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 ⓘ

Dec 17, 2023 – 05:50 pm GMT

PDB ID	:	3ZO5
Title	:	Structure of SENP2-Loop1 in complex with preSUMO-2
Authors	:	Alegre, K.O.; Reverter, D.
Deposited on	:	2013-02-20
Resolution	:	2.15 Å(reported)

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	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.15 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.
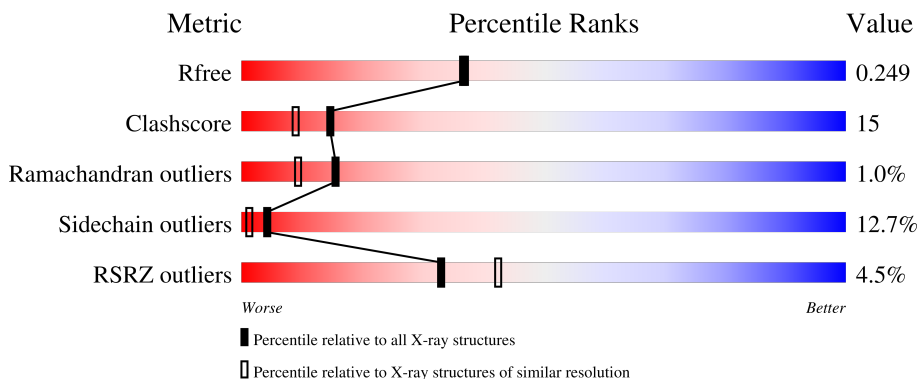
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	238	2% 60% 28% 8% · ·
2	B	89	10% 55% 31% · 9%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2595 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 SENTRIN-SPECIFIC PROTEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total 1898	C 1219	N 332	O 337	S 10	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	GLY	-	expression tag	UNP Q9HC62
A	359	SER	-	expression tag	UNP Q9HC62
A	360	HIS	-	expression tag	UNP Q9HC62
A	361	MET	-	expression tag	UNP Q9HC62
A	362	ALA	-	expression tag	UNP Q9HC62
A	393	PRO	-	insertion	UNP Q9HC62
A	394	PRO	-	insertion	UNP Q9HC62
A	395	PRO	-	insertion	UNP Q9HC62
A	396	PRO	-	insertion	UNP Q9HC62
A	397	ALA	-	insertion	UNP Q9HC62
A	398	LYS	-	insertion	UNP Q9HC62
A	399	GLY	-	insertion	UNP Q9HC62
A	400	GLY	-	insertion	UNP Q9HC62
A	554	SER	CYS	engineered mutation	UNP Q9HC62

- Molecule 2 is a protein called SMALL UBIQUITIN-RELATED MODIFIER 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total 652	C 406	N 116	O 126	S 4	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	MET	-	expression tag	UNP P61956
B	14	ALA	-	expression tag	UNP P61956

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ASN	-	expression tag	UNP P61956
B	96	LEU	-	expression tag	UNP P61956
B	97	GLU	-	expression tag	UNP P61956
B	98	HIS	-	expression tag	UNP P61956
B	99	HIS	-	expression tag	UNP P61956
B	100	HIS	-	expression tag	UNP P61956
B	101	HIS	-	expression tag	UNP P61956

