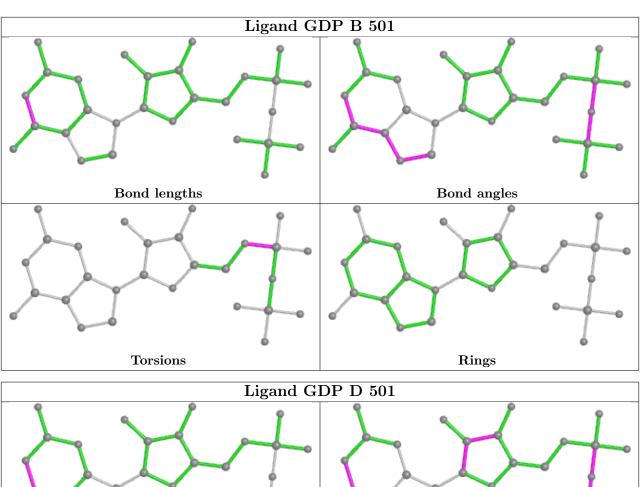
There are no ring outliers.

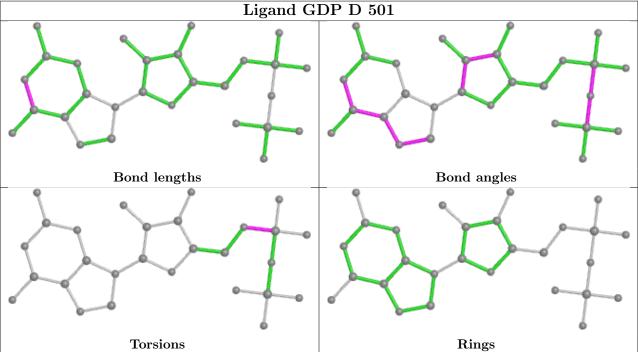
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
9	В	504	MES	5	0
5	A	501	GTP	1	0

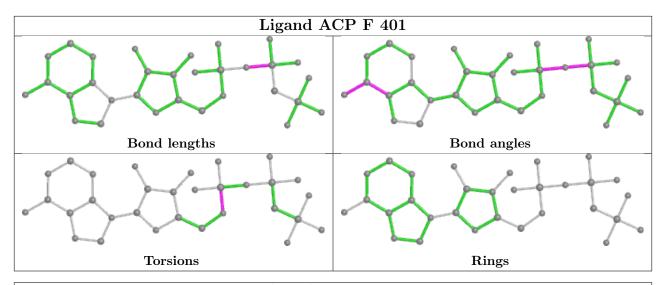
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

