



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:13 AM GMT

PDB ID : 3HKE
Title : Tubulin-T138067: RB3 stathmin-like domain complex
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.
Deposited on : 2009-05-23
Resolution : 3.60 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

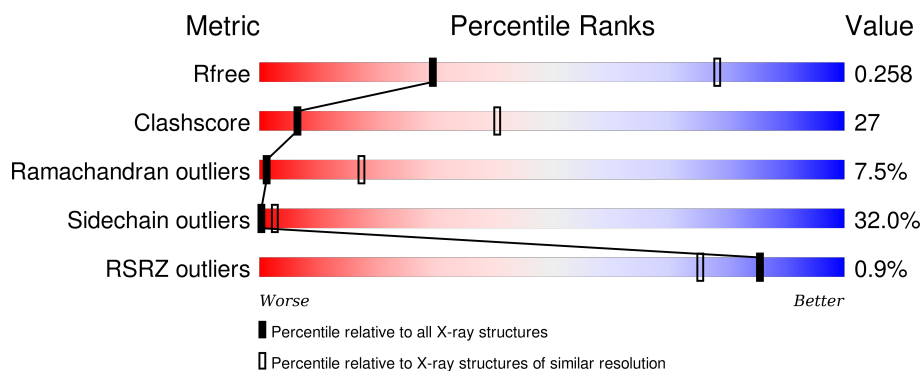
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 13%, orange 13% 38%, yellow 38% 41%, green 41%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 41% 38% 13% • 5% </div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5% 15%, yellow 15% 33%, green 33% 46%, grey 46%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 46% 33% 15% • 5% </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 6% 17%, yellow 17% 39%, green 39% 37%, grey 37%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 37% 39% 17% • 6% </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 17%, orange 17% 38%, yellow 38% 39%, green 39%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 39% 38% 17% • • </div> </div>
3	E	142	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 12%, orange 12% 37%, yellow 37% 37%, green 37%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 37% 37% 12% • 13% </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14244 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3297	2095	559	622	21			
1	C	428	Total	C	N	O	S	0	0	0
			3269	2075	553	621	20			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3248	2043	547	633	25			
2	D	427	Total	C	N	O	S	0	0	0
			3296	2071	557	644	24			

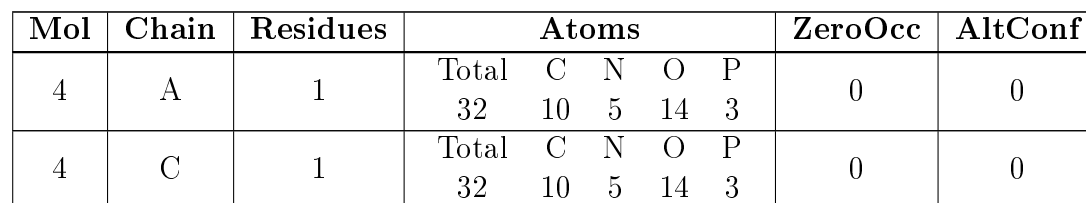
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			917	555	174	183	5			

There is a discrepancy between the modelled and reference sequences:

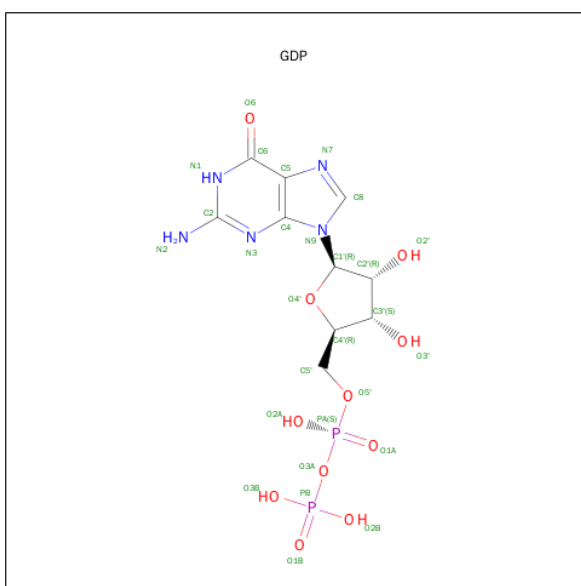
Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

