W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2017 – 06:54 PM EDT

PDB ID	:	5XHC
Title	:	Crystal structure of T2R-TTL-PO10 complex
Authors	:	Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on	:	unknown
Resolution	:	2.75 Å(reported)

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

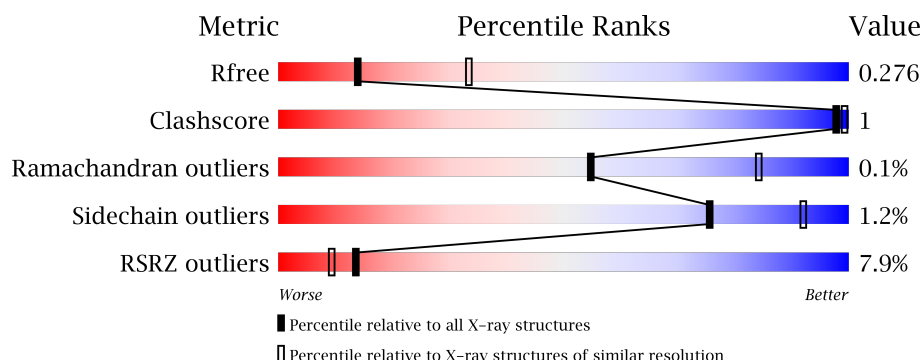|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.75 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		1.2%
RSRZ outliers		7.9%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 <=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	450	4% / 94% · ·
1	C	450	95% · ·
2	B	445	3% / 92% · 5%
2	D	445	12% / 92% · 5%
3	E	184	6% / 64% · 35%

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Mol	Chain	Length	Quality of chain
4	F	384	

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
9	MES	B	507	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17462 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	437	Total 3441	C 2179	N 586	O 652	S 24	0	4	0
1	C	440	Total 3482	C 2200	N 589	O 668	S 25	0	9	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total 3353	C 2107	N 574	O 645	S 27	0	2	0
2	D	421	Total 3306	C 2079	N 562	O 638	S 27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total 1004	C 621	N 181	O 196	S 6	0	2	0

- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total 2553	C 1645	N 438	O 455	S 15	0	3	0

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_{10}H_{16}N_5O_{14}P_3$).
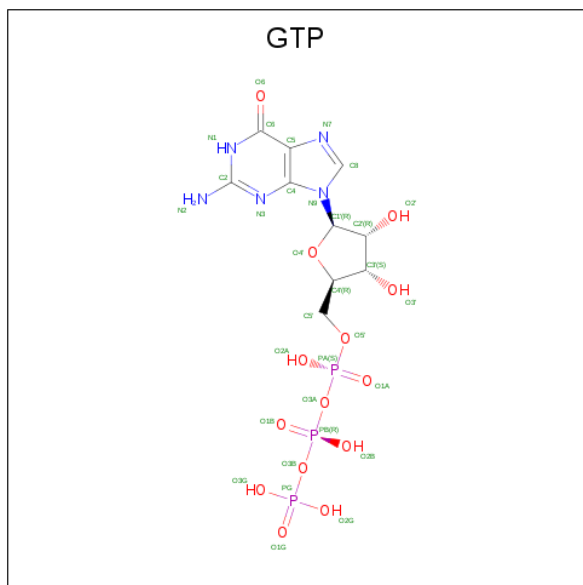
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

MES

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(4-fluoroph enyl)carbonylphenyl]methylidene]piperazine-2,5-dione (three-letter code: 87U) (formula: $C_{26}H_{23}FN_4O_3$).

