



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 12:46 pm GMT

PDB ID : 3UIO
Title : Complex between human RanGAP1-SUMO2, UBC9 and the IR1 domain from RanBP2 containing IR2 Motif II
Authors : Gareau, J.R.; Reverter, D.; Lima, C.D.
Deposited on : 2011-11-05
Resolution : 2.60 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

<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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

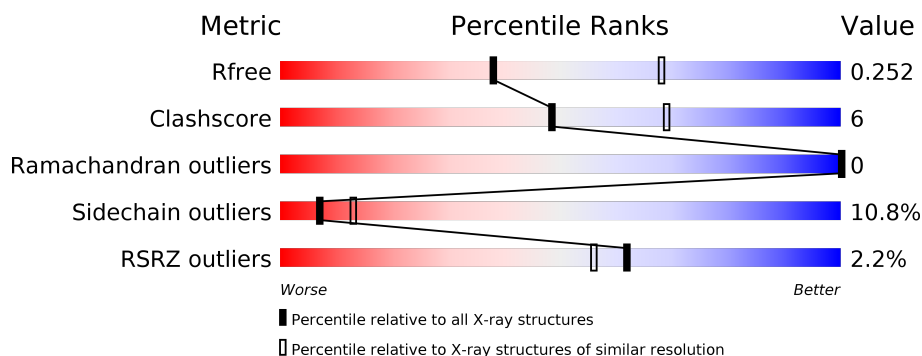
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	158	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>
2	B	80	<div> <div>6%</div> <div>71%</div> <div>21%</div> <div>6%</div> <div>.</div> </div>
3	C	171	<div> <div>71%</div> <div>18%</div> <div>.</div> <div>9%</div> </div>
4	D	67	<div> <div>7%</div> <div>73%</div> <div>16%</div> <div>6%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3768 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 SUMO-conjugating enzyme UBC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1258	807	216	228	7			

- Molecule 2 is a protein called Small ubiquitin-related modifier 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			633	390	115	124	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	MET	VAL	SEE REMARK 999	UNP P61956

- Molecule 3 is a protein called Ran GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1204	775	199	224	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	417	SER	-	EXPRESSION TAG	UNP P46060
C	418	LEU	-	EXPRESSION TAG	UNP P46060

- Molecule 4 is a protein called E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	65	Total	C	N	O	S	0	0	0
			530	338	77	114	1			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2629	SER	-	EXPRESSION TAG	UNP P49792
D	2630	LEU	-	EXPRESSION TAG	UNP P49792
D	2642	VAL	ALA	ENGINEERED MUTATION	UNP P49792
D	2644	GLU	GLN	ENGINEERED MUTATION	UNP P49792
D	2647	LYS	LEU	ENGINEERED MUTATION	UNP P49792
D	2649	ASP	THR	ENGINEERED MUTATION	UNP P49792
D	2650	THR	LYS	ENGINEERED MUTATION	UNP P49792

- Molecule 5 is water.

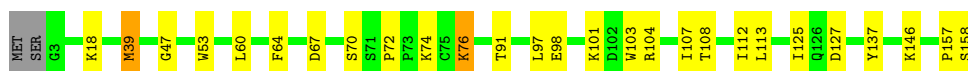
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	84	Total O 84 84	0	0
5	B	10	Total O 10 10	0	0
5	C	25	Total O 25 25	0	0
5	D	24	Total O 24 24	0	0

3 Residue-property plots [i](#)

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: SUMO-conjugating enzyme UBC9

Chain A: 



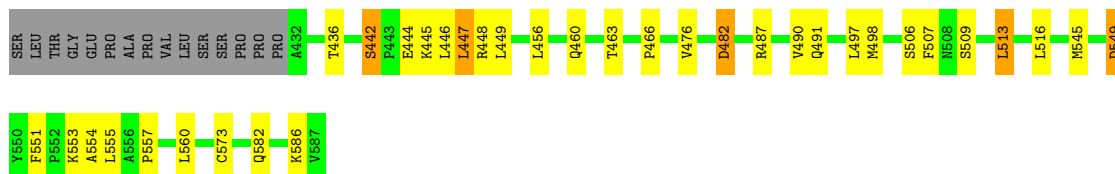
- Molecule 2: Small ubiquitin-related modifier 2

