

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 - 01:09 PM EDT

PDB ID	:	3HSV
Title	:	Structures of SPOP-Substrate Complexes: Insights into Molecular Architec-
		tures of BTB-Cul3 Ubiquitin Ligases: SPOPMATHx-MacroH2ASBCpep
		2
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Deposited on		
Resolution	:	1.43 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 (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:

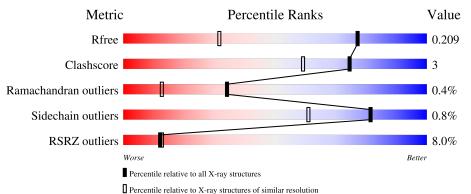
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.43 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	А	145	8%	7% • 8%
1	В	145	3% 86%	5% 9%
2	М	16	<u>31%</u> 69% 6%	25%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2740 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	133	Total	С	Ν	0	S	0	11	0
		155	1140	742	183	208	$\overline{7}$	0		
1	р	132	Total	С	Ν	0	S	0	7	0
1	I B	132	1110	722	183	198	$\overline{7}$	0		

• Molecule 1 is a protein called Speckle-type POZ protein.

GLY			
GLI	-	expression tag	UNP O43791
SER	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
SER	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
GLY	ASP	engineered mutation	UNP O43791
GLY	-	expression tag	UNP O43791
SER	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
SER	-	expression tag	UNP O43791
GLY	-	expression tag	UNP O43791
GLY	ASP	engineered mutation	UNP O43791
	GLY GLY SER GLY GLY SER GLY GLY SER GLY	GLY-GLY-SER-GLY-GLY-SER-GLY-GLY-GLY-GLY-GLY-GLY-GLY-GLY-SER-GLY-	GLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-engineered mutationGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagSER-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tagGLY-expression tag

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Core histone macro-H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	М	12	Total 76	C 43	N 11	O 22	0	1	0

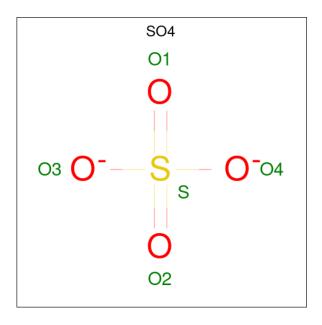
There is a discrepancy between the modelled and reference sequences:



С	hain	Residue	Modelled	Actual	Comment	Reference
	М	170	ACE	ALA	conflict	UNP 075367

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 2 2	0	1
3	В	1	Total Zn 2 2	0	1
3	М	1	Total Zn 1 1	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 5	$\begin{array}{c} \mathrm{O} \\ 4 \end{array}$	S 1	0	0

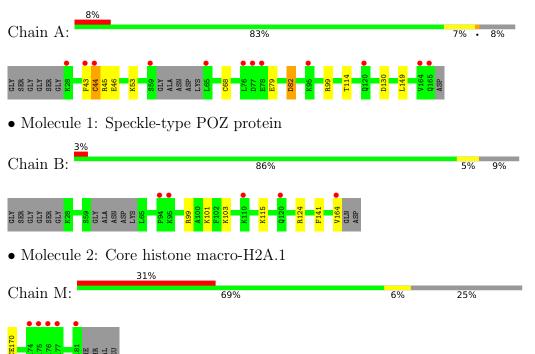
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	177	Total O 180 180	0	3
5	В	199	Total O 199 199	0	0
5	М	24	TotalO2525	0	1



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: Speckle-type POZ protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	88.95Å 43.09Å 87.45Å	Depositor
a, b, c, α , β , γ	90.00° 118.15° 90.00°	Depositor
Resolution (Å)	31.23 - 1.43	Depositor
Resolution (A)	31.23 - 1.43	EDS
% Data completeness	99.4 (31.23-1.43)	Depositor
(in resolution range)	99.3 (31.23-1.43)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$9.79 (at 1.43 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.174 , 0.206	Depositor
R, R_{free}	0.184 , 0.209	DCC
R_{free} test set	2741 reflections (5.10%)	wwPDB-VP
Wilson B-factor $(Å^2)$	9.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 50.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2740	wwPDB-VP
Average B, all atoms $(Å^2)$	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 31.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0369e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: SO4, ZN, ACE

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/1187	0.64	0/1590	
1	В	0.45	0/1146	0.63	0/1532	
2	М	0.41	0/77	0.89	1/106~(0.9%)	
All	All	0.45	0/2410	0.65	1/3228~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	М	170	ACE	C-N-CA	5.25	134.84	121.70

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	А	1140	0	1148	10	0
1	В	1110	0	1138	5	0
2	М	76	0	61	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
3	М	1	0	0	0	0
4	В	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
5	А	180	0	0	6	0		
5	В	199	0	0	1	0		
5	М	25	0	0	0	0		
All	All	2740	0	2347	15	0		

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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 3.

The worst 5 of 15 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:A:130[B]:ASP:OD1	5:A:397:HOH:O	1.81	0.97
1:A:44[B]:CYS:CB	5:A:266:HOH:O	2.38	0.71
1:A:44[A]:CYS:CB	5:A:266:HOH:O	2.40	0.70
1:B:103[B]:LYS:NZ	5:B:191:HOH:O	2.29	0.66
1:B:99:ARG:CD	1:B:124[A]:ARG:HG2	2.28	0.64

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	А	140/145~(97%)	135~(96%)	3~(2%)	2(1%)	11 1
1	В	134/145~(92%)	132~(98%)	2(2%)	0	100 100
2	М	11/16~(69%)	11 (100%)	0	0	100 100
All	All	285/306~(93%)	278~(98%)	5 (2%)	2 (1%)	34 4

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	44[A]	CYS
1	А	44[B]	CYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	128/127~(101%)	125~(98%)	3~(2%)	50 16
1	В	125/127~(98%)	125 (100%)	0	100 100
2	М	8/12~(67%)	8 (100%)	0	100 100
All	All	261/266~(98%)	258~(99%)	3 (1%)	81 47

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	79	GLU
1	А	82[A]	ASP
1	А	82[B]	ASP

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)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	B	ond leng	gths	В	ond ang	gles
IVIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	SO4	В	1	-	4,4,4	0.22	0	$6,\!6,\!6$	0.26	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.

No monomer is involved in short contacts.

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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	133/145~(91%)	0.43	12 (9%) 9 9	4, 7, 15, 21	0
1	В	132/145~(91%)	0.25	5 (3%) 40 42	3, 6, 14, 17	0
2	М	11/16 (68%)	1.55	5(45%) 0 0	3, 6, 14, 14	0
All	All	276/306~(90%)	0.39	22 (7%) 12 13	3, 7, 14, 21	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	44[A]	CYS	9.4
1	В	94	PRO	7.1
2	М	176	GLY	6.0
1	А	78	GLU	3.8
2	М	175	GLU	3.6

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	ZN	В	3[A]	1/1	0.94	0.11	8,8,8,8	1
3	ZN	В	3[B]	1/1	0.94	0.11	11,11,11,11	1
3	ZN	А	2[A]	1/1	0.95	0.09	11,11,11,11	1
3	ZN	А	2[B]	1/1	0.95	0.09	12,12,12,12	1
4	SO4	В	1	5/5	0.98	0.11	8,9,11,12	0
3	ZN	М	1	1/1	0.99	0.32	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.