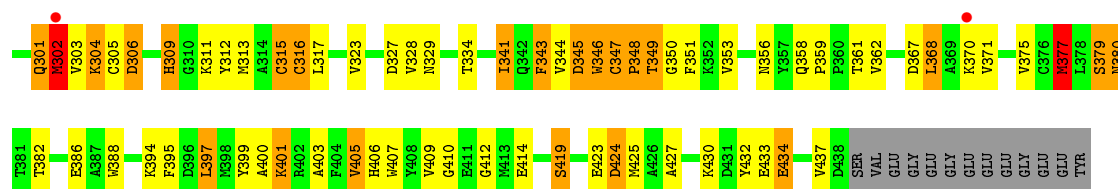


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | B | 1 | Total Mg
1 1 | 0 | 0 |
| 5 | A | 1 | Total Mg
1 1 | 0 | 0 |
| 5 | C | 1 | Total Mg
1 1 | 0 | 0 |

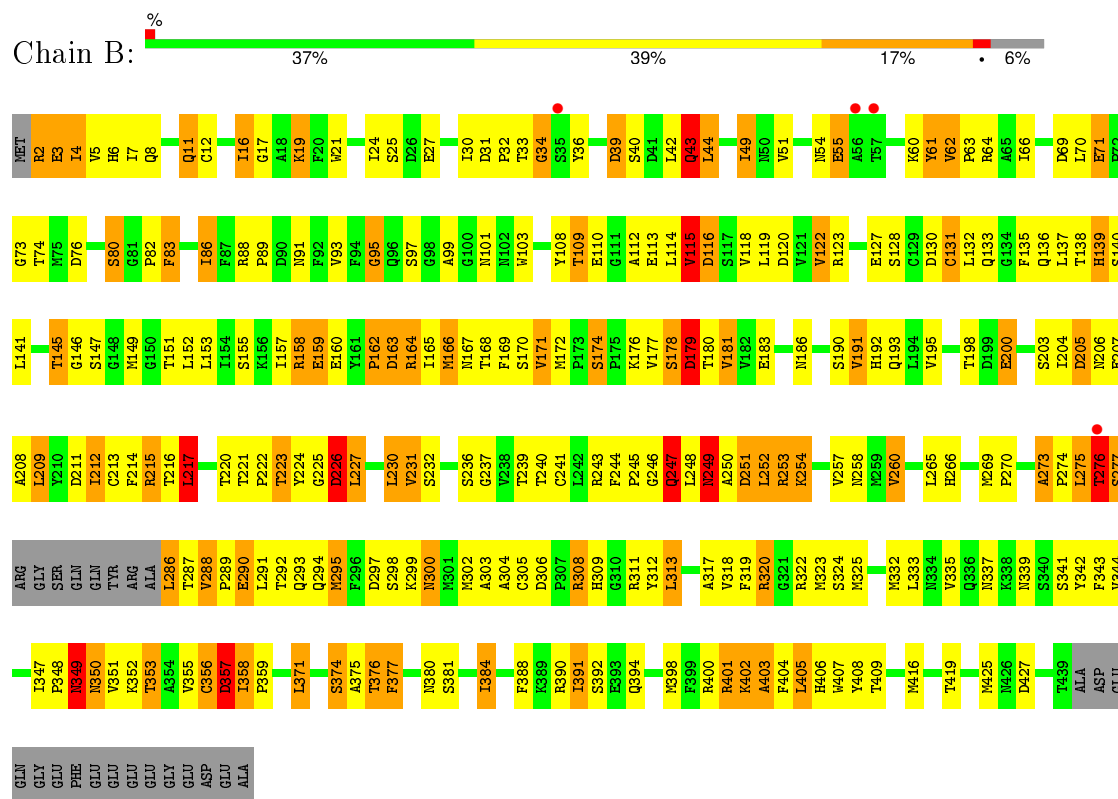
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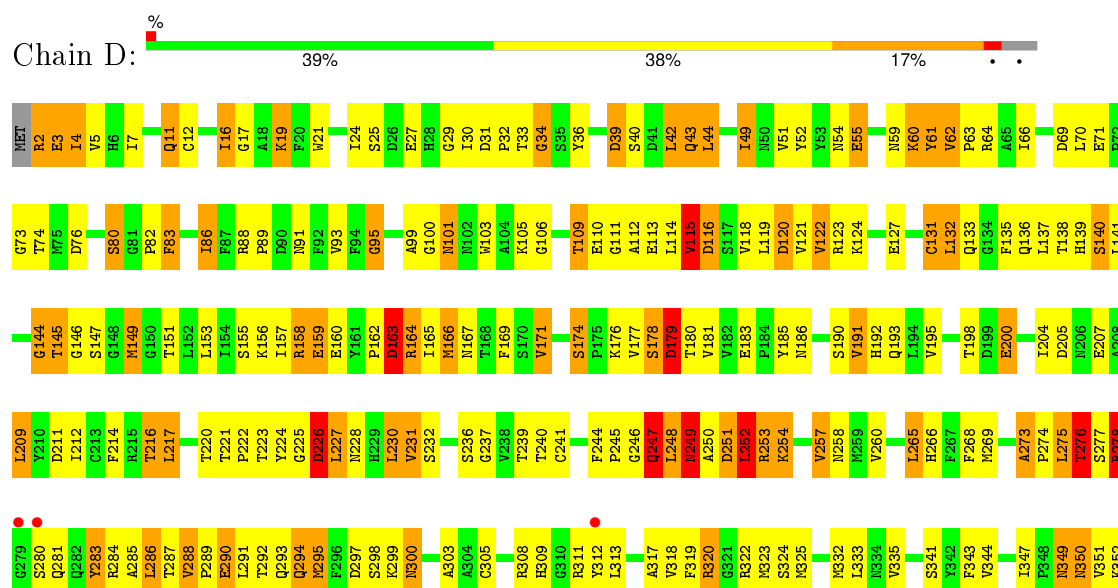
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

