



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:44 PM GMT

PDB ID : 1SA1
Title : Tubulin-podophyllotoxin:stathmin-like domain complex
Authors : Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.
Deposited on : 2004-02-06
Resolution : 4.20 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

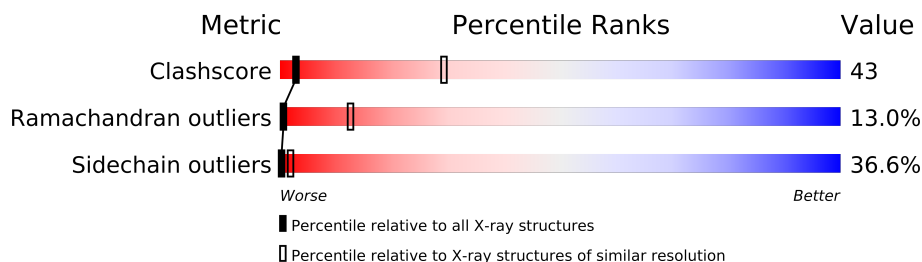
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 4.20 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))
Clashscore	79885	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)

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.

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	142	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14180 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3299	2089	559	631	20			
1	C	430	Total	C	N	O	S	0	0	0
			3275	2072	555	628	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ILE	ALA	SEE REMARK 999	UNP P02550
C	265	ILE	ALA	SEE REMARK 999	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3241	2040	545	631	25			
2	D	426	Total	C	N	O	S	0	0	0
			3278	2059	556	638	25			

- Molecule 3 is a protein called Stathmin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	134	Total	C	N	O	S	0	0	0
			905	555	169	176	5			

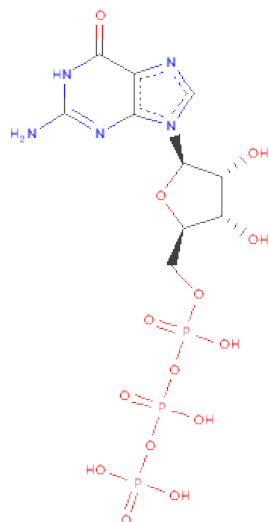
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P02554

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

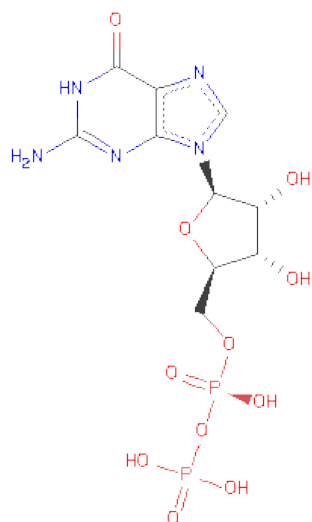
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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



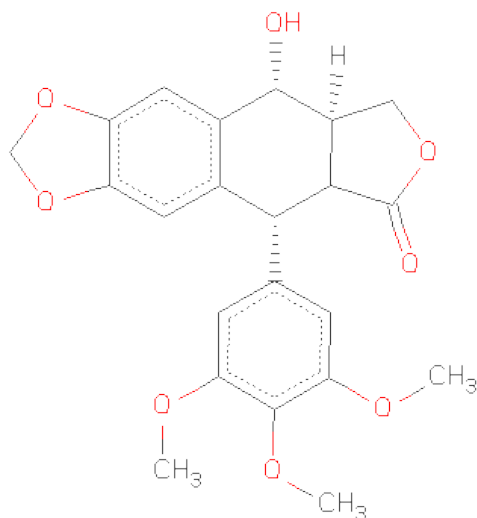
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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



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

- Molecule 7 is 9-HYDROXY-5-(3,4,5-TRIMETHOXYPHENYL)-5,8,8A,9-TETRAHYDR OFURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-6(5AH)-ONE (three-letter code: POD) (formula: C₂₂H₂₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			30	22	8		