• Molecule 3 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	6	Total O 6 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: SENTRIN-SPECIFIC PROTEASE 2
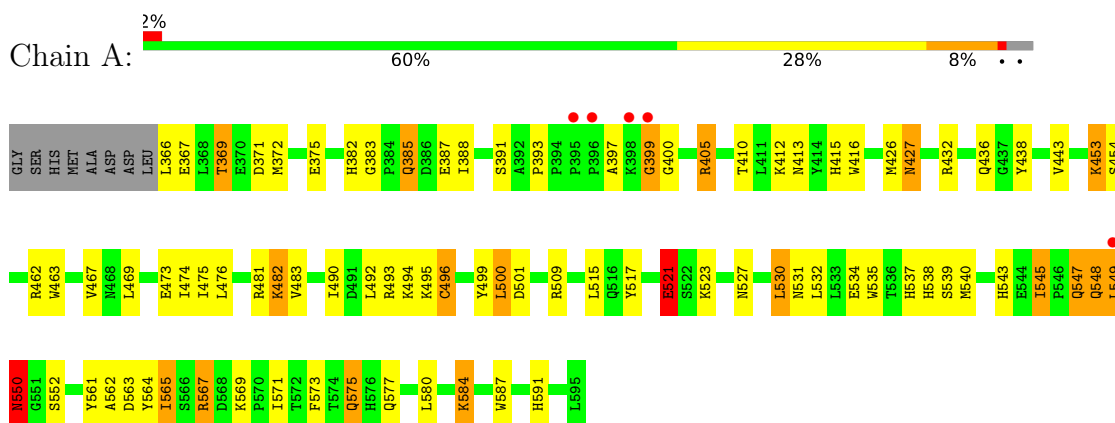
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 2
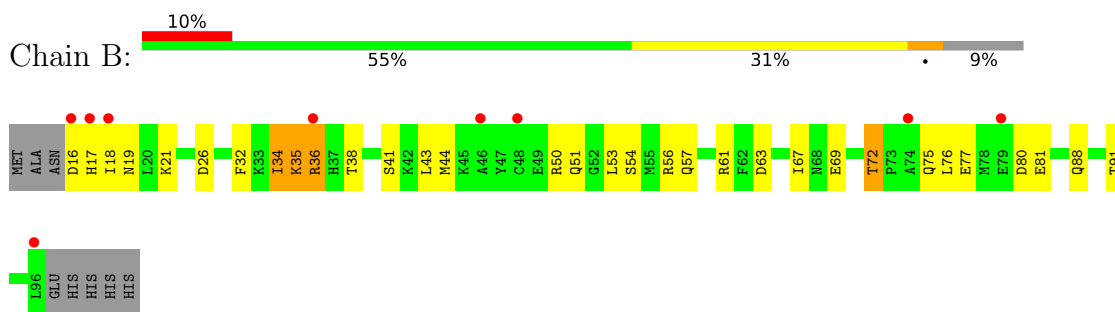
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	145.52Å 145.52Å 104.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.52 – 2.15 48.33 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.52-2.15) 99.7 (48.33-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.188 , 0.236 0.213 , 0.249	Depositor DCC
R_{free} test set	1193 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2595	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.12	7/1947 (0.4%)	1.19	10/2627 (0.4%)
2	B	0.87	0/662	1.10	1/889 (0.1%)
All	All	1.06	7/2609 (0.3%)	1.17	11/3516 (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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	TRP	CD2-CE2	6.52	1.49	1.41
1	A	427	ASN	CB-CG	-6.45	1.36	1.51
1	A	539	SER	CB-OG	6.30	1.50	1.42
1	A	567	ARG	CD-NE	-5.31	1.37	1.46
1	A	587	TRP	CD2-CE2	5.13	1.47	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ARG	NE-CZ-NH2	-10.14	115.23	120.30
2	B	61	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	A	567	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	550	ASN	N-CA-C	6.02	127.26	111.00
1	A	530	LEU	CB-CG-CD1	5.86	120.96	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	ARG	Sidechain

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	1898	0	1911	56	0
2	B	652	0	641	26	0
3	A	39	0	0	0	0
3	B	6	0	0	0	0
All	All	2595	0	2552	78	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 15.

The worst 5 of 78 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	1.15	1.09
1:A:369:THR:HG22	1:A:372:MET:H	1.16	1.05
1:A:547:GLN:HE22	1:A:549:LEU:HD12	1.34	0.91
1:A:547:GLN:NE2	1:A:549:LEU:HD12	1.86	0.89
1:A:547:GLN:OE1	1:A:550:ASN:N	2.11	0.83

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	228/238 (96%)	220 (96%)	6 (3%)	2 (1%)	17	11
2	B	79/89 (89%)	74 (94%)	4 (5%)	1 (1%)	12	6
All	All	307/327 (94%)	294 (96%)	10 (3%)	3 (1%)	15	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ILE
1	A	399	GLY
2	B	26	ASP

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	211/217 (97%)	182 (86%)	29 (14%)	3	1
2	B	72/79 (91%)	65 (90%)	7 (10%)	8	4
All	All	283/296 (96%)	247 (87%)	36 (13%)	4	1

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	584	LYS
2	B	91	THR
2	B	17	HIS
2	B	36	ARG
1	A	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	HIS
1	A	550	ASN
2	B	89	GLN

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Mol	Chain	Res	Type
2	B	57	GLN
1	A	415	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	230/238 (96%)	0.29	5 (2%) 62	69	26, 42, 74, 100	0
2	B	81/89 (91%)	0.64	9 (11%) 5	7	32, 44, 63, 79	0
All	All	311/327 (95%)	0.39	14 (4%) 33	42	26, 42, 73, 100	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	LEU	5.1
1	A	396	PRO	4.6
1	A	398	LYS	3.4
2	B	48	CYS	3.1
2	B	16	ASP	3.1

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 monosaccharides 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.

WORLDWIDE
PDB
PROTEIN DATA BANK