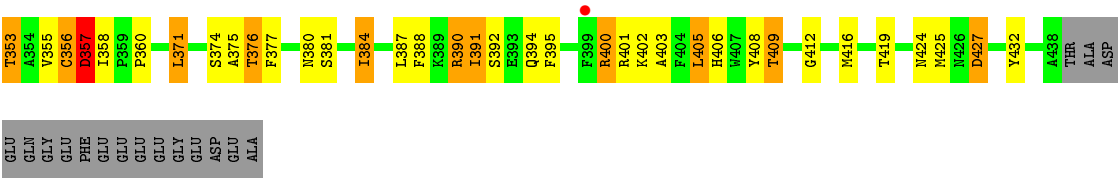


• Molecule 2: Tubulin beta chain

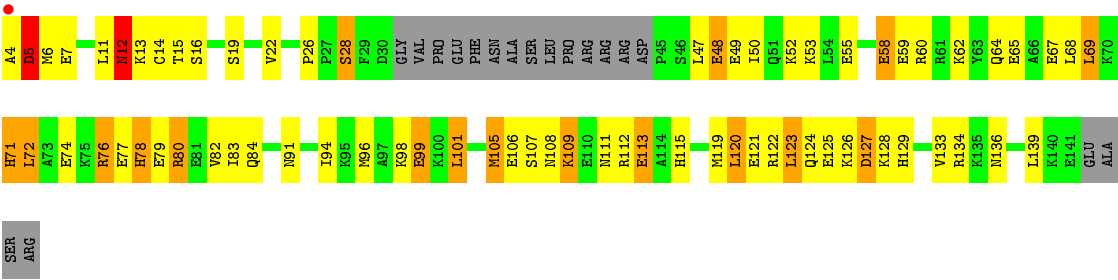


• Molecule 2: Tubulin beta chain





● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	326.71 Å 326.71 Å 54.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 48.29 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.60) 98.6 (48.29-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.57 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.253 0.219 , 0.258	Depositor DCC
R_{free} test set	1940 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	133.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 131.8	EDS
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 38704 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14244	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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, T13