87U

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	0	0
			34	26	1	4	3		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	20	Total 20	O 20	0	0
12	B	22	Total 22	O 22	0	0
12	C	55	Total 55	O 55	0	0
12	E	2	Total 2	O 2	0	0
12	F	4	Total 4	O 4	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 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.
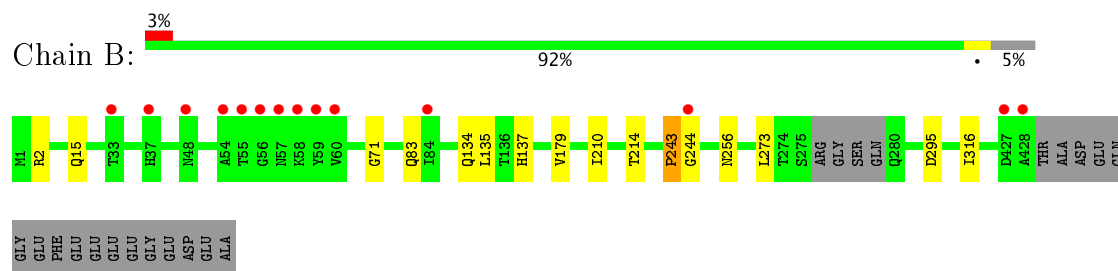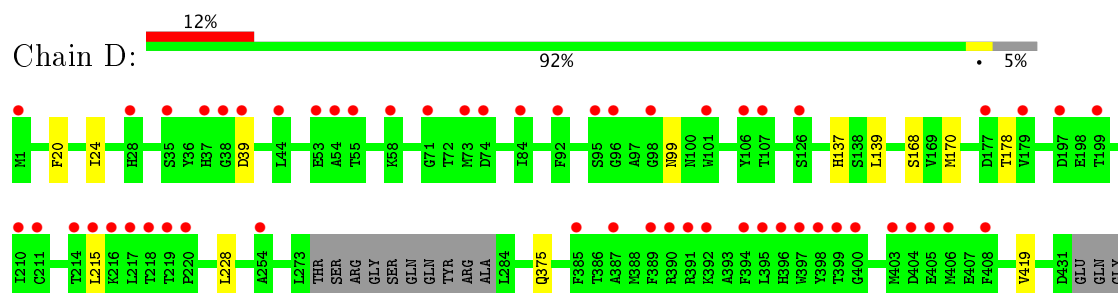
- Molecule 1: Tubulin alpha chain
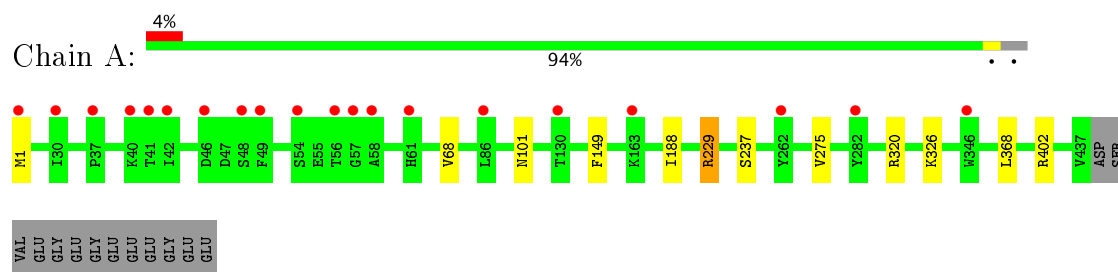
- Molecule 1: Tubulin alpha chain
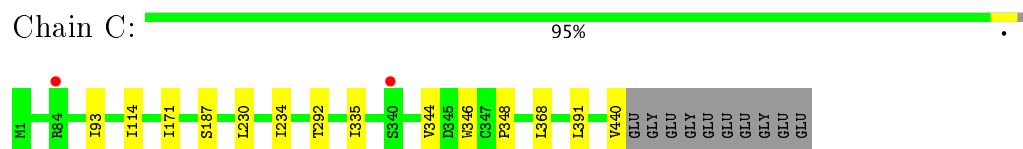
- Molecule 2: Tubulin beta chain

- Molecule 2: Tubulin beta chain

GLU PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

● **Molecule 3: Stathmin-4**

Chain E:

TYR LYS GLU LYS MET LYS GLU LEU PRO LEU VAL SER LEU PHE CYS SER CYS PHE LEU SER ASP PRO LEU ASN LYS SER TYR LYS GLU ALA ASP THR VAL ASP ASN LEU ASN TRP CYS VAL ILE SER ASP M6 P26 P27 SER PHE ASP GLY VAL PRO GLU PHE ASN ALA SER LEU