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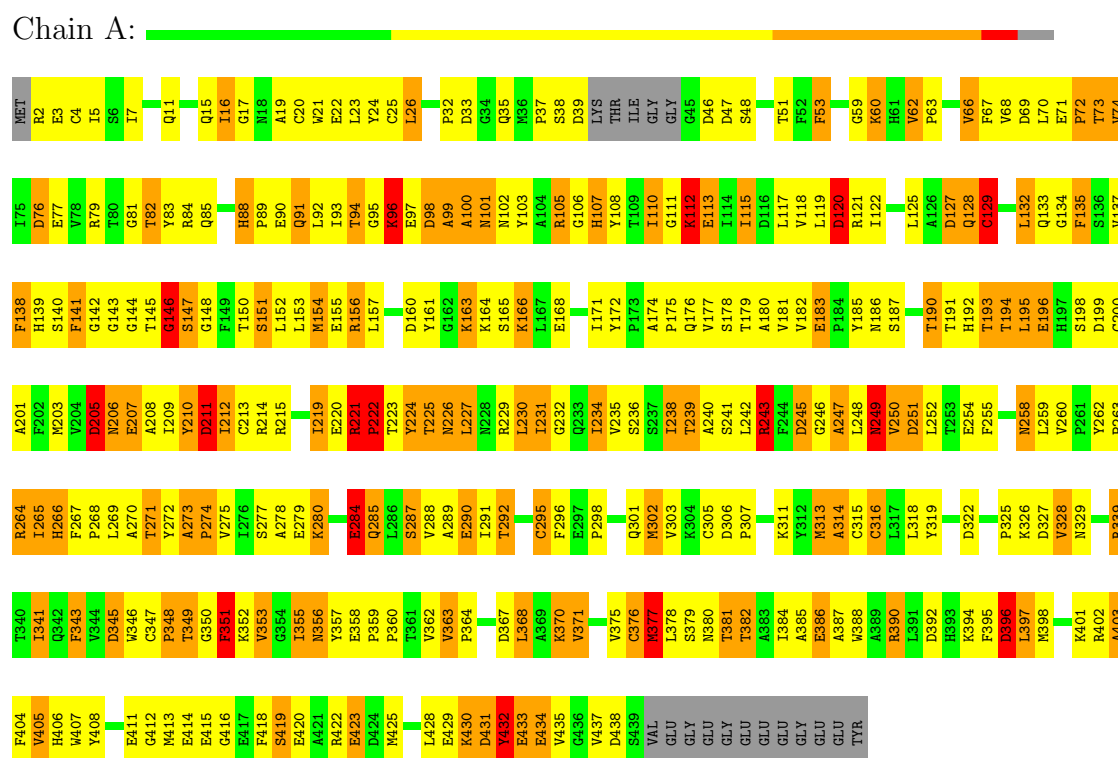
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	30	22	8	0	0

3 Residue-property plots

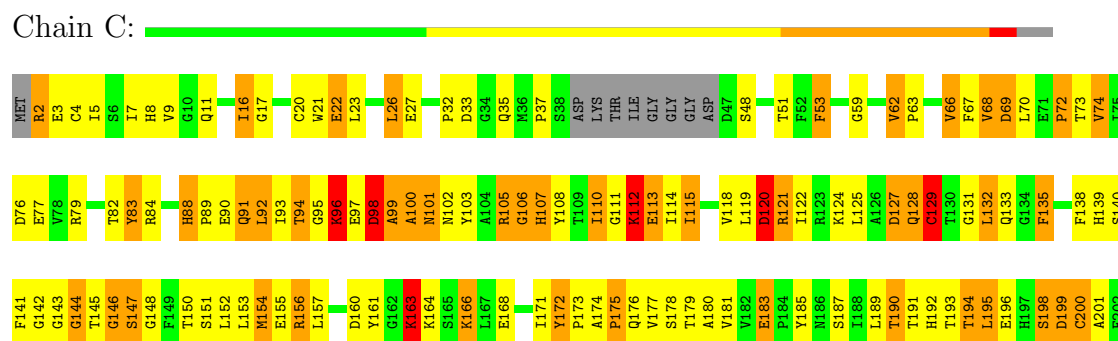
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Tubulin alpha chain