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	0.69	0/3374	0.94	14/4588 (0.3%)
1	C	0.59	1/3342 (0.0%)	0.89	12/4550 (0.3%)
2	B	0.62	0/3320	0.91	14/4508 (0.3%)
2	D	0.57	0/3370	0.87	15/4577 (0.3%)
3	E	0.65	0/925	0.82	1/1241 (0.1%)
All	All	0.62	1/14331 (0.0%)	0.90	56/19464 (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	1
1	C	0	1
2	B	0	2
2	D	0	2
3	E	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	302	MET	SD-CE	5.27	2.07	1.77

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	CYS	CA-CB-SG	-10.22	95.61	114.00
1	A	424	ASP	CB-CG-OD2	7.49	125.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LEU	CA-CB-CG	7.08	131.57	115.30
1	C	397	LEU	CA-CB-CG	7.05	131.51	115.30
1	C	120	ASP	CB-CG-OD2	6.98	124.58	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	HIS	Peptide
2	B	162	PRO	Peptide
2	B	247	GLN	Peptide
1	C	266	HIS	Peptide
2	D	162	PRO	Peptide

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	3297	0	3167	173	0
1	C	3269	0	3118	161	0
2	B	3248	0	3064	213	0
2	D	3296	0	3100	199	0
3	E	917	0	803	41	0
4	A	32	0	12	4	0
4	C	32	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	47	0	14	6	0
6	D	47	0	14	6	0
7	B	28	0	12	5	0
7	D	28	0	12	4	0
All	All	14244	0	13328	756	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 27.

The worst 5 of 756 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)
3:E:105:MET:SD	3:E:105:MET:CE	2.04	1.45
1:C:302:MET:SD	1:C:302:MET:CE	2.07	1.41
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.17	1.15
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.26	1.14
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.30	1.12

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	423/451 (94%)	337 (80%)	56 (13%)	30 (7%)	1	19
1	C	422/451 (94%)	332 (79%)	58 (14%)	32 (8%)	1	17
2	B	416/445 (94%)	324 (78%)	60 (14%)	32 (8%)	1	16
2	D	425/445 (96%)	339 (80%)	56 (13%)	30 (7%)	1	19
3	E	120/142 (84%)	81 (68%)	27 (22%)	12 (10%)	1	11
All	All	1806/1934 (93%)	1413 (78%)	257 (14%)	136 (8%)	1	17

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	62	VAL
1	A	112	LYS
1	A	247	ALA
1	A	265	ILE

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	346/378 (92%)	242 (70%)	104 (30%)	0	3
1	C	340/378 (90%)	236 (69%)	104 (31%)	0	3
2	B	349/383 (91%)	240 (69%)	109 (31%)	0	3
2	D	352/383 (92%)	237 (67%)	115 (33%)	0	2
3	E	80/126 (64%)	43 (54%)	37 (46%)	0	0
All	All	1467/1648 (89%)	998 (68%)	469 (32%)	0	2

