



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:22 PM UTC

PDB ID : 8XK6 / pdb_00008xk6
Title : S2A5 Fab bound to SFTSV glycoprotein Gn
Authors : Deng, Z.
Deposited on : 2023-12-22
Resolution : 2.45 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

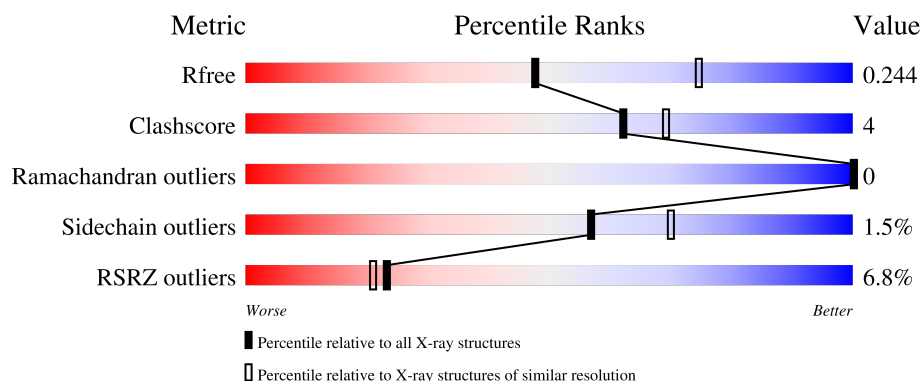
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	A	357	
2	H	251	
3	L	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4333 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2402	1506	416	454	26			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	LEU	PHE	conflict	UNP R4V2Q5
A	18	GLY	SER	conflict	UNP R4V2Q5
A	21	THR	SER	conflict	UNP R4V2Q5
A	161	ARG	GLY	conflict	UNP R4V2Q5
A	340	SER	ASN	conflict	UNP R4V2Q5
A	341	GLY	-	expression tag	UNP R4V2Q5
A	342	SER	-	expression tag	UNP R4V2Q5
A	343	THR	-	expression tag	UNP R4V2Q5
A	344	LEU	-	expression tag	UNP R4V2Q5
A	345	GLU	-	expression tag	UNP R4V2Q5
A	346	VAL	-	expression tag	UNP R4V2Q5
A	347	LEU	-	expression tag	UNP R4V2Q5
A	348	PHE	-	expression tag	UNP R4V2Q5
A	349	GLN	-	expression tag	UNP R4V2Q5
A	350	GLY	-	expression tag	UNP R4V2Q5
A	351	PRO	-	expression tag	UNP R4V2Q5
A	352	HIS	-	expression tag	UNP R4V2Q5
A	353	HIS	-	expression tag	UNP R4V2Q5
A	354	HIS	-	expression tag	UNP R4V2Q5
A	355	HIS	-	expression tag	UNP R4V2Q5
A	356	HIS	-	expression tag	UNP R4V2Q5
A	357	HIS	-	expression tag	UNP R4V2Q5

- Molecule 2 is a protein called mAb S2A5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	120	Total	C	N	O	S	0	0	0
			927	579	152	191	5			

- Molecule 3 is a protein called mAb S2A5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	111	Total	C	N	O	S	0	0	0
			844	529	140	172	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	H	30	Total	O	0	0
			30	30		
4	L	30	Total	O	0	0
			30	30		

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.02Å 158.02Å 190.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 2.45 49.49 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.49-2.45) 97.3 (49.49-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.231 , 0.250 (Not available) , 0.244	Depositor DCC
R_{free} test set	2504 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4333	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

5.1 Standard geometry

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	0.38	0/2462	0.61	1/3321 (0.0%)
2	H	0.31	0/949	0.49	0/1283
3	L	0.35	0/863	0.54	0/1173
All	All	0.36	0/4274	0.57	1/5777 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	PRO	N-CA-C	-5.34	101.46	112.47

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	A	2402	0	2307	20	0
2	H	927	0	868	10	0
3	L	844	0	809	6	0
4	A	100	0	0	5	1
4	H	30	0	0	1	1
4	L	30	0	0	1	0
All	All	4333	0	3984	33	1

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 4.

