Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 10:09 pm BST

PDB ID	:	8BE2
Title	:	Crystal structure of SOS1-Nanobody77
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Deposited on	:	2022-10-21
Resolution	:	1.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

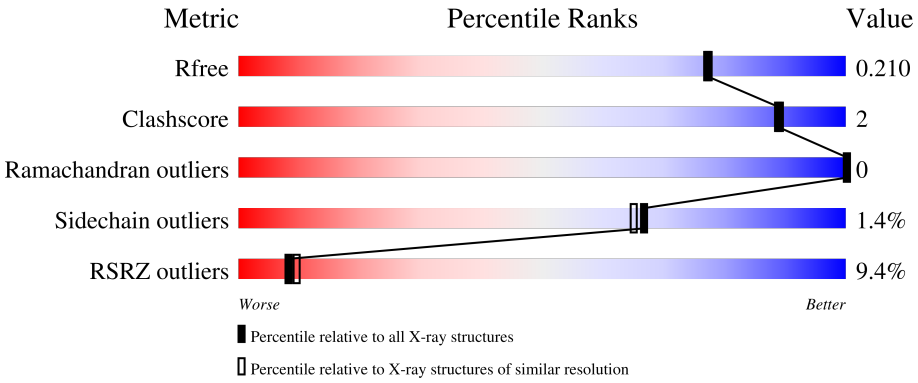
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	S	507	10% 83% 5% 11%
2	N	127	2% 84% 7% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5130 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 Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	449	Total	C	N	O	S	0	7	0
			3784	2428	651	692	13			

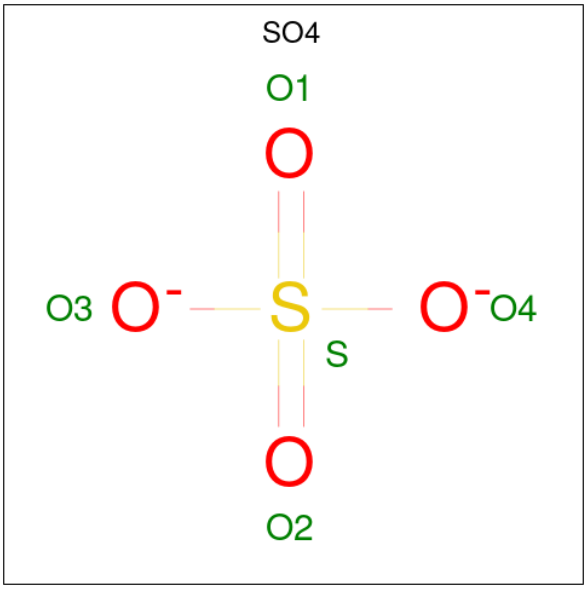
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	543	MET	-	initiating methionine	UNP Q07889
S	544	GLY	-	expression tag	UNP Q07889
S	545	SER	-	expression tag	UNP Q07889
S	546	SER	-	expression tag	UNP Q07889
S	547	HIS	-	expression tag	UNP Q07889
S	548	HIS	-	expression tag	UNP Q07889
S	549	HIS	-	expression tag	UNP Q07889
S	550	HIS	-	expression tag	UNP Q07889
S	551	HIS	-	expression tag	UNP Q07889
S	552	HIS	-	expression tag	UNP Q07889
S	553	SER	-	expression tag	UNP Q07889
S	554	SER	-	expression tag	UNP Q07889
S	555	GLY	-	expression tag	UNP Q07889
S	556	LEU	-	expression tag	UNP Q07889
S	557	VAL	-	expression tag	UNP Q07889
S	558	PRO	-	expression tag	UNP Q07889
S	559	ARG	-	expression tag	UNP Q07889
S	560	GLY	-	expression tag	UNP Q07889
S	561	SER	-	expression tag	UNP Q07889
S	562	HIS	-	expression tag	UNP Q07889
S	563	MET	-	expression tag	UNP Q07889

- Molecule 2 is a protein called Nanobody 77.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	116	Total	C	N	O	S	0	3	0
			912	558	171	179	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	O	S		0	0
			5	4	1			
3	S	1	Total	O	S		0	0
			5	4	1			
3	S	1	Total	O	S		0	0
			5	4	1			
3	S	1	Total	O	S		0	0
			5	4	1			
3	N	1	Total	O	S		0	0
			5	4	1			

