



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FFX  
Title : TUBULIN:STATHMIN-LIKE DOMAIN COMPLEX  
Authors : Gigant, B.; Martin-Barbey, C.; Knossow, M.  
Deposited on : 2000-07-26  
Resolution : 3.95 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

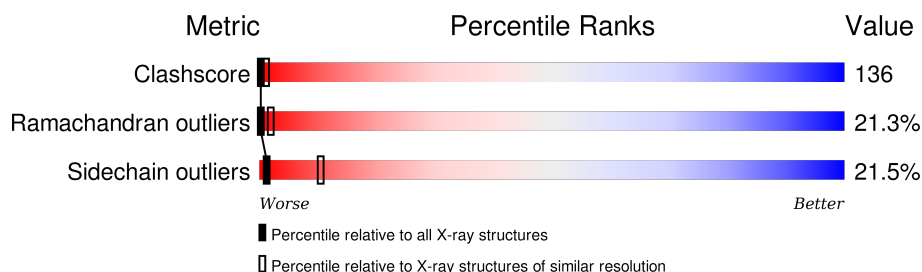
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.95 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))
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	91	

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
5	GDP	D	503	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13568 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3295	2082	559	632	22			
1	C	423	Total	C	N	O	S	0	0	0
			3295	2082	559	632	22			

- Molecule 2 is a protein called PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3201	2014	550	611	26			
2	D	410	Total	C	N	O	S	0	0	0
			3201	2014	550	611	26			

- Molecule 3 is a protein called PROTEIN (STATHMIN-LIKE DOMAIN OF RB3).

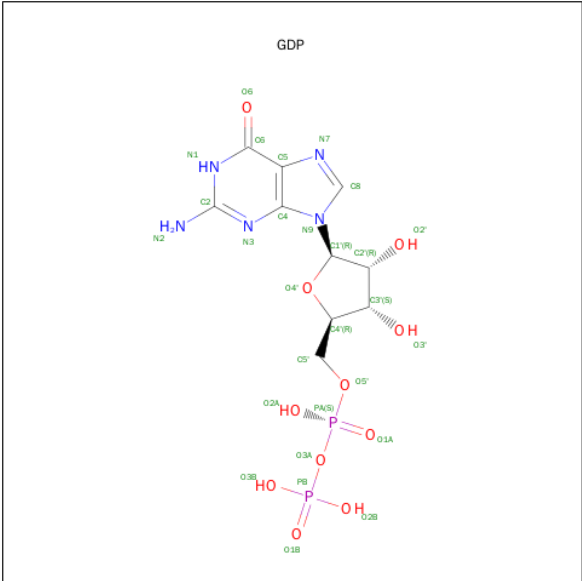
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	91	Total	C	N	O	0	0	0
			456	273	91	92			

- 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 GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

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

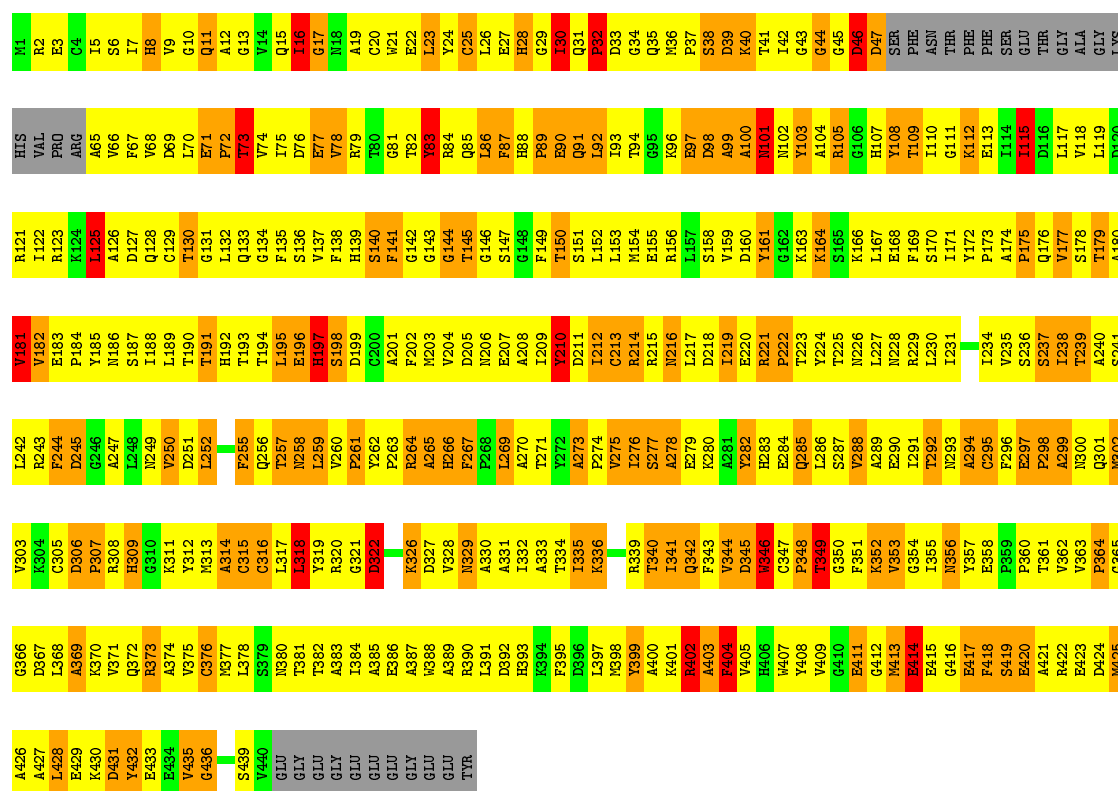
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