All (33) 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:H:46:GLU:OE2	4:H:301:HOH:O	1.90	0.90
1:A:154:GLU:HG3	2:H:100(A):ARG:HH22	1.49	0.78
3:L:94:ASP:OD1	4:L:301:HOH:O	2.04	0.75
1:A:66:GLN:NE2	4:A:403:HOH:O	2.20	0.74
1:A:291:GLY:O	4:A:401:HOH:O	2.10	0.68
1:A:301:ALA:N	4:A:405:HOH:O	2.28	0.66
1:A:249:GLN:OE1	4:A:402:HOH:O	2.13	0.66
1:A:38:ILE:CD1	1:A:59:SER:HB2	2.26	0.66
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.30	0.64
1:A:38:ILE:HD12	1:A:59:SER:HB2	1.82	0.61
2:H:51:ILE:HD13	2:H:71:VAL:HG13	1.83	0.60
1:A:269:SER:HA	1:A:272:LYS:HE2	1.87	0.57
1:A:205:ILE:O	1:A:214:ASN:HB2	2.06	0.56
1:A:154:GLU:HG3	2:H:100(A):ARG:NH2	2.20	0.55
1:A:83:TYR:CD1	1:A:83:TYR:C	2.87	0.53
1:A:184:THR:HG23	1:A:324:ARG:HD2	1.90	0.53
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.19	0.51
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.94	0.49
1:A:242:GLU:OE1	1:A:244:LYS:NZ	2.45	0.49
2:H:84:SER:O	2:H:87:SER:OG	2.31	0.48
2:H:100:SER:HB2	3:L:49:TYR:CG	2.48	0.47
3:L:81:GLU:OE2	3:L:81:GLU:N	2.27	0.47
1:A:37:ASP:HA	1:A:62:ARG:HH12	1.80	0.47
2:H:80:MET:HE1	2:H:90:TYR:CD2	2.51	0.46
1:A:207:LYS:HE2	1:A:219:GLU:OE2	2.17	0.45
2:H:80:MET:HE3	2:H:82:LEU:HD11	1.99	0.45
1:A:317:SER:HA	1:A:321:MET:O	2.19	0.42
2:H:43:LYS:HE3	2:H:43:LYS:HB3	1.80	0.42
1:A:49:CYS:SG	1:A:53:ARG:NH1	2.93	0.42
1:A:278:GLY:HA2	4:A:401:HOH:O	2.21	0.41
1:A:95:LEU:HD21	1:A:311:PRO:HD2	2.03	0.41
1:A:274:CYS:SG	1:A:303:CYS:HB2	2.60	0.40
3:L:31:SER:O	3:L:50:ALA:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:492:HOH:O	4:H:330:HOH:O[3_655]	1.93	0.27

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	A	309/357 (87%)	294 (95%)	15 (5%)	0	100	100
2	H	118/251 (47%)	114 (97%)	4 (3%)	0	100	100
3	L	109/237 (46%)	104 (95%)	5 (5%)	0	100	100
All	All	536/845 (63%)	512 (96%)	24 (4%)	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	A	268/309 (87%)	263 (98%)	5 (2%)	50	64
2	H	102/215 (47%)	101 (99%)	1 (1%)	68	77
3	L	91/202 (45%)	90 (99%)	1 (1%)	65	76
All	All	461/726 (64%)	454 (98%)	7 (2%)	57	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	169	SER
1	A	217	GLU
1	A	269	SER
1	A	331	SER
2	H	87	SER
3	L	67	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
3	L	76	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	313/357 (87%)	0.34	27 (8%) 16 14	30, 46, 73, 83	0
2	H	120/251 (47%)	0.47	7 (5%) 29 26	38, 48, 71, 77	0
3	L	111/237 (46%)	0.22	3 (2%) 56 57	33, 45, 61, 72	0
All	All	544/845 (64%)	0.34	37 (6%) 23 21	30, 46, 71, 83	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ALA	5.7
2	H	113	SER	5.5
1	A	293	GLU	5.3
1	A	284	MET	3.7
3	L	56	SER	3.6
1	A	340	SER	3.5
1	A	249	GLN	3.5
3	L	105	GLU	3.5
1	A	21	THR	3.3
1	A	339	VAL	3.2
1	A	197	PHE	3.1
1	A	266	CYS	2.9
1	A	262	GLY	2.7
1	A	25	ILE	2.7
1	A	216	CYS	2.6
1	A	306	SER	2.6
1	A	217	GLU	2.5
1	A	250	GLU	2.5
1	A	84	PRO	2.4
2	H	41	HIS	2.4
1	A	38	ILE	2.4
1	A	276	THR	2.4
1	A	218	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	204	ASP	2.4
1	A	292	CYS	2.4
2	H	112	SER	2.3
2	H	61	GLN	2.3
1	A	272	LYS	2.3
1	A	52	ASP	2.2
2	H	1	GLU	2.2
1	A	91	ARG	2.2
2	H	13	LYS	2.2
2	H	42	GLY	2.1
1	A	303	CYS	2.1
3	L	107	LYS	2.1
1	A	33	ASN	2.1
1	A	83	TYR	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.