



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:52 PM GMT

PDB ID : 1XTS
Title : Structure of small GTPase human Rheb in complex with GTP
Authors : Yu, Y.; Ding, J.
Deposited on : 2004-10-24
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

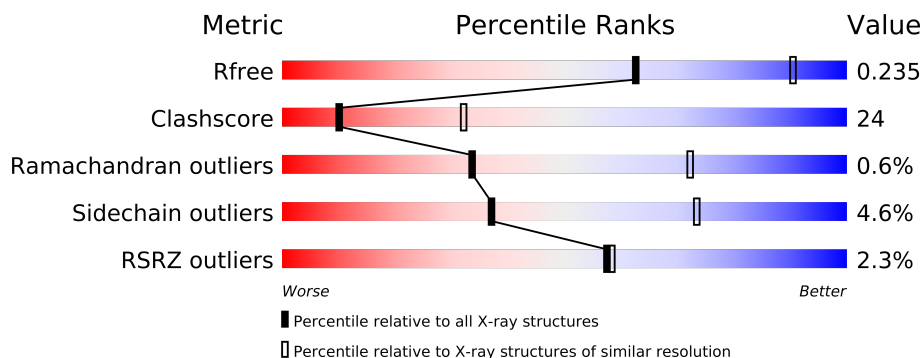
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	177	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1424 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 GTP-binding protein Rheb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1361	873	223	262	3			

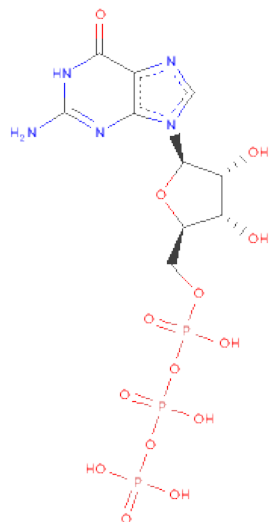
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	LEU	-	EXPRESSION TAG	UNP Q15382
A	171	GLU	-	EXPRESSION TAG	UNP Q15382
A	172	HIS	-	EXPRESSION TAG	UNP Q15382
A	173	HIS	-	EXPRESSION TAG	UNP Q15382
A	174	HIS	-	EXPRESSION TAG	UNP Q15382
A	175	HIS	-	EXPRESSION TAG	UNP Q15382
A	176	HIS	-	EXPRESSION TAG	UNP Q15382
A	177	HIS	-	EXPRESSION TAG	UNP Q15382

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		

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- Molecule 1: GTP-binding protein Rheb

HIS	P2	R7	K8	I9	A10	G18	K19	S20	I24	Q25	F26	V27	E28	G29	F31	V32	I39	E40	K45	L46	I47	E53	Y54	H55	L56	Q57	L58	D65	E66	I69	F70	P71	Q72	T73	Y74	S75	I76	D77	I78	N79	G80	Y81	I82	L83	Y84	Y85	S86	V87	T88	E89		
HIS	I90	K91	S92	F93	I96	A97	V98	K102	L103	L104	D105	M106	V107	G108	K109	V110	Q111	I112	P113	I114	M115	L116	K120	K121	D122	L123	H124	M125	E126	R127	V128	I129	A138	M142	A143	A144	F145	L146	E147	M153	Q154	F160	R161	R162	I163	I164	L165	E166	K169	L170	E171	E172

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.41Å 98.39Å 47.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.80 18.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.80-2.80) 98.7 (18.99-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.277 0.231 , 0.235	Depositor DCC
R_{free} test set	287 reflections (4.68%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.8	EDS
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 6137 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1424	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1385	0.65	0/1870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1361	0	1375	66	1
2	A	1	0	0	0	0
3	A	32	0	12	4	0
4	A	30	0	0	0	0
All	All	1424	0	1387	66	1

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 24.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:LYS:H	1:A:79:ASN:ND2	1.68	0.91
1:A:10:ALA:HB2	1:A:78:ILE:HD13	1.55	0.90
1:A:8:LYS:H	1:A:79:ASN:HD22	1.24	0.83
1:A:81:TYR:HE1	1:A:112:ILE:HG12	1.49	0.77
1:A:25:GLN:HE21	1:A:153:ASN:HD22	1.35	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:GLN:OE1	1:A:30:GLN:OE1[4_572]	1.71	0.49

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	169/177 (96%)	157 (93%)	11 (6%)	1 (1%)	33 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	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	152/158 (96%)	145 (95%)	7 (5%)	37 73

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	166	GLU
1	A	115	MET
1	A	76	ILE
1	A	142	ASN

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	25	GLN
1	A	50	ASN
1	A	79	ASN
1	A	119	ASN
1	A	172	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	GTP	A	179	2	34,34,34	1.21	3 (8%)	51,54,54	1.98	9 (17%)

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
3	GTP	A	179	2	-	0/22/38/38	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	179	GTP	C4-N9	-2.95	1.33	1.37
3	A	179	GTP	C2-N1	2.36	1.40	1.36
3	A	179	GTP	C8-N9	-2.04	1.33	1.36

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	179	GTP	C6-C5-N7	-9.05	132.92	134.14
3	A	179	GTP	C2-N3-C4	4.68	121.66	115.09
3	A	179	GTP	PB-O3B-PG	-3.85	120.41	131.68
3	A	179	GTP	N3-C4-N9	3.78	132.45	126.91
3	A	179	GTP	C5-C4-N3	-3.63	120.68	125.94

There are no chirality outliers.

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 ⓘ

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	171/177 (96%)	-0.31	4 (2%) 57 58	22, 37, 58, 70	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	HIS	4.0
1	A	109	LYS	3.5
1	A	125	MET	3.0
1	A	111	GLN	2.5

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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	178	1/1	0.15	-0.61	35,35,35,35	0
3	GTP	A	179	32/32	0.12	-1.29	29,34,38,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.