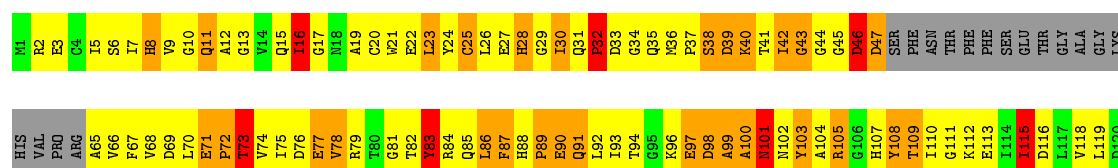
#### • Molecule 1: PROTEIN (TUBULIN)

Chain A: 



#### • Molecule 1: PROTEIN (TUBULIN)

Chain C: 



R121	R181	S241	X302	P364	D424
I122	V182	L242	V303	G365	M425
R123	E183	R243	R304	G366	A426
K124	P184	R244	C305	G367	A427
L125	Y185	D245	D306	L368	L428
A126	M186	G246	P307	A369	E429
D127	S187	K247	R308	K370	K430
Q128	L188	L248	R309	K371	D431
G129	L189	L249	G310	G372	D432
T130	T190	V250	K311	K373	E433
G131	T191	D251	Y312	A374	E434
L132	H192	L252	K313	G375	V435
Q133	T193	T253	A314	G376	G436
G134	T194	E254	C315	K377	
F135	L195	F255	C316	L378	S439
E136	E196	Q256	L317	S379	V440
V137	H197	T257	L318	K380	GLU
F138	S198	N258	Y319	T381	GLY
H139	D199	L259	R320	T382	GLU
S140	G200	V260	G321	K383	GLY
F141	A201	P261	R322	L384	GLU
G142	F202	Y262	K326	I385	GLU
G143	M203	P263	D327	E386	GLU
L144	V204	R264	R328	A387	GLY
T145	D205	G265	V328	K388	GLU
G146	N206	H266	N329	A389	GLU
S147	E207	T267	A330	K390	
G148	A208	P268	A331	L391	TYR
F149	T209	L269	I332	R392	
	Y210	K270	A333	H393	
S151	D211	A271	T334	K394	
L152	I212	A273	I335	P395	
L153	C213	P274	K336	D396	
M154	R214	V275	T337	L397	
E155	R215	L276	K338	K398	
R156	N216	S277	R339	Y399	
L157	L217	A278	T340	GLY	
S158	D218	E279	I341	A400	
V159	I219	K280	Q342	R402	
D160	E220	A281	F343	A403	
Y161	R221	Y282	V344	F404	
G162	P222	H283	D345	V405	
K163	T223	E284	K346	H406	
K164	Y224	Q285	C347	H407	
S165	T225	L286	P348	Y408	
K166	N226	S287	T349	V409	
L167	L227	V288	G350	G410	
E168	N228	A289	F351	E411	
F169	R229	E290	K352	G412	
S170	L230	L291	V353	H413	
I171	I231	T292	G354	E414	
Y172	G232	N293	I355	E415	
P173	Q233	A294	N356	A416	
A174	I234	C295	Y357	A417	
P175	V235	F296	E358	G418	
O176	S236	E297	P359	S419	
V177	S237	P298	P360	E420	
T178	L238	A299	T361	A421	
S179	T239	N300	V362	L242	
A180	A240	Q301	V363	E423	

