Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2025 – 01:06 pm BST

PDB ID	:	9HZK / pdb_00009hzk
Title	:	sdAb9 in complex with PfCSP aTSR domain
Authors	:	Sterckx, Y.G.-J.; Geens, R.
Deposited on	:	2025-01-13
Resolution	:	2.07 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 ⓘ 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:

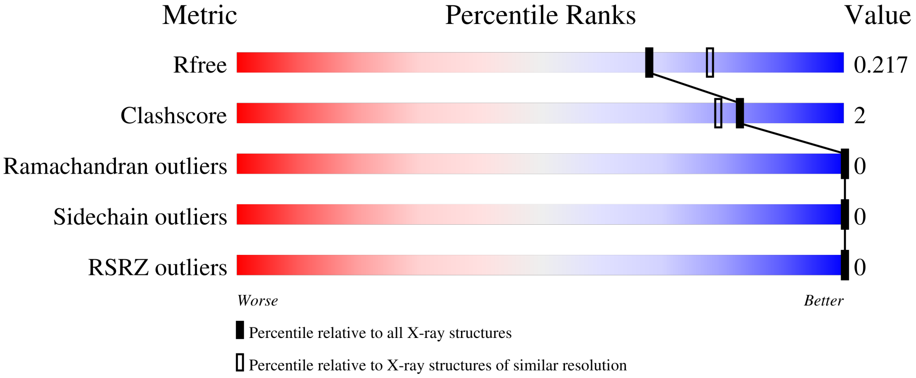
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.07 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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	B	91	
2	A	144	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 1641 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 Circumsporozoite protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	67	523	322	90	106	5	0	0	0

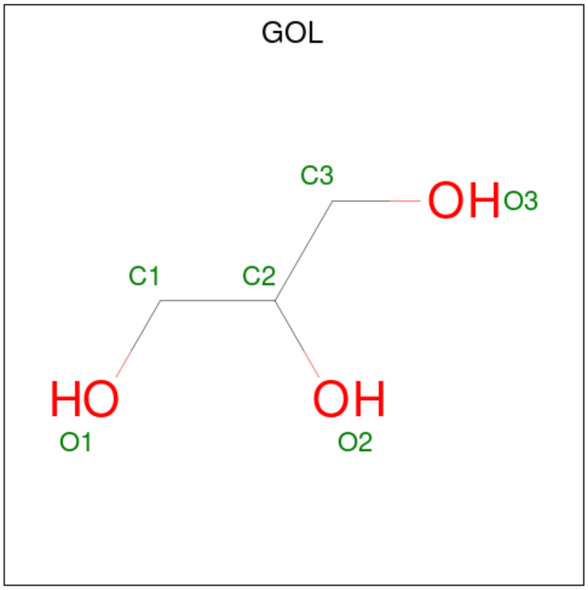
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	309	MET	-	initiating methionine	UNP P19597
B	385	GLU	-	expression tag	UNP P19597
B	386	ASN	-	expression tag	UNP P19597
B	387	LEU	-	expression tag	UNP P19597
B	388	TYR	-	expression tag	UNP P19597
B	389	PHE	-	expression tag	UNP P19597
B	390	GLN	-	expression tag	UNP P19597
B	391	SER	-	expression tag	UNP P19597
B	392	GLY	-	expression tag	UNP P19597
B	393	GLY	-	expression tag	UNP P19597
B	394	HIS	-	expression tag	UNP P19597
B	395	HIS	-	expression tag	UNP P19597
B	396	HIS	-	expression tag	UNP P19597
B	397	HIS	-	expression tag	UNP P19597
B	398	HIS	-	expression tag	UNP P19597
B	399	HIS	-	expression tag	UNP P19597

- Molecule 2 is a protein called sdAb9.

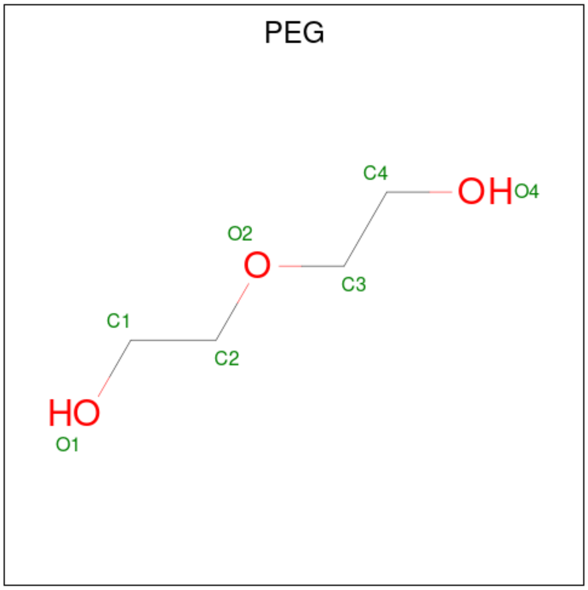
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	125	951	588	168	191	4	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is water.

