



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 10, 2025 – 06:04 PM EST

PDB ID : 9OC7 / pdb_00009oc7
Title : Crystal structure of FcRn in complex with Human Astrovirus 2 spike
Authors : Agrawal, S.; Wilson, I.A.
Deposited on : 2025-04-23
Resolution : 3.07 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

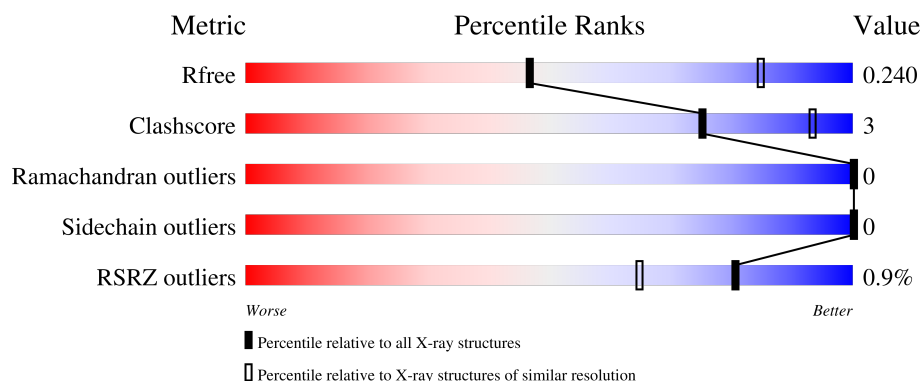
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	1842 (3.10-3.06)
Clashscore	180529	1965 (3.10-3.06)
Ramachandran outliers	177936	1859 (3.10-3.06)
Sidechain outliers	177891	1858 (3.10-3.06)
RSRZ outliers	164620	1842 (3.10-3.06)

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	D	249	
1	X	249	
2	E	274	
2	Y	274	
3	F	99	

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Mol	Chain	Length	Quality of chain
3	Z	99	 <div>94%6%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9228 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 Spike protein VP25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	218	Total	C	N	O	S	0	0	0
			1760	1128	292	331	9			
1	D	218	Total	C	N	O	S	0	0	0
			1760	1128	292	331	9			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	427	MET	-	initiating methionine	UNP Q82446
X	648	GLY	-	expression tag	UNP Q82446
X	649	SER	-	expression tag	UNP Q82446
X	650	GLY	-	expression tag	UNP Q82446
X	651	LEU	-	expression tag	UNP Q82446
X	652	ASN	-	expression tag	UNP Q82446
X	653	ASP	-	expression tag	UNP Q82446
X	654	ILE	-	expression tag	UNP Q82446
X	655	PHE	-	expression tag	UNP Q82446
X	656	GLU	-	expression tag	UNP Q82446
X	657	ALA	-	expression tag	UNP Q82446
X	658	GLN	-	expression tag	UNP Q82446
X	659	LYS	-	expression tag	UNP Q82446
X	660	ILE	-	expression tag	UNP Q82446
X	661	GLU	-	expression tag	UNP Q82446
X	662	TRP	-	expression tag	UNP Q82446
X	663	HIS	-	expression tag	UNP Q82446
X	664	GLU	-	expression tag	UNP Q82446
X	665	GLY	-	expression tag	UNP Q82446
X	666	HIS	-	expression tag	UNP Q82446
X	667	HIS	-	expression tag	UNP Q82446
X	668	HIS	-	expression tag	UNP Q82446
X	669	HIS	-	expression tag	UNP Q82446
X	670	HIS	-	expression tag	UNP Q82446
X	671	HIS	-	expression tag	UNP Q82446

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Chain	Residue	Modelled	Actual	Comment	Reference
X	672	HIS	-	expression tag	UNP Q82446
X	673	HIS	-	expression tag	UNP Q82446
X	674	HIS	-	expression tag	UNP Q82446
X	675	HIS	-	expression tag	UNP Q82446
D	427	MET	-	initiating methionine	UNP Q82446
D	648	GLY	-	expression tag	UNP Q82446
D	649	SER	-	expression tag	UNP Q82446
D	650	GLY	-	expression tag	UNP Q82446
D	651	LEU	-	expression tag	UNP Q82446
D	652	ASN	-	expression tag	UNP Q82446
D	653	ASP	-	expression tag	UNP Q82446
D	654	ILE	-	expression tag	UNP Q82446
D	655	PHE	-	expression tag	UNP Q82446
D	656	GLU	-	expression tag	UNP Q82446
D	657	ALA	-	expression tag	UNP Q82446
D	658	GLN	-	expression tag	UNP Q82446
D	659	LYS	-	expression tag	UNP Q82446
D	660	ILE	-	expression tag	UNP Q82446
D	661	GLU	-	expression tag	UNP Q82446
D	662	TRP	-	expression tag	UNP Q82446
D	663	HIS	-	expression tag	UNP Q82446
D	664	GLU	-	expression tag	UNP Q82446
D	665	GLY	-	expression tag	UNP Q82446
D	666	HIS	-	expression tag	UNP Q82446
D	667	HIS	-	expression tag	UNP Q82446
D	668	HIS	-	expression tag	UNP Q82446
D	669	HIS	-	expression tag	UNP Q82446
D	670	HIS	-	expression tag	UNP Q82446
D	671	HIS	-	expression tag	UNP Q82446
D	672	HIS	-	expression tag	UNP Q82446
D	673	HIS	-	expression tag	UNP Q82446
D	674	HIS	-	expression tag	UNP Q82446
D	675	HIS	-	expression tag	UNP Q82446