• Molecule 2: PROTEIN (TUBULIN)

Chain B: 6% 57% 25% 5% 8%

M1	R2	R64	K124	P184	F244	A304	M373	Q433
R2	A65	A65	E125	Y185	P245	C305	S374	Q434
I4	L67	L66	E126	N186	Q246	D306	A375	Y435
H5	V68	V68	S128	T188	Q247	P307	T376	Q436
I7	D69	D69	L248	L189	N249	R309	F377	D437
I7	L70	L70	D130	S190	A250	G310	K378	ALA
Q8	E71	E71	C131	Y191	D251	R311	G379	THR
G10	P72	P72	L132	H192	L252	Y312	N380	ALA
Q11	G73	G73	Q133	Q193	R253	L133	S381	ASP
Q12	T74	T74	K134	L194	K254	T314	T382	GLU
C13	M75	M75	F135	V195	L255	V315	K383	GLN
N14	S77	S77	L136	E196	A256	A316	K384	GLY
Q15	N78	N78	T138	N197	V257	K317	K385	GLU
I16	R79	R79	H139	T198	N258	V318	E386	PHE
G17	S80	S80	L141	E200	M259	F319	L387	GLU
A18	G81	G81	S140	E201	V260	R320	F388	GLU
K19	P82	P82	G142	T201	P261	G321	K389	GLU
F20	F83	F83	G143	Y202	F262	R322	K390	GLY
W21	G84	G84	G144	C203	P263	K323	I391	GLU
K31	D90	D90	T145	L204	R264	S324	S392	GLU
V23	Q85	Q85	T146	D205	H266	K325	E393	ASP
I24	F87	F87	G146	N206	H267	K326	Q394	GLU
S25	K88	K88	G148	A208	F267	E327	T396	ALA
D26	P89	P89	M149	L209	M269	E330	T397	
E27	D90	D90	G150	Y210	P270	K331	K398	
I30	F92	F92	T151	D211	G271	K332	F399	
D31	V93	V93	L152	T212	F272	L333	R400	
P90	F94	F94	L153	C213	A273	K334	R401	
THR	G95	G95	I154	F214	P274	V335	K402	
GLY	Q96	Q96	S155	R215	L275	Q336	A403	
SER	S97	S97	T157	L216	T276	R337	R404	
HIS	A99	A99	R158	K218	S277	K338	L405	
ASP	G100	G100	E159	L219	G279	S340	H407	
ASP	N101	N101	A104	T220	S280	S341	Y408	
SER	M102	M102	Y161	T221	Q281	Y342	T409	
LEU	M103	M103	P162	P222	Q282	F343	G410	
LEU	A104	A104	R164	T223	Y283	V344	E411	
LEU	K105	K105	G225	Y224	R284	E345	G412	
LEU	G106	G106	M166	D226	A285	K346	M413	
GLU	H107	H107	M167	L227	L286	L347	D414	
ARG	Y108	Y108	T168	N228	T287	P348	E415	
ILE	T109	T109	F169	H229	V288	R349	M416	
V51	G110	G110	S170	E110	P289	N350	E417	
Y52	G111	G111	V171	L230	E290	V351	F418	
Y53	A112	A112	V172	V231	L291	K352	T419	
E54	E113	E113	P173	S232	T292	T353	A421	
E55	L114	L114	S174	Q233	Q293	A354	E422	
A56	V115	V115	P175	T234	Q294	V355	S423	
D116	K176	K176	K176	M235	M295	C356	R424	
S117	V177	V177	S178	S236	F296	D357	M425	
V118	G58	G58	S178	Q237	D297	L358	M426	
L119	D179	D179	T180	V238	A298	P359	D427	
D120	E180	E180	V181	K299	K300	P360	L428	
V121	V121	V121	V182	T240	R301	R369	V429	
R123	V122	V122	L242	C241	M302	G370	S430	
			E183	R243	L242	L371	E431	
					A303	K372	Y432	

• Molecule 2: PROTEIN (TUBULIN)