PRO ARG ARG ARG D44 P45 S46 L47 E48 Q51 E59 K128 E131 E132 V133 N136 K137 E138 L139 K140 E141 GLU ALA SER ARG

● **Molecule 4: TUBULIN TYROSINE LIGASE**

Chain F:
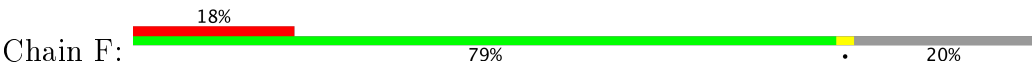
M1 V6 E9 N10 Y14 L20 L21 L22 W27 R31 K32 Y98 V99 I100 Y101 P102 THR ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR ASP GLU ARG GLU VAL PHE LEU ALA TYR ASN ARG ARG

GLU GLY ARG GLU G144 N145 V146 W147 I148 A149 K150 S151 SER ALA GLY ALA LYS GLY GLU G159 I160 L161 I162 S163 S164 E165 A166 SER GLU LEU LEU ASP PHE ILE ASP GLU GLN GLY GLN VAL H180 V181 I182 Q183 K184 L191 L192 E193 P194 G195 H196 R197 K198 F199 Y211 T223 S224

S225 E226 P227 Y228 N229 S230 A231 N232 P233 Q234 D235 K236 T237 C238 H239 L240 T241 N242 H243 C244 I245 Q246 K247 GLU TYR SER LYS N252 Y253 G254 R255 Y256 E257 E258 G259 N260 M320 A335 G349 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO THR S373 I374 H384

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.26Å 157.88Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.38 – 2.75 49.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (119.38-2.75) 98.5 (49.93-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.227 , 0.277 0.228 , 0.276	Depositor DCC
R_{free} test set	3932 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.8	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	0.91	EDS
Total number of atoms	17462	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical 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.

wwPDB X-ray Structure Validation Summary Report

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, 87U, GTP, ACP, 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	0.37	0/3525	0.59	0/4784
1	C	0.37	0/3572	0.60	0/4850
2	B	0.39	0/3427	0.60	0/4640
2	D	0.38	0/3379	0.55	0/4577
3	E	0.38	0/1018	0.53	0/1350
4	F	0.38	0/2618	0.54	0/3537
All	All	0.38	0/17539	0.57	0/23738

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 ⓘ

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	3441	0	3363	9	0
1	C	3482	0	3384	7	0
2	B	3353	0	3228	7	0
2	D	3306	0	3181	6	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	2	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	1	0
10	B	34	0	0	2	0
11	F	31	0	14	0	0
12	A	20	0	0	0	0
12	B	22	0	0	0	0
12	C	55	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17462	0	16791	30	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 1.

The worst 5 of 30 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:A:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.07	1.20
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.75	0.98
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.87	0.84
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.67	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.22	0.69

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	439/450 (98%)	426 (97%)	13 (3%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	407 (96%)	13 (3%)	2 (0%)	32	64
2	D	417/445 (94%)	404 (97%)	12 (3%)	1 (0%)	51	81
3	E	118/184 (64%)	116 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	286 (95%)	14 (5%)	0	100	100
All	All	2142/2358 (91%)	2074 (97%)	65 (3%)	3 (0%)	55	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	71	GLY
2	D	39	ASP

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	372/378 (98%)	364 (98%)	8 (2%)	57	85
1	C	379/378 (100%)	377 (100%)	2 (0%)	91	96
2	B	367/383 (96%)	360 (98%)	7 (2%)	62	87
2	D	362/383 (94%)	361 (100%)	1 (0%)	94	98
3	E	110/168 (66%)	107 (97%)	3 (3%)	50	80
4	F	281/342 (82%)	278 (99%)	3 (1%)	78	92
All	All	1871/2032 (92%)	1847 (99%)	24 (1%)	75	91

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	83	GLN
2	B	214	THR
4	F	32	LYS
2	B	135	LEU
2	B	137	HIS