• Molecule 1: Tubulin alpha chain



V409	D345	L289	M203
G410	W346	A270	V204
E411	C347	T271	V205
G412	T348	V272	M206
M413	G349	A273	E207
E414	G350	P274	A208
E415	F351	V275	I209
G416	G352	I276	Y210
E417	G353	S277	D211
F418	G354	A278	I212
S419	I355	E279	C213
E220	N356	K280	R214
A421	Y357	A281	
E422	E358		I219
E423	P359	E284	E220
D424	P360	Q285	R221
M425	T361	L286	P222
	V362	S287	T223
L428	V363	V288	Y224
E429	P364	A289	T225
D430		E290	N226
D431	D367	I291	I227
Y432	L368	T292	N228
E433	A369		R229
E434	K370		
E435	V371	C286	L230
G436		Q301	I231
V437	V375	M302	Q232
D438	G376	V303	Q233
	R377	K304	I234
S439	L378	C305	V235
VAL	S379	P307	S236
GLU	N380		S237
GLY	T381		T239
GLY	L382	K311	
GLU	A383	Y312	A240
GLU	L384	M313	S241
GLY	A385	A314	L242
GLY	E386	C315	R243
GLY	L387	C316	
GLU	K388	L317	L248
	A389	L318	N249
TYR	R390	T319	V250
	L391	R320	D251
	D392		L252
	G393	P325	T253
	K394	K326	E254
	F395	D327	F255
	D396	V328	Q256
	L397		T257
	M398	A333	N258
			L259
	K401	K336	V260
	R402		P261
	A403	R339	A262
	F404	T340	P263
	V405	I341	R264
	H406	Q342	I265
	W407	F343	H266
	Y408	V244	F267
			V268

• Molecule 2: Tubulin beta chain

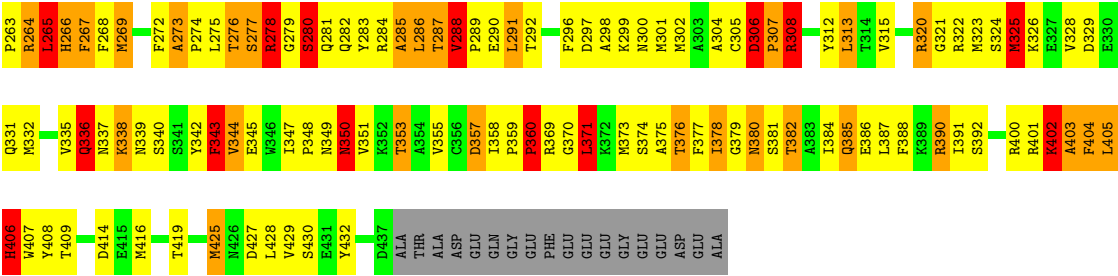
Chain B:

R401	R402	A403	F404	L405	R406	Y407	Y408	T409	G410		D411	S412	M413		T414																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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• Molecule 2: Tubulin beta chain

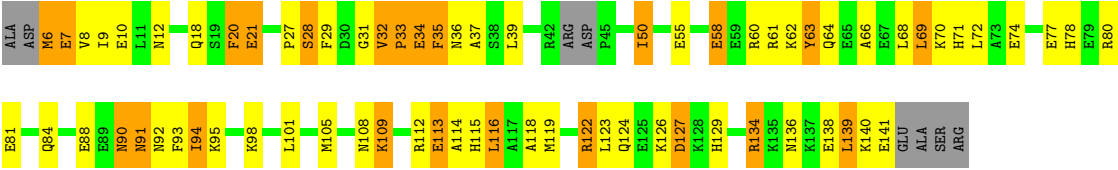
Chain D:

D193	E200	T201	Y202	C203	L204	L205	G206	F207	A208	L209	Y210	D211	T216	L217	K218	L219	T220	T221	P222	T223	G224	D225	D226	L227	N228	H229	L230	S231	S232	S233	S234	M235	S236	V237	T238	M239	M302	A303	A304	C305	D306	P307	R308	Y312	L313	L314	V315	T316	A317	A318	A319	V320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R
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• Molecule 3: Stathmin 4

Chain E:



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, α , β , γ	328.06Å 328.06Å 54.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	98.3 (20.00-4.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14180	wwPDB-VP
Average B, all atoms (Å ²)	116.0	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, MG, POD

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	0.89	1/3374 (0.0%)	1.09	19/4593 (0.4%)
1	C	0.74	0/3349	1.00	11/4561 (0.2%)
2	B	0.86	3/3314 (0.1%)	1.08	25/4506 (0.6%)
2	D	0.76	2/3352 (0.1%)	1.04	20/4556 (0.4%)
3	E	0.87	0/914	0.95	2/1238 (0.2%)
All	All	0.82	6/14303 (0.0%)	1.05	77/19454 (0.4%)

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	4
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	15