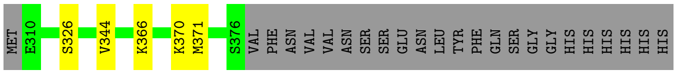
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	30	Total O 30 30	0	0
5	A	56	Total O 56 56	0	0

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: Circumsporozoite protein

Chain B:



- Molecule 2: sdAb9

Chain A:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	53.74Å 53.74Å 60.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.46 – 2.07 25.46 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.46-2.07) 99.6 (25.46-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.184 , 0.226 0.179 , 0.217	Depositor DCC
R_{free} test set	592 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.047 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1641	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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)

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

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	B	0.34	0/531	0.49	0/712
2	A	0.42	0/970	0.62	0/1312
All	All	0.40	0/1501	0.58	0/2024

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 (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	B	523	0	518	4	0
2	A	951	0	891	3	0
3	A	30	0	40	1	0
3	B	30	0	40	1	0
4	A	21	0	30	1	0
5	A	56	0	0	0	0
5	B	30	0	0	2	0
All	All	1641	0	1519	7	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 (7) 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:A:57:ASN:HA	4:A:207:PEG:H22	1.72	0.71
1:B:371:MET:HE3	5:B:522:HOH:O	2.01	0.59
1:B:344:VAL:HG12	1:B:366:LYS:HG2	1.85	0.57
2:A:3:GLN:HG2	3:A:202:GOL:H2	1.87	0.57
1:B:370:LYS:NZ	5:B:501:HOH:O	2.40	0.55
2:A:89:GLU:H	2:A:89:GLU:CD	2.23	0.42
1:B:326:SER:HB3	3:B:403:GOL:H2	2.02	0.40

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	B	65/91 (71%)	64 (98%)	1 (2%)	0	100	100
2	A	123/144 (85%)	122 (99%)	1 (1%)	0	100	100
All	All	188/235 (80%)	186 (99%)	2 (1%)	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	B	62/84 (74%)	62 (100%)	0	100	100
2	A	97/114 (85%)	97 (100%)	0	100	100
All	All	159/198 (80%)	159 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	GOL	A	205	-	5,5,5	0.35	0	5,5,5	0.59	0
3	GOL	A	204	-	5,5,5	0.30	0	5,5,5	0.38	0
3	GOL	B	403	-	5,5,5	0.29	0	5,5,5	0.41	0
3	GOL	B	404	-	5,5,5	0.25	0	5,5,5	0.40	0
3	GOL	B	401	-	5,5,5	0.24	0	5,5,5	0.31	0
4	PEG	A	203	-	6,6,6	0.26	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GOL	B	402	-	5,5,5	0.32	0	5,5,5	0.15	0
3	GOL	A	208	-	5,5,5	0.31	0	5,5,5	0.36	0
3	GOL	B	405	-	5,5,5	0.43	0	5,5,5	0.43	0
4	PEG	A	207	-	6,6,6	0.24	0	5,5,5	0.33	0
3	GOL	A	206	-	5,5,5	0.32	0	5,5,5	0.60	0
4	PEG	A	201	-	6,6,6	0.26	0	5,5,5	0.35	0
3	GOL	A	202	-	5,5,5	0.34	0	5,5,5	0.37	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
3	GOL	A	205	-	-	4/4/4/4	-
3	GOL	A	204	-	-	1/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	B	401	-	-	2/4/4/4	-
4	PEG	A	203	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	208	-	-	4/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
4	PEG	A	207	-	-	0/4/4/4	-
3	GOL	A	206	-	-	4/4/4/4	-
4	PEG	A	201	-	-	1/4/4/4	-
3	GOL	A	202	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
3	A	205	GOL	C1-C2-C3-O3
3	A	208	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	208	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	A	205	GOL	O1-C1-C2-C3
3	A	206	GOL	O1-C1-C2-C3
3	A	206	GOL	C1-C2-C3-O3
3	A	208	GOL	C1-C2-C3-O3
3	B	401	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-O2
3	A	205	GOL	O2-C2-C3-O3
3	A	205	GOL	O1-C1-C2-O2
3	A	208	GOL	O1-C1-C2-O2
3	A	206	GOL	O2-C2-C3-O3
3	A	204	GOL	O1-C1-C2-C3
3	A	206	GOL	O1-C1-C2-O2
4	A	201	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	GOL	1	0
4	A	207	PEG	1	0
3	A	202	GOL	1	0

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

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, 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($\AA^2$)	Q<0.9
1	B	67/91 (73%)	-0.35	0	100	100	31, 38, 54, 73	0
2	A	125/144 (86%)	-0.30	0	100	100	28, 37, 52, 76	0
All	All	192/235 (81%)	-0.32	0	100	100	28, 38, 54, 76	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	GOL	B	405	6/6	0.77	0.13	56,66,85,112	0
3	GOL	A	208	6/6	0.81	0.16	63,71,76,131	0
3	GOL	A	204	6/6	0.84	0.11	50,56,61,80	0
3	GOL	A	205	6/6	0.85	0.12	50,59,61,62	0
3	GOL	B	402	6/6	0.85	0.12	50,60,63,74	0
4	PEG	A	207	7/7	0.85	0.12	64,66,68,76	0
4	PEG	A	201	7/7	0.87	0.11	46,52,66,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	206	6/6	0.88	0.12	58,64,84,87	0
3	GOL	B	401	6/6	0.88	0.10	50,52,59,67	0
3	GOL	B	404	6/6	0.89	0.10	45,63,65,88	0
4	PEG	A	203	7/7	0.91	0.09	50,52,56,64	0
3	GOL	A	202	6/6	0.92	0.17	36,63,91,209	0
3	GOL	B	403	6/6	0.92	0.10	45,48,50,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.