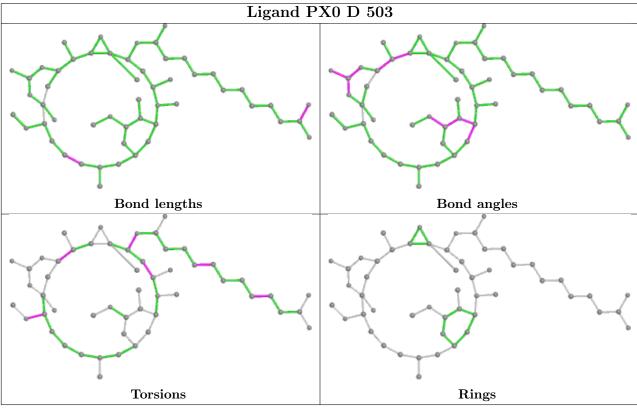




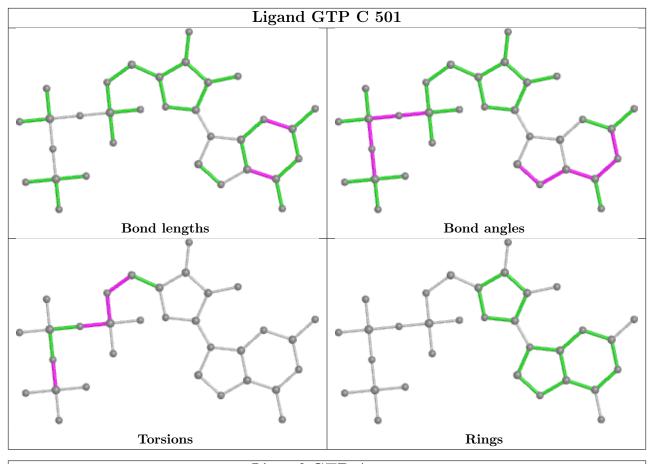


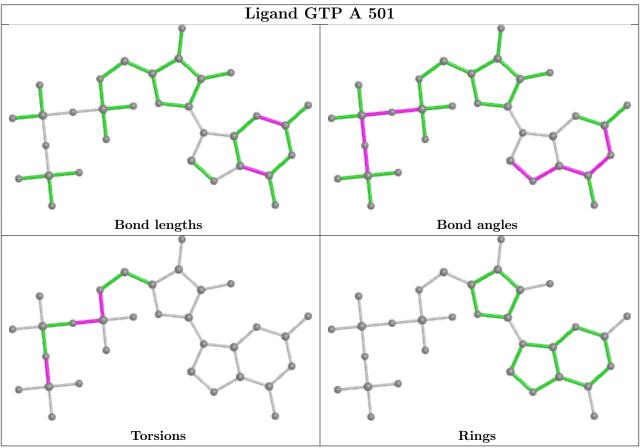














5.7 Other polymers (i)

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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	438/451 (97%)	0.14	15 (3%) 45 47	40, 59, 90, 144	0
1	С	440/451 (97%)	-0.05	5 (1%) 80 82	36, 49, 73, 129	0
2	В	425/445~(95%)	0.13	19 (4%) 33 36	37, 54, 87, 133	0
2	D	426/445~(95%)	0.34	36 (8%) 10 12	47, 75, 114, 146	0
3	E	123/143 (86%)	0.39	9 (7%) 15 15	52, 74, 112, 147	0
4	F	328/384 (85%)	1.28	104 (31%) 0 0	54, 86, 147, 180	0
All	All	2180/2319 (94%)	0.32	188 (8%) 10 11	36, 63, 115, 180	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	10.4
1	A	282	TYR	8.5
4	F	249	TYR	8.5
2	В	57	THR	7.9
4	F	132	LEU	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 monosaccharides in this entry.



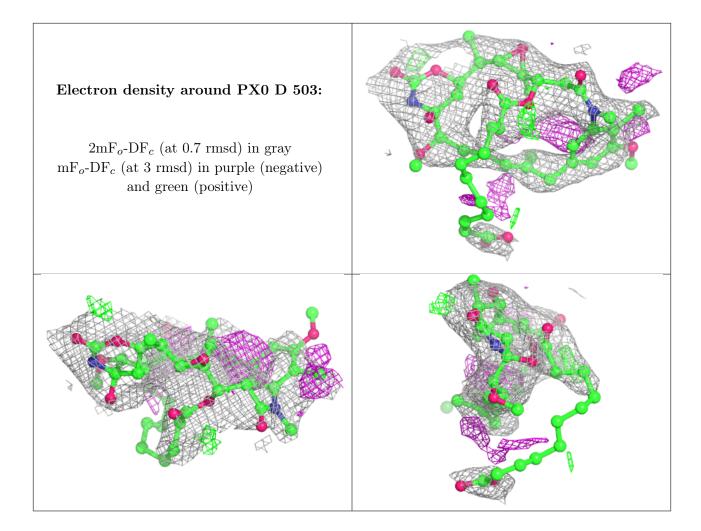
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
11	PX0	D	503	53/53	0.83	0.32	67,94,109,114	0
7	CA	E	201	1/1	0.85	0.16	106,106,106,106	0
10	GOL	С	504	6/6	0.89	0.23	66,82,98,99	0
7	CA	В	505	1/1	0.89	0.05	106,106,106,106	0
12	ACP	F	401	31/31	0.92	0.14	85,96,111,118	0
8	GDP	D	501	28/28	0.93	0.13	66,71,89,108	0
7	CA	A	503	1/1	0.96	0.03	79,79,79,79	0
7	CA	В	503	1/1	0.96	0.11	93,93,93,93	0
9	MES	В	504	12/12	0.97	0.11	37,54,61,63	0
6	MG	F	402	1/1	0.97	0.07	92,92,92,92	0
6	MG	В	502	1/1	0.98	0.18	41,41,41,41	0
5	GTP	A	501	32/32	0.98	0.21	36,44,53,55	0
7	CA	С	503	1/1	0.98	0.09	66,66,66,66	0
6	MG	A	502	1/1	0.98	0.17	42,42,42,42	0
8	GDP	В	501	28/28	0.98	0.22	36,43,47,50	0
5	GTP	С	501	32/32	0.99	0.16	32,39,48,52	0
6	MG	С	502	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	502	1/1	0.99	0.04	65,65,65,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

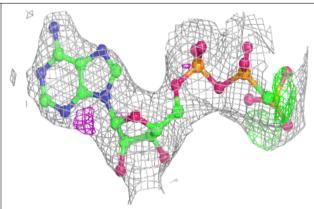


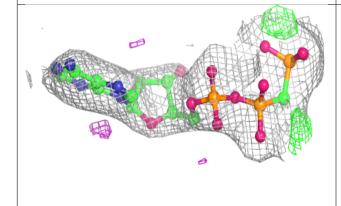


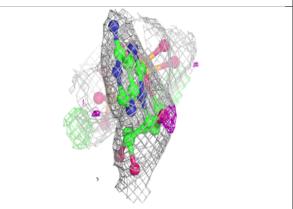


Electron density around ACP F 401:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

