Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2020 – 06:02 PM BST

PDB ID	:	6SQ2
Title	:	Structure of a phosphomimetic switch 2 variant of Rab8a in complex with the phospho-Rab binding domain of RILPL2
Authors	:	Khan, A.R.; Waschbusch, D.
Deposited on	:	2019-09-03
Resolution	:	1.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

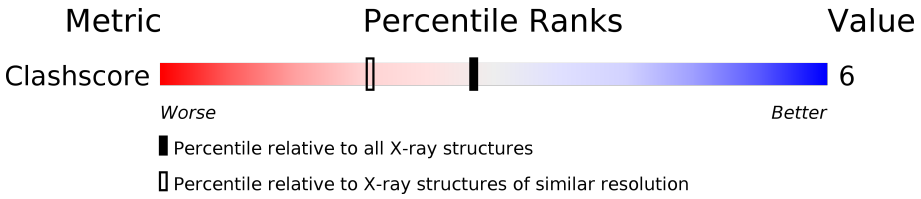
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	141614	7310 (1.70-1.66)

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3974 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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	5	0
			1447	925	246	269	7			
1	B	173	Total	C	N	O	S	0	0	0
			1401	893	239	262	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P61006
A	-1	SER	-	expression tag	UNP P61006
A	0	HIS	-	expression tag	UNP P61006
A	67	LEU	GLN	engineered mutation	UNP P61006
A	72	GLU	THR	engineered mutation	UNP P61006
B	-2	GLY	-	expression tag	UNP P61006
B	-1	SER	-	expression tag	UNP P61006
B	0	HIS	-	expression tag	UNP P61006
B	67	LEU	GLN	engineered mutation	UNP P61006
B	72	GLU	THR	engineered mutation	UNP P61006

- Molecule 2 is a protein called RILP-like protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	31	Total	C	N	O	0	1	0
			272	170	52	50			
2	E	32	Total	C	N	O	0	0	0
			275	171	53	51			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	123	HIS	-	expression tag	UNP Q969X0
D	124	HIS	-	expression tag	UNP Q969X0

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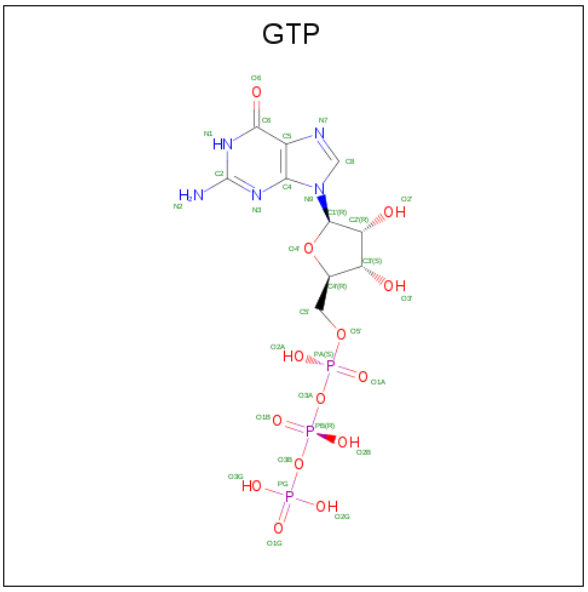
Chain	Residue	Modelled	Actual	Comment	Reference
D	125	HIS	-	expression tag	UNP Q969X0
D	126	HIS	-	expression tag	UNP Q969X0
D	127	HIS	-	expression tag	UNP Q969X0
D	128	HIS	-	expression tag	UNP Q969X0
E	123	HIS	-	expression tag	UNP Q969X0
E	124	HIS	-	expression tag	UNP Q969X0
E	125	HIS	-	expression tag	UNP Q969X0
E	126	HIS	-	expression tag	UNP Q969X0
E	127	HIS	-	expression tag	UNP Q969X0
E	128	HIS	-	expression tag	UNP Q969X0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	222	Total O 222 222	0	0
5	B	226	Total O 226 226	0	0
5	D	32	Total O 32 32	0	0
5	E	33	Total O 33 33	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.70Å 71.73Å 116.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.07 – 1.68	Depositor
% Data completeness (in resolution range)	93.6 (61.07-1.68)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.181 , 0.202	Depositor
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.259	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

4 Model quality

4.1 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	0.46	0/1483	0.57	0/1987
1	B	0.39	0/1422	0.54	0/1905
2	D	1.04	2/276 (0.7%)	0.86	1/369 (0.3%)
2	E	0.84	1/276 (0.4%)	0.80	1/369 (0.3%)
All	All	0.54	3/3457 (0.1%)	0.61	2/4630 (0.0%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	157	GLU	CD-OE1	-5.99	1.19	1.25
2	D	143[A]	GLN	N-CA	5.79	1.57	1.46
2	D	143[B]	GLN	N-CA	5.79	1.57	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	132	ARG	CB-CA-C	-5.49	99.42	110.40
2	E	157	GLU	CB-CA-C	-5.40	99.59	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39[A]	SER	Mainchain
1	A	39[B]	SER	Mainchain