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

Mol	Chain	Res	Type
1	A	101	ASN
2	B	83	GLN
1	C	249	ASN
3	E	136	ASN
4	F	252	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 15 ligands modelled in this entry, 7 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
5	GTP	A	501	7	27,34,34	1.19	2 (7%)	27,54,54	2.07	8 (29%)
8	GDP	B	502	7	25,30,30	1.22	2 (8%)	26,47,47	2.13	6 (23%)
9	MES	B	504	-	12,12,12	1.94	1 (8%)	14,16,16	9.62	10 (71%)
10	87U	B	505	-	29,37,37	2.45	8 (27%)	35,54,54	1.74	9 (25%)
9	MES	B	507	-	12,12,12	1.95	2 (16%)	14,16,16	7.23	8 (57%)
5	GTP	C	501	7	27,34,34	1.13	2 (7%)	27,54,54	2.08	8 (29%)
5	GTP	D	501	7	27,34,34	1.25	2 (7%)	27,54,54	2.04	6 (22%)
11	ACP	F	401	-	27,33,33	1.97	8 (29%)	30,52,52	1.65	2 (6%)

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	7	-	0/18/38/38	0/3/3/3
8	GDP	B	502	7	-	0/12/32/32	0/3/3/3
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	87U	B	505	-	-	0/18/22/22	0/4/4/4
9	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	7	-	0/18/38/38	0/3/3/3
5	GTP	D	501	7	-	0/18/38/38	0/3/3/3
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-6.07	1.68	1.77
9	B	507	MES	C8-S	-6.03	1.68	1.77
10	B	505	87U	FAG-CAX	-5.56	1.23	1.36
10	B	505	87U	CBA-CAW	-4.80	1.41	1.49
10	B	505	87U	CBB-CAW	-4.08	1.42	1.49

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	504	MES	O1S-S-C8	-26.16	84.32	106.79
9	B	507	MES	O3S-S-O1S	-14.30	78.60	111.37
9	B	507	MES	O1S-S-C8	-14.13	94.65	106.79
9	B	504	MES	O3S-S-O1S	-11.38	85.27	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	504	MES	O2S-S-O1S	-8.77	83.47	113.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	87U	2	0
9	B	507	MES	1	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 ⓘ

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(Å²)	Q<0.9
1	A	437/450 (97%)	0.20	20 (4%)	33	27	23, 45, 71, 91	0
1	C	440/450 (97%)	-0.09	2 (0%)	90	89	19, 36, 58, 80	1 (0%)
2	B	424/445 (95%)	0.21	14 (3%)	47	41	25, 45, 75, 102	1 (0%)
2	D	421/445 (94%)	0.79	55 (13%)	4	3	35, 64, 96, 126	4 (0%)
3	E	120/184 (65%)	0.65	11 (9%)	10	7	34, 64, 95, 106	0
4	F	309/384 (80%)	1.05	69 (22%)	1	1	35, 68, 107, 122	0
All	All	2151/2358 (91%)	0.41	171 (7%)	13	9	19, 51, 92, 126	6 (0%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	9.0
2	D	37	HIS	8.2
4	F	233	PHE	6.6
2	D	395	LEU	5.6
4	F	244	CYS	5.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
9	MES	B	507	12/12	0.89	0.43	6.75	95,97,101,104	0
9	MES	B	504	12/12	0.89	0.21	1.35	70,74,76,78	0
7	MG	B	501	1/1	0.98	0.18	0.19	22,22,22,22	0
10	87U	B	505	34/34	0.94	0.20	0.14	48,54,55,55	0
11	ACP	F	401	31/31	0.85	0.29	-0.26	79,83,112,115	0
8	GDP	B	502	28/28	0.98	0.15	-0.55	22,25,26,28	0
5	GTP	D	501	32/32	0.93	0.17	-0.85	45,49,67,70	0
5	GTP	C	501	32/32	0.98	0.14	-0.93	24,26,28,30	0
5	GTP	A	501	32/32	0.98	0.15	-1.77	26,28,30,30	0
6	CA	C	503	1/1	0.89	0.10	-1.90	56,56,56,56	0
6	CA	A	502	1/1	0.96	0.13	-2.84	67,67,67,67	0
6	CA	B	506	1/1	0.88	0.16	-	78,78,78,78	0
7	MG	B	503	1/1	0.97	0.11	-	24,24,24,24	0
7	MG	D	502	1/1	0.85	0.12	-	52,52,52,52	0
7	MG	C	502	1/1	0.98	0.11	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.