



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 7Z89
Title : Sam68
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Deposited on : 2022-03-16
Resolution : 2.76 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

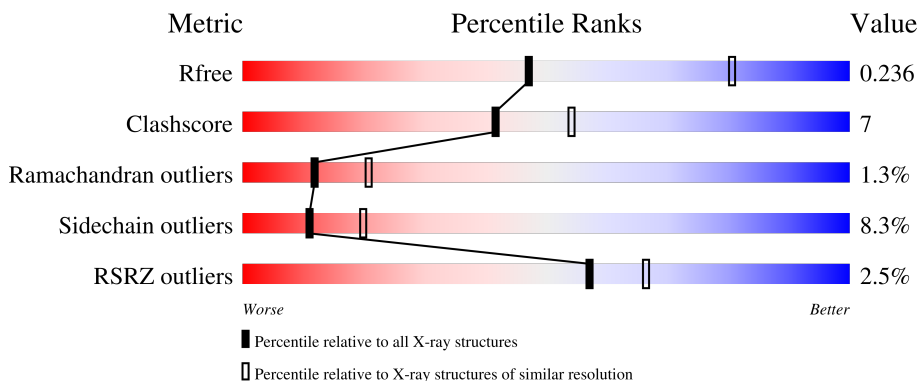
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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	AAA	118	
1	BBB	118	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1981 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 Isoform 2 of KH domain-containing, RNA-binding, signal transduction-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	118	942	606	161	166	9	0	0	0
1	BBB	118	942	606	161	166	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	249	CYS	GLU	conflict	UNP Q07666
BBB	249	CYS	GLU	conflict	UNP Q07666

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	I	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0

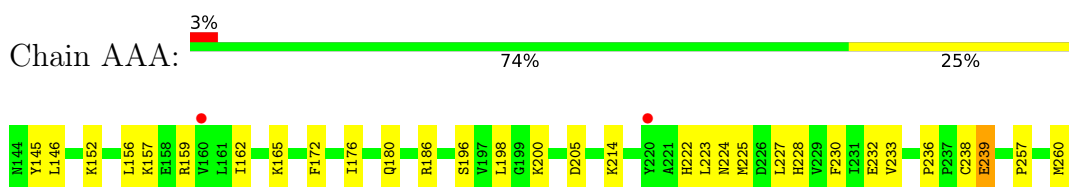
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	8	Total O 8 8	0	0
5	BBB	13	Total O 13 13	0	0

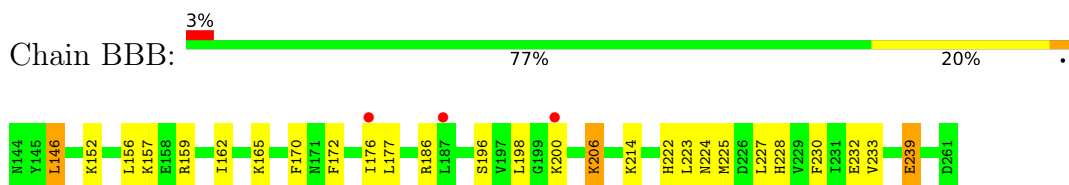
3 Residue-property plots [i](#)

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: Isoform 2 of KH domain-containing, RNA-binding, signal transduction-associated protein 1



- Molecule 1: Isoform 2 of KH domain-containing, RNA-binding, signal transduction-associated protein 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.78Å 97.50Å 81.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.76 48.89 – 2.76	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.94-2.76) 91.5 (48.89-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.236 0.199 , 0.236	Depositor DCC
R_{free} test set	942 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtrriage
Anisotropy	0.393	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.467 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1981	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.66% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	AAA	0.46	0/962	0.92	2/1286 (0.2%)
1	BBB	0.43	0/962	0.91	0/1286
All	All	0.45	0/1924	0.92	2/2572 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	260	MET	C-N-CA	6.75	138.57	121.70
1	AAA	145	TYR	CB-CA-C	-5.45	99.50	110.40

There are no chirality outliers.

There are no planarity outliers.

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	AAA	942	0	968	14	0
1	BBB	942	0	968	15	0
2	AAA	1	0	0	0	0
3	AAA	10	0	0	0	0
3	BBB	5	0	0	0	0
4	AAA	36	0	54	0	0
4	BBB	24	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	8	0	0	0	0
5	BBB	13	0	0	0	0
All	All	1981	0	2026	28	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 7.

The worst 5 of 28 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:BBB:239:GLU:N	1:BBB:239:GLU:OE2	1.92	1.02
1:AAA:172:PHE:O	1:AAA:176:ILE:HG13	1.83	0.77
1:BBB:172:PHE:O	1:BBB:176:ILE:HG13	1.84	0.76
1:AAA:239:GLU:N	1:AAA:239:GLU:OE2	2.35	0.59
1:AAA:238:CYS:HB3	1:AAA:239:GLU:OE2	2.05	0.57

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	AAA	116/118 (98%)	111 (96%)	3 (3%)	2 (2%)	9	16
1	BBB	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	17	31
All	All	232/236 (98%)	222 (96%)	7 (3%)	3 (1%)	12	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	223	LEU
1	AAA	223	LEU

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Mol	Chain	Res	Type
1	AAA	205	ASP

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	AAA	102/102 (100%)	93 (91%)	9 (9%)	10	17
1	BBB	102/102 (100%)	94 (92%)	8 (8%)	12	22
All	All	204/204 (100%)	187 (92%)	17 (8%)	11	20