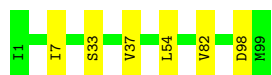
- Molecule 2 is a protein called IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	271	Total	C	N	O	S	0	0	0
			2069	1319	353	389	8			
2	E	264	Total	C	N	O	S	0	0	0
			2021	1291	345	377	8			

- Molecule 3 is a protein called Beta-2-microglobulin.

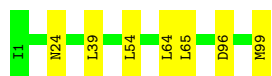
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	99	Total 809	C 514	N 136	O 156	S 3	0	0	0
3	F	99	Total 809	C 514	N 136	O 156	S 3	0	0	0

Chain Z:  94% 6%



● Molecule 3: Beta-2-microglobulin

Chain F:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.88Å 86.22Å 157.09Å 90.00° 122.08° 90.00°	Depositor
Resolution (Å)	29.52 – 3.07 29.52 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.52-3.07) 96.6 (29.52-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.05Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.194 , 0.239 0.194 , 0.240	Depositor DCC
R_{free} test set	2009 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9228	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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](#)

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	D	0.10	0/1807	0.29	0/2462
1	X	0.11	0/1807	0.28	0/2462
2	E	0.09	0/2085	0.25	0/2844
2	Y	0.09	0/2134	0.26	0/2910
3	F	0.09	0/832	0.25	0/1131
3	Z	0.09	0/832	0.23	0/1131
All	All	0.10	0/9497	0.26	0/12940

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	D	1760	0	1727	15	0
1	X	1760	0	1727	12	0
2	E	2021	0	1877	13	0
2	Y	2069	0	1923	11	0
3	F	809	0	746	4	0
3	Z	809	0	746	4	0
All	All	9228	0	8746	52	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 3.

The worst 5 of 52 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:Y:185:LYS:HD2	3:Z:98:ASP:HA	1.79	0.65
2:Y:8:LEU:HD23	2:Y:95:GLY:HA3	1.83	0.60
2:E:57:VAL:HG12	2:E:60:TYR:HB2	1.84	0.60
1:X:458:ALA:HB1	1:X:466:ASN:HB2	1.84	0.59
1:D:510:VAL:HB	1:D:518:ALA:HB3	1.87	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	D	216/249 (87%)	209 (97%)	7 (3%)	0	100	100
1	X	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
2	E	262/274 (96%)	258 (98%)	4 (2%)	0	100	100
2	Y	269/274 (98%)	258 (96%)	11 (4%)	0	100	100
3	F	97/99 (98%)	97 (100%)	0	0	100	100
3	Z	97/99 (98%)	97 (100%)	0	0	100	100
All	All	1157/1244 (93%)	1129 (98%)	28 (2%)	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	D	199/226 (88%)	199 (100%)	0	100	100
1	X	199/226 (88%)	199 (100%)	0	100	100
2	E	206/226 (91%)	206 (100%)	0	100	100
2	Y	212/226 (94%)	212 (100%)	0	100	100
3	F	89/94 (95%)	89 (100%)	0	100	100
3	Z	89/94 (95%)	89 (100%)	0	100	100
All	All	994/1092 (91%)	994 (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. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	17	ASN
2	E	223	GLN
2	E	55	ASN
2	E	33	GLN
2	E	161	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 [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	D	218/249 (87%)	-0.62	1 (0%) 87 74	35, 53, 93, 117	0
1	X	218/249 (87%)	-0.59	0 100 100	35, 52, 90, 116	0
2	E	264/274 (96%)	0.09	6 (2%) 61 41	48, 83, 125, 140	0
2	Y	271/274 (98%)	-0.03	3 (1%) 77 60	50, 84, 114, 138	0
3	F	99/99 (100%)	0.08	0 100 100	58, 86, 115, 130	0
3	Z	99/99 (100%)	-0.10	0 100 100	66, 85, 114, 123	0
All	All	1169/1244 (93%)	-0.21	10 (0%) 81 65	35, 73, 114, 140	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	269	SER	2.9
1	D	645	THR	2.6
2	E	243	LYS	2.6
2	E	267	LEU	2.5
2	E	189	SER	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.