4.2 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	1447	0	1479	13	0
1	B	1401	0	1414	4	0
2	D	272	0	289	12	0
2	E	275	0	289	18	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	222	0	0	3	2
5	B	226	0	0	0	1
5	D	32	0	0	0	0
5	E	33	0	0	2	0
All	All	3974	0	3495	43	3

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 6.

All (43) 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:E:154:VAL:O	2:E:157:GLU:HG3	1.58	1.03
2:E:154:VAL:O	2:E:157:GLU:CG	2.15	0.95
2:E:158:GLU:O	2:E:160:GLN:N	2.03	0.91
2:D:158:GLU:C	2:D:159:LEU:HD23	1.94	0.86
1:A:172:LYS:HD3	1:A:172:LYS:N	1.90	0.84
2:D:158:GLU:O	2:D:159:LEU:HD23	1.84	0.77
2:D:157:GLU:C	2:D:159:LEU:H	1.94	0.69
2:E:157:GLU:OE1	2:E:158:GLU:HA	1.96	0.66
2:D:157:GLU:O	2:D:159:LEU:N	2.30	0.65
2:E:154:VAL:O	2:E:157:GLU:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:GLU:OE1	2:E:158:GLU:N	2.31	0.64
2:E:135:LEU:HD21	2:E:139:ARG:NH1	2.15	0.61
2:D:157:GLU:C	2:D:159:LEU:N	2.52	0.61
1:B:45:PHE:O	2:D:149:LYS:NZ	2.37	0.57
2:E:157:GLU:OE1	2:E:158:GLU:CA	2.55	0.54
1:A:69:ARG:HH12	2:D:137:GLU:CD	2.13	0.52
2:E:160:GLN:OE1	2:E:160:GLN:HA	2.10	0.52
1:A:100:ARG:NH1	1:A:143:TYR:OH	2.43	0.51
2:E:151:GLN:HG3	5:E:214:HOH:O	2.13	0.49
1:B:43:ILE:HD13	1:B:77:TYR:CD2	2.48	0.48
2:D:129:ASN:N	2:D:129:ASN:OD1	2.46	0.48
1:A:167:ARG:NH2	5:A:1004:HOH:O	2.40	0.48
2:D:141:VAL:HG12	2:E:141:VAL:HG12	1.97	0.47
1:A:13[B]:LEU:HD23	1:A:85:MET:HB2	1.97	0.46
1:A:3:LYS:HE2	1:A:5:TYR:O	2.16	0.45
2:E:139:ARG:HD3	5:E:212:HOH:O	2.16	0.45
2:E:158:GLU:C	2:E:160:GLN:N	2.69	0.45
2:D:149:LYS:O	2:D:153:LEU:HG	2.17	0.45
1:A:71:ARG:HA	1:A:71:ARG:HD3	1.80	0.44
2:E:157:GLU:O	2:E:159:LEU:N	2.51	0.44
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.86	0.43
2:E:157:GLU:C	2:E:159:LEU:H	2.21	0.43
1:A:167:ARG:NE	5:A:1004:HOH:O	2.38	0.43
1:A:94:LYS:HE3	1:A:94:LYS:O	2.19	0.42
2:D:159:LEU:HD23	2:D:159:LEU:N	2.31	0.42
1:A:172:LYS:HD3	1:A:172:LYS:H	1.76	0.42
1:A:140:ALA:HB1	1:A:145:ILE:O	2.20	0.42
1:B:4:THR:HB	1:B:5:TYR:H	1.47	0.41
2:E:151:GLN:HA	2:E:154:VAL:HG22	2.02	0.41
2:E:157:GLU:CD	2:E:158:GLU:N	2.73	0.41
1:B:103:ILE:HD13	1:B:143:TYR:CZ	2.55	0.41
1:A:159:GLU:HG3	5:A:1112:HOH:O	2.21	0.41
2:D:155:VAL:HG12	2:E:155:VAL:HG12	2.03	0.40

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
5:B:1026:HOH:O	5:B:1033:HOH:O[4_535]	1.73	0.47
5:A:1094:HOH:O	5:A:1163:HOH:O[4_525]	1.92	0.28
5:A:1102:HOH:O	5:A:1201:HOH:O[4_425]	2.05	0.15

4.3 Torsion angles

4.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.