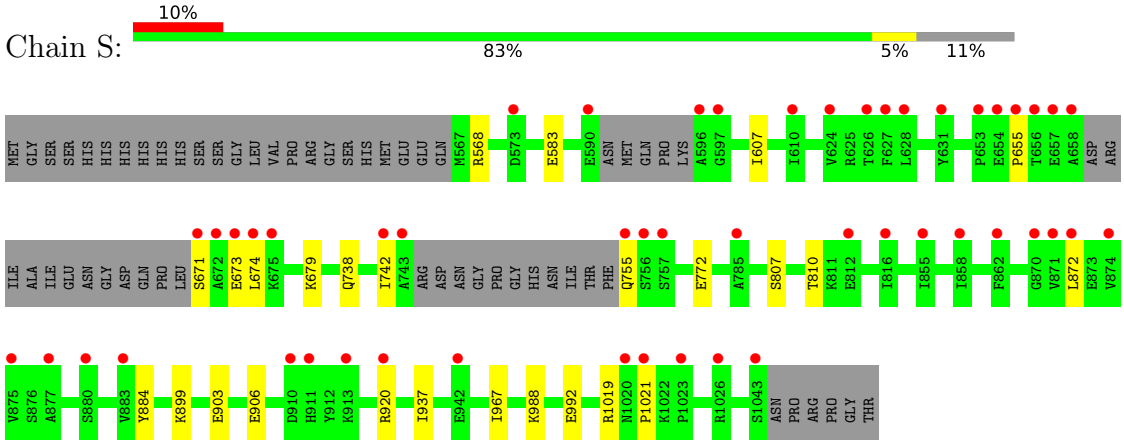
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	339	Total	O	0	0
			339	339		
4	N	70	Total	O	0	0
			70	70		

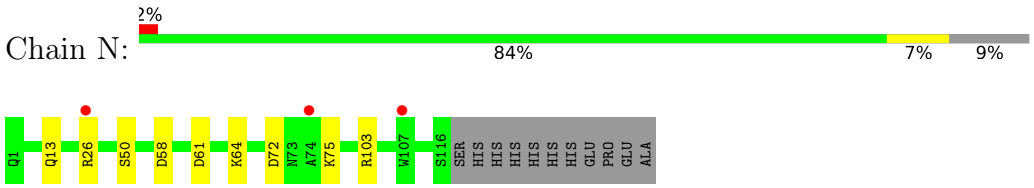
3 Residue-property plots (i)

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: Son of sevenless homolog 1



• Molecule 2: Nanobody 77



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.53Å 102.93Å 108.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 1.90 29.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.59-1.90) 99.9 (29.59-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.181 , 0.211 0.181 , 0.210	Depositor DCC
R_{free} test set	3595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	S	0.41	0/3876	0.50	0/5240
2	N	0.37	0/927	0.57	0/1252
All	All	0.40	0/4803	0.52	0/6492

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	S	3784	0	3803	14	0
2	N	912	0	896	5	0
3	N	5	0	0	1	0
3	S	20	0	0	0	0
4	N	70	0	0	1	0
4	S	339	0	0	0	0
All	All	5130	0	4699	18	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 2.

All (18) 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:S:903:GLU:O	1:S:906[B]:GLU:HG3	2.01	0.61
2:N:103[A]:ARG:HD3	3:N:201:SO4:O4	2.03	0.59
1:S:671:SER:HA	1:S:674:LEU:HB2	1.87	0.57
1:S:568:ARG:NH2	1:S:655:PRO:HA	2.19	0.56
1:S:772:GLU:H	1:S:772:GLU:CD	2.11	0.54
1:S:1021:PRO:HG3	4:N:312:HOH:O	2.06	0.54
1:S:884:TYR:O	2:N:103[A]:ARG:NH2	2.37	0.47
2:N:61:ASP:HA	2:N:64:LYS:HD2	1.98	0.45
1:S:807:SER:HG	1:S:810:THR:HG1	1.64	0.45
1:S:738:GLN:O	1:S:742:ILE:HG12	2.16	0.45
2:N:50:SER:OG	2:N:58:ASP:OD1	2.32	0.45
2:N:72:ASP:OD2	2:N:75:LYS:HG3	2.17	0.44
1:S:679:LYS:HD3	1:S:679:LYS:O	2.18	0.43
1:S:988:LYS:HE2	1:S:992:GLU:OE2	2.18	0.43
1:S:937:ILE:HG13	1:S:967:ILE:HG21	2.01	0.42
1:S:607:ILE:HD13	1:S:607:ILE:HA	1.82	0.41
1:S:568:ARG:HD3	1:S:673:GLU:OE1	2.21	0.41
1:S:872:LEU:HD13	1:S:872:LEU:HA	1.94	0.40