Chain B: 




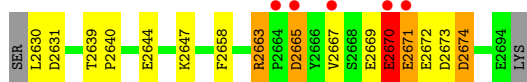
- Molecule 3: Ran GTPase-activating protein 1

Chain C: 



- Molecule 4: E3 SUMO-protein ligase RanBP2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.35Å 151.35Å 57.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.77 – 2.60 34.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.77-2.60) 98.1 (34.78-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.204 , 0.251 0.203 , 0.252	Depositor DCC
R_{free} test set	1198 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3768	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 3.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CSD

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	0.49	0/1279	0.61	0/1734
2	B	0.41	0/642	0.54	0/861
3	C	0.40	0/1227	0.54	0/1661
4	D	0.49	0/532	0.59	0/721
All	All	0.45	0/3680	0.57	0/4977

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
4	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	PRO	Peptide
4	D	2670	GLU	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	1258	0	1249	15	0
2	B	633	0	618	11	0
3	C	1204	0	1238	15	0
4	D	530	0	508	6	0
5	A	84	0	0	3	0
5	B	10	0	0	0	0
5	C	25	0	0	0	0
5	D	24	0	0	0	0
All	All	3768	0	3613	47	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 6.

The worst 5 of 47 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:B:72:THR:HG22	2:B:75:GLN:H	1.39	0.84
2:B:41:SER:HB3	2:B:69:GLU:HB3	1.62	0.81
3:C:509:SER:HB3	3:C:555:LEU:HD11	1.81	0.62
2:B:45:LYS:HA	2:B:55:MET:HE1	1.82	0.62
1:A:18:LYS:NZ	5:A:271:HOH:O	2.32	0.61

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	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
2	B	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	C	154/171 (90%)	152 (99%)	2 (1%)	0	100	100
4	D	62/67 (92%)	62 (100%)	0	0	100	100
All	All	445/476 (94%)	438 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	133/135 (98%)	128 (96%)	5 (4%)	36	63
2	B	70/71 (99%)	60 (86%)	10 (14%)	3	6
3	C	136/149 (91%)	120 (88%)	16 (12%)	6	10
4	D	59/61 (97%)	47 (80%)	12 (20%)	1	2
All	All	398/416 (96%)	355 (89%)	43 (11%)	7	13

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	449	LEU
3	C	506	SER
4	D	2671	GLU
3	C	456	LEU
3	C	460	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSD	A	138	1	4,7,8	1.04	0	2,8,10	2.13	1 (50%)
1	CSD	A	93	1	4,7,8	1.05	0	2,8,10	2.78	1 (50%)
4	CSD	D	2659	4	4,7,8	1.00	0	2,8,10	3.23	1 (50%)

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
1	CSD	A	138	1	-	0/2/6/8	0/0/0/0
1	CSD	A	93	1	-	0/2/6/8	0/0/0/0
4	CSD	D	2659	4	-	0/2/6/8	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	CSD	OD1-SG-CB	2.27	109.86	105.54
1	A	93	CSD	OD1-SG-CB	3.65	112.48	105.54
4	D	2659	CSD	OD1-SG-CB	4.16	113.44	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	154/158 (97%)	-0.37	0 100 100	22, 35, 52, 72	0
2	B	79/80 (98%)	0.26	5 (6%) 20 15	32, 63, 88, 100	0
3	C	156/171 (91%)	-0.17	0 100 100	41, 62, 83, 92	0
4	D	64/67 (95%)	0.16	5 (7%) 13 9	33, 51, 104, 122	0
All	All	453/476 (95%)	-0.12	10 (2%) 62 56	22, 51, 84, 122	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2670	GLU	4.4
4	D	2671	GLU	4.2
2	B	15	ASN	3.6
4	D	2667	VAL	3.6
4	D	2665	ASP	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
4	CSD	D	2659	8/9	0.92	0.14	61,65,66,78	0
1	CSD	A	138	8/9	0.93	0.15	38,47,55,60	0
1	CSD	A	93	8/9	0.95	0.15	31,35,62,77	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.