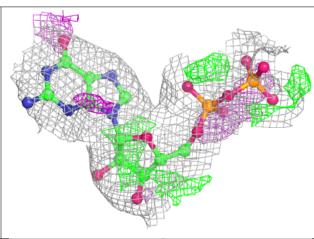


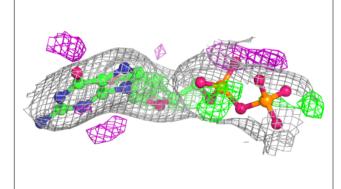


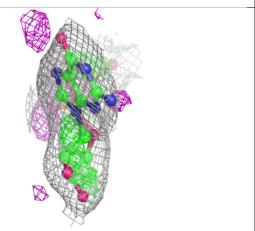


Electron density around GDP D 501:

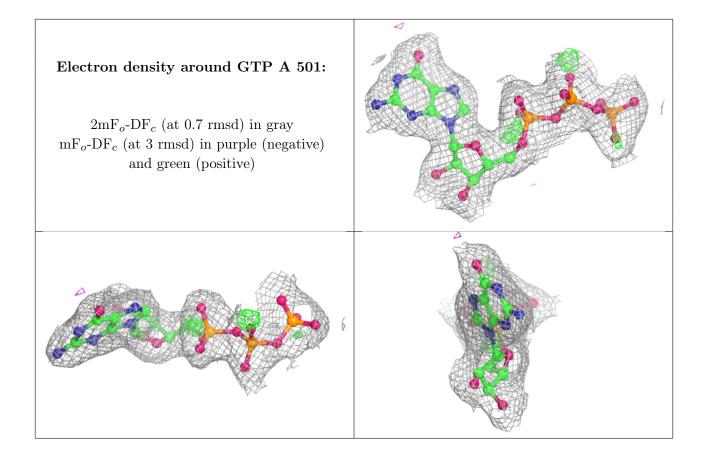
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



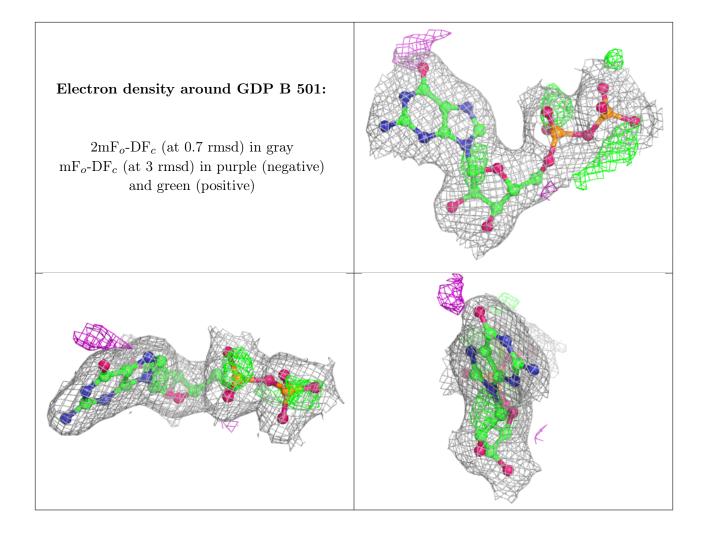




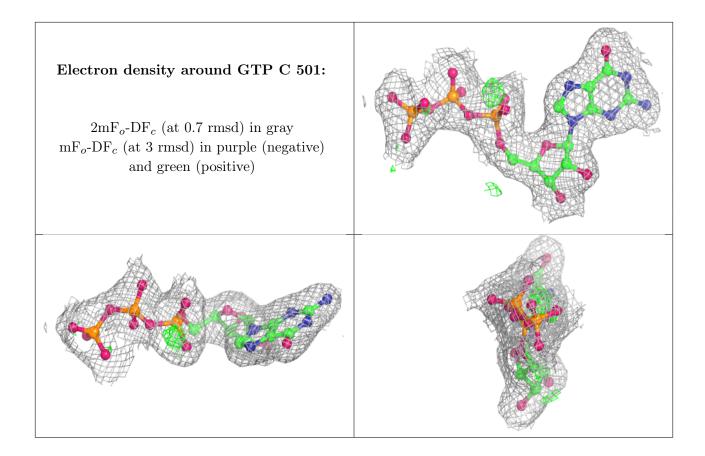












6.5 Other polymers (i)

There are no such residues in this entry.