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	S	448/507 (88%)	440 (98%)	8 (2%)	0	100	100
2	N	117/127 (92%)	117 (100%)	0	0	100	100
All	All	565/634 (89%)	557 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	S	426/469 (91%)	421 (99%)	5 (1%)	71 70
2	N	100/107 (94%)	97 (97%)	3 (3%)	41 33
All	All	526/576 (91%)	518 (98%)	8 (2%)	67 62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	583	GLU
1	S	755	GLN
1	S	899	LYS
1	S	920	ARG
1	S	1019	ARG
2	N	13	GLN
2	N	26[A]	ARG
2	N	26[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
3	SO4	N	201	-	4,4,4	0.17	0	6,6,6	0.39	0
3	SO4	S	1102	-	4,4,4	0.17	0	6,6,6	0.22	0
3	SO4	S	1104	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	S	1101	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	S	1103	-	4,4,4	0.12	0	6,6,6	0.12	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	201	SO4	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, 95^{th} 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	S	449/507 (88%)	0.57	50 (11%) 5 6	26, 39, 73, 99	0
2	N	116/127 (91%)	0.33	3 (2%) 56 58	30, 42, 61, 70	0
All	All	565/634 (89%)	0.52	53 (9%) 8 9	26, 40, 70, 99	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	596	ALA	8.1
1	S	742	ILE	6.5
1	S	743	ALA	6.1
1	S	655	PRO	5.9
1	S	674	LEU	5.7
1	S	597	GLY	5.3
1	S	590	GLU	5.2
1	S	657	GLU	4.9
1	S	672	ALA	4.6
1	S	910	ASP	4.3
1	S	1021	PRO	4.2
1	S	658	ALA	4.0
1	S	656	THR	3.9
1	S	756	SER	3.8
1	S	755	GLN	3.6
1	S	673	GLU	3.6
1	S	875	VAL	3.6
1	S	874	VAL	3.5
2	N	74	ALA	3.5
1	S	1026	ARG	3.3
1	S	883	VAL	3.2
1	S	855	ILE	3.2
2	N	26[A]	ARG	3.0
1	S	1020	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	S	1023	PRO	2.9
1	S	913	LYS	2.8
1	S	624	VAL	2.8
1	S	627	PHE	2.8
1	S	911	HIS	2.7
1	S	610	ILE	2.7
1	S	653	PRO	2.7
1	S	812	GLU	2.7
1	S	858	ILE	2.6
1	S	877	ALA	2.5
1	S	1043	SER	2.5
1	S	631	TYR	2.4
1	S	675	LYS	2.4
1	S	628	LEU	2.4
1	S	942	GLU	2.3
1	S	816	ILE	2.3
1	S	871	VAL	2.3
1	S	757	SER	2.3
1	S	626	THR	2.2
1	S	880	SER	2.2
1	S	872	LEU	2.2
1	S	654	GLU	2.1
1	S	671	SER	2.1
1	S	920	ARG	2.1
1	S	870	GLY	2.1
1	S	573	ASP	2.1
1	S	785	ALA	2.1
1	S	862	PHE	2.0
2	N	107	TRP	2.0

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)

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, 95^{th} 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
3	SO4	S	1102	5/5	0.85	0.23	47,50,85,107	0
3	SO4	S	1103	5/5	0.91	0.27	68,79,102,119	0
3	SO4	S	1104	5/5	0.92	0.14	78,80,95,132	0
3	SO4	S	1101	5/5	0.96	0.19	69,73,80,86	0
3	SO4	N	201	5/5	0.97	0.09	43,50,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.