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	206	LYS
1	BBB	239	GLU
1	AAA	214	LYS
1	AAA	239	GLU
1	BBB	146	LEU

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

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
4	EDO	AAA	1005	-	3,3,3	0.15	0	2,2,2	0.18	0
4	EDO	BBB	303	-	3,3,3	0.20	0	2,2,2	0.25	0
4	EDO	BBB	305	-	3,3,3	0.12	0	2,2,2	0.43	0
4	EDO	AAA	1006	-	3,3,3	0.08	0	2,2,2	0.05	0
4	EDO	AAA	1012	-	3,3,3	0.19	0	2,2,2	0.65	0
4	EDO	BBB	302	-	3,3,3	0.18	0	2,2,2	0.61	0
4	EDO	BBB	307	-	3,3,3	0.08	0	2,2,2	0.76	0
4	EDO	AAA	1008	-	3,3,3	0.12	0	2,2,2	0.39	0
3	SO4	AAA	1003	-	4,4,4	0.35	0	6,6,6	0.09	0
4	EDO	AAA	1007	-	3,3,3	0.19	0	2,2,2	0.26	0
3	SO4	AAA	1002	-	4,4,4	0.35	0	6,6,6	0.19	0
4	EDO	AAA	1009	-	3,3,3	0.28	0	2,2,2	0.53	0
4	EDO	AAA	1010	-	3,3,3	0.11	0	2,2,2	0.48	0
4	EDO	AAA	1011	-	3,3,3	0.10	0	2,2,2	0.21	0
4	EDO	BBB	304	-	3,3,3	0.04	0	2,2,2	0.04	0
4	EDO	BBB	306	-	3,3,3	0.13	0	2,2,2	0.62	0
3	SO4	BBB	301	-	4,4,4	0.32	0	6,6,6	0.14	0
4	EDO	AAA	1004	-	3,3,3	0.17	0	2,2,2	0.52	0

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
4	EDO	AAA	1005	-	-	1/1/1/1	-
4	EDO	BBB	303	-	-	1/1/1/1	-
4	EDO	BBB	305	-	-	0/1/1/1	-
4	EDO	AAA	1006	-	-	0/1/1/1	-
4	EDO	AAA	1012	-	-	1/1/1/1	-
4	EDO	BBB	302	-	-	1/1/1/1	-
4	EDO	BBB	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	1008	-	-	1/1/1/1	-
4	EDO	AAA	1007	-	-	1/1/1/1	-
4	EDO	AAA	1009	-	-	1/1/1/1	-
4	EDO	AAA	1010	-	-	1/1/1/1	-
4	EDO	AAA	1011	-	-	0/1/1/1	-
4	EDO	BBB	304	-	-	1/1/1/1	-
4	EDO	BBB	306	-	-	0/1/1/1	-
4	EDO	AAA	1004	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	1008	EDO	O1-C1-C2-O2
4	BBB	307	EDO	O1-C1-C2-O2
4	AAA	1009	EDO	O1-C1-C2-O2
4	AAA	1010	EDO	O1-C1-C2-O2
4	AAA	1005	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	305	EDO	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 [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	AAA	118/118 (100%)	0.65	3 (2%) 57 66	64, 85, 121, 150	0
1	BBB	118/118 (100%)	0.66	3 (2%) 57 66	67, 84, 122, 152	0
All	All	236/236 (100%)	0.66	6 (2%) 57 66	64, 85, 121, 152	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	261	ASP	3.5
1	AAA	160	VAL	2.2
1	AAA	220	TYR	2.1
1	BBB	176	ILE	2.1
1	BBB	200	LYS	2.1

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](#)

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(\AA^2)	Q<0.9
4	EDO	AAA	1005	4/4	0.65	0.30	119,126,130,131	0
4	EDO	AAA	1012	4/4	0.73	0.34	114,117,119,139	0
4	EDO	AAA	1011	4/4	0.78	0.31	105,116,122,129	0
3	SO4	AAA	1003	5/5	0.80	0.15	157,165,174,193	0
4	EDO	AAA	1006	4/4	0.83	0.44	100,109,110,128	0
4	EDO	BBB	302	4/4	0.84	0.24	97,104,108,112	0
4	EDO	BBB	305	4/4	0.86	0.22	120,124,128,128	0
4	EDO	AAA	1009	4/4	0.87	0.49	78,95,104,111	0
4	EDO	AAA	1008	4/4	0.89	0.22	92,97,114,116	0
4	EDO	BBB	306	4/4	0.89	0.28	104,105,108,115	0
4	EDO	BBB	304	4/4	0.90	0.21	105,107,119,119	0
3	SO4	AAA	1002	5/5	0.91	0.14	142,153,154,199	0
3	SO4	BBB	301	5/5	0.92	0.17	120,140,150,186	0
4	EDO	AAA	1010	4/4	0.92	0.19	94,96,103,107	0
4	EDO	AAA	1004	4/4	0.94	0.16	92,95,103,106	0
4	EDO	AAA	1007	4/4	0.95	0.34	92,100,119,126	0
4	EDO	BBB	303	4/4	0.96	0.27	96,97,114,121	0
4	EDO	BBB	307	4/4	0.96	0.36	111,112,117,117	0
2	IOD	AAA	1001	1/1	1.00	0.30	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.