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	419	THR
1	C	206	ASN
3	E	11	LEU
1	C	41	THR
1	C	116	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	349	ASN
1	C	91	GLN
2	D	394	GLN
2	B	350	ASN
2	B	436	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	A	600	-	25,34,34	0.97	2 (8%)	34,54,54	1.66	9 (26%)
6	T13	B	1241	2	24,24,25	2.44	4 (16%)	31,36,38	2.12	8 (25%)
7	GDP	B	600	-	23,30,30	1.08	1 (4%)	30,47,47	1.71	7 (23%)
6	T13	B	700	-	25,25,25	2.66	4 (16%)	33,38,38	1.86	7 (21%)
4	GTP	C	600	-	25,34,34	1.02	2 (8%)	34,54,54	1.85	8 (23%)
6	T13	D	1241	2	24,24,25	2.37	4 (16%)	31,36,38	1.73	7 (22%)
7	GDP	D	600	-	23,30,30	0.94	1 (4%)	30,47,47	1.83	7 (23%)
6	T13	D	700	-	25,25,25	2.50	4 (16%)	33,38,38	2.15	8 (24%)

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	-	-	0/18/38/38	0/3/3/3
6	T13	B	1241	2	-	0/13/13/13	0/2/2/2
7	GDP	B	600	-	-	0/12/32/32	0/3/3/3
6	T13	B	700	-	-	0/13/13/13	0/2/2/2
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	T13	D	1241	2	-	0/13/13/13	0/2/2/2
7	GDP	D	600	-	-	0/12/32/32	0/3/3/3
6	T13	D	700	-	-	0/13/13/13	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1241	T13	CAO-NAM	-7.09	1.31	1.43
6	B	1241	T13	CAO-NAM	-6.95	1.31	1.43
6	B	700	T13	CAO-NAM	-6.22	1.32	1.43
6	D	700	T13	CAO-NAM	-5.20	1.34	1.43
6	D	700	T13	CAW-SAX	-4.98	1.70	1.79

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	700	T13	CAA-OAN-CAV	-7.85	105.64	117.54
6	D	700	T13	OAC-SAX-OAB	-6.19	111.33	119.54
6	B	1241	T13	OAC-SAX-OAB	-6.06	111.51	119.54
6	B	700	T13	CAA-OAN-CAV	-5.93	108.55	117.54
6	B	1241	T13	CAA-OAN-CAV	-5.46	109.26	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	4	0
6	B	1241	T13	4	0
7	B	600	GDP	5	0
6	B	700	T13	2	0
4	C	600	GTP	4	0
6	D	1241	T13	5	0
7	D	600	GDP	4	0
6	D	700	T13	1	0

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 [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	427/451 (94%)	-0.31	2 (0%) 91 86	63, 66, 67, 73	0
1	C	428/451 (94%)	-0.10	6 (1%) 78 65	60, 66, 67, 77	0
2	B	420/445 (94%)	-0.15	4 (0%) 84 73	64, 66, 67, 72	0
2	D	427/445 (95%)	-0.23	4 (0%) 85 75	64, 66, 67, 73	0
3	E	124/142 (87%)	-0.44	1 (0%) 87 78	59, 66, 71, 74	0
All	All	1826/1934 (94%)	-0.22	17 (0%) 85 75	59, 66, 68, 77	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	3.7
1	C	30	ILE	3.0
2	B	57	THR	2.6
1	A	351	PHE	2.6
1	C	370	LYS	2.6

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
6	T13	B	1241	23/24	0.84	0.28	0.18	68,69,100,100	23
6	T13	B	700	24/24	0.89	0.24	-0.22	62,71,76,77	24
6	T13	D	700	24/24	0.90	0.23	-0.51	61,65,67,69	24
7	GDP	D	600	28/28	0.96	0.13	-1.19	64,65,67,67	0
4	GTP	C	600	32/32	0.94	0.15	-1.40	63,65,66,66	0
7	GDP	B	600	28/28	0.94	0.13	-1.42	64,65,67,67	0
4	GTP	A	600	32/32	0.97	0.13	-1.68	63,65,66,66	0
6	T13	D	1241	23/24	0.94	0.15	-1.69	64,66,100,100	23
5	MG	C	601	1/1	0.98	0.19	-1.85	30,30,30,30	0
5	MG	A	601	1/1	0.99	0.11	-5.43	30,30,30,30	0
5	MG	B	601	1/1	0.97	1.04	-	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.