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	LEU	C-N	11.14	1.59	1.34
2	B	44	LEU	C-N	9.19	1.55	1.34
2	B	360	PRO	C-N	8.02	1.52	1.34
2	D	360	PRO	C-N	6.55	1.49	1.34
2	B	2	ARG	NE-CZ	5.14	1.39	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.82	126.24	118.30
2	D	205	ASP	CB-CG-OD2	8.78	126.20	118.30
2	D	163	ASP	CB-CG-OD2	8.20	125.68	118.30
2	B	205	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	211	ASP	CB-CG-OD2	7.70	125.22	118.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLY	Peptide
1	A	220	GLU	Peptide
1	A	221	ARG	Peptide
1	A	339	ARG	Peptide
2	B	49	ILE	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	3299	0	3129	275	0
1	C	3275	0	3104	271	0
2	B	3241	0	3033	321	0
2	D	3278	0	3074	297	0
3	E	905	0	730	59	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	3	0
5	C	32	0	12	2	0
6	B	28	0	12	1	0
6	D	28	0	12	2	0
7	B	30	0	19	5	0
7	D	30	0	19	4	0
All	All	14180	0	13156	1177	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 43.

The worst 5 of 1177 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:33:PRO:HB3	3:E:35:PHE:CZ	1.64	1.33
1:C:240:ALA:HB2	1:C:243:ARG:NH1	1.39	1.33
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.18
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.22	1.15
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.22	1.14

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	429/451 (95%)	288 (67%)	88 (20%)	53 (12%)	1	14
1	C	426/451 (94%)	289 (68%)	90 (21%)	47 (11%)	1	17
2	B	418/445 (94%)	274 (66%)	87 (21%)	57 (14%)	0	11
2	D	424/445 (95%)	276 (65%)	87 (20%)	61 (14%)	0	10
3	E	130/142 (92%)	81 (62%)	29 (22%)	20 (15%)	0	8
All	All	1827/1934 (94%)	1208 (66%)	381 (21%)	238 (13%)	0	12

5 of 238 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	47	ASP
1	A	62	VAL
1	A	73	THR
1	A	96	LYS

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	342/378 (90%)	217 (64%)	125 (36%)	0	2
1	C	340/378 (90%)	219 (64%)	121 (36%)	0	2
2	B	343/381 (90%)	216 (63%)	127 (37%)	0	1
2	D	348/381 (91%)	214 (62%)	134 (38%)	0	1
3	E	65/126 (52%)	45 (69%)	20 (31%)	0	5
All	All	1438/1644 (88%)	911 (63%)	527 (37%)	0	2

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	382	THR
1	C	178	SER
2	D	373	MET
2	B	406	HIS
1	C	92	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	406	HIS
1	C	133	GLN
2	D	309	HIS
1	C	8	HIS
1	C	88	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 8 ligands modelled in this entry, 2 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	600	4	34,34,34	1.28	3 (8%)	51,54,54	2.00	14 (27%)
6	GDP	B	602	-	30,30,30	0.95	1 (3%)	44,47,47	2.06	13 (29%)
7	POD	B	700	-	34,34,34	3.14	11 (32%)	51,51,51	4.15	23 (45%)
5	GTP	C	601	4	34,34,34	1.13	4 (11%)	51,54,54	1.68	10 (19%)
6	GDP	D	603	-	30,30,30	1.03	2 (6%)	44,47,47	1.87	12 (27%)
7	POD	D	701	-	34,34,34	3.10	11 (32%)	51,51,51	3.93	22 (43%)

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	600	4	-	0/22/38/38	0/1/3/3
6	GDP	B	602	-	-	0/16/32/32	0/1/3/3
7	POD	B	700	-	1/1/5/5	0/10/45/45	0/1/5/5
5	GTP	C	601	4	-	0/22/38/38	0/1/3/3
6	GDP	D	603	-	-	0/16/32/32	0/1/3/3
7	POD	D	701	-	1/1/5/5	0/10/45/45	0/1/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	POD	C7-C6	-9.80	1.21	1.39
7	D	701	POD	C7-C2	-8.95	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	POD	C7-C6	-8.72	1.23	1.39
7	B	700	POD	C7-C2	-8.49	1.22	1.38
7	B	700	POD	C10-C11	-6.52	1.45	1.56

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	POD	C2-C7-C6	13.51	149.06	119.53
7	D	701	POD	C2-C7-C6	12.96	147.85	119.53
7	D	701	POD	C7-C6-C5	-12.11	103.81	120.16
7	B	700	POD	C7-C6-C5	-11.80	104.22	120.16
7	B	700	POD	C7-C2-C3	-10.72	107.77	122.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	701	POD	C10
7	B	700	POD	C10

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 ⓘ

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.