Chain D: 6% 56% 24% 6% 8%





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.50Å 328.50Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 3.95	Depositor
% Data completeness (in resolution range)	94.3 (7.00-3.95)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.267 , 0.367	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.59	0/3367	0.86	5/4570 (0.1%)
1	C	0.56	0/3367	0.84	5/4570 (0.1%)
2	B	0.56	0/3270	0.82	1/4428 (0.0%)
2	D	0.58	0/3270	0.84	0/4428
All	All	0.57	0/13274	0.84	11/17996 (0.1%)

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	1
1	C	0	2
2	B	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	417	GLU	N-CA-C	-5.93	94.99	111.00
1	C	318	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	417	GLU	N-CA-C	-5.77	95.43	111.00
1	A	318	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	294	ALA	N-CA-C	-5.38	96.46	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain
2	B	61	TYR	Sidechain
1	C	108	TYR	Sidechain
1	C	210	TYR	Sidechain
2	D	312	TYR	Sidechain

## 5.2 Too-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 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	3295	0	3202	883	0
1	C	3295	0	3202	910	0
2	B	3201	0	3091	916	0
2	D	3201	0	3091	883	0
3	E	456	0	103	79	0
4	A	32	0	12	4	0
4	C	32	0	12	8	0
5	B	28	0	12	5	0
5	D	28	0	12	9	0
All	All	13568	0	12737	3585	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 136.

The worst 5 of 3585 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)
2:B:175:PRO:HD2	2:B:207:GLU:HB2	1.23	1.16
2:D:158:ARG:HD3	2:D:197:ASN:ND2	1.63	1.14
1:A:214:ARG:HH21	1:A:220:GLU:HA	1.04	1.14
2:D:311:ARG:HH21	2:D:437:ASP:HB2	1.03	1.13
1:C:222:PRO:HB2	1:C:227:LEU:HD11	1.31	1.12

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	419/451 (93%)	221 (53%)	111 (26%)	87 (21%)	0	2
1	C	419/451 (93%)	219 (52%)	114 (27%)	86 (20%)	0	2
2	B	406/445 (91%)	184 (45%)	133 (33%)	89 (22%)	0	1
2	D	406/445 (91%)	186 (46%)	130 (32%)	90 (22%)	0	1
All	All	1650/1792 (92%)	810 (49%)	488 (30%)	352 (21%)	0	2

5 of 352 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	32	PRO
1	A	46	ASP
1	A	83	TYR
1	A	90	GLU

### 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	354/377 (94%)	278 (78%)	76 (22%)	1	10
1	C	354/377 (94%)	279 (79%)	75 (21%)	1	11
2	B	347/381 (91%)	274 (79%)	73 (21%)	1	11
2	D	347/381 (91%)	270 (78%)	77 (22%)	1	10
All	All	1402/1516 (92%)	1101 (78%)	301 (22%)	1	10

5 of 301 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	395	PHE
1	C	115	ILE
2	D	346	TRP
2	B	407	TRP
1	C	25	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	380	ASN
1	C	133	GLN
2	D	349	ASN
2	B	426	ASN
1	C	15	GLN

### 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 ⓘ

4 ligands are modelled in this entry.

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	500	-	25,34,34	1.48	4 (16%)	34,54,54	2.14	5 (14%)
5	GDP	B	501	-	23,30,30	1.72	4 (17%)	30,47,47	2.45	6 (20%)
4	GTP	C	502	-	25,34,34	1.55	3 (12%)	34,54,54	2.22	6 (17%)
5	GDP	D	503	-	23,30,30	1.56	3 (13%)	30,47,47	2.18	4 (13%)

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	500	-	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
4	GTP	C	502	-	-	0/18/38/38	0/3/3/3
5	GDP	D	503	-	-	0/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	O4'-C1'	-3.12	1.37	1.41
5	D	503	GDP	PA-O2A	-2.23	1.45	1.54
4	A	500	GTP	PA-O2A	-2.20	1.45	1.54
5	B	501	GDP	PA-O2A	-2.15	1.45	1.54
4	A	500	GTP	O5'-C5'	-2.11	1.36	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C6-N1	-8.42	112.08	123.59
5	D	503	GDP	C5-C6-N1	-7.99	112.67	123.59
4	C	502	GTP	C5-C6-N1	-7.92	112.76	123.59
4	A	500	GTP	C5-C6-N1	-7.76	112.99	123.59
5	B	501	GDP	C4'-O4'-C1'	-4.77	104.48	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	GTP	4	0
5	B	501	GDP	5	0
4	C	502	GTP	8	0
5	D	503	GDP	9	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.