



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2023 – 01:25 pm BST

PDB ID : 7QUH
Title : Siglec-8 in complex with therapeutic Fab AK002.
Authors : Lenza, M.P.; Oyenarte, I.; Jimenez Barbero, J.; Ereno Orbea, J.
Deposited on : 2022-01-18
Resolution : 2.87 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
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

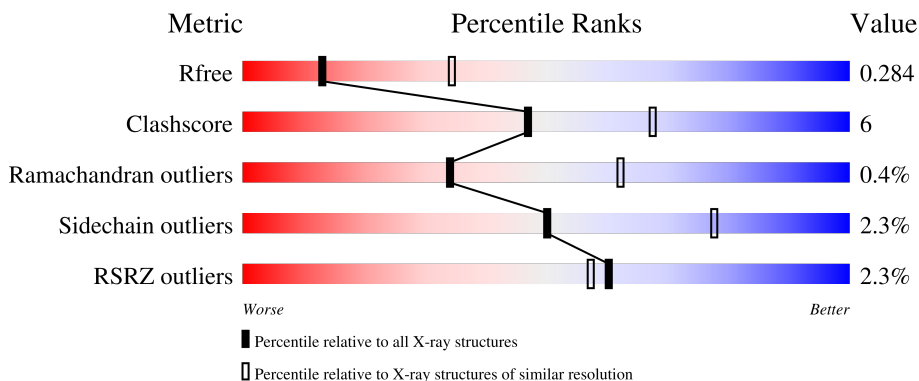
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	H	223	
2	L	213	
3	A	350	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4329 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 Sialic acid-binding immunoglobulin-type lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	216	1610	1016	269	318	7	0	0	0

- Molecule 2 is a protein called Sialic acid-binding immunoglobulin-type lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1621	1018	269	329	5	0	0	0

- Molecule 3 is a protein called Sialic acid-binding Ig-like lectin 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	135	1098	691	194	210	3	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	CYS	conflict	UNP Q9NYZ4
A	353	GLY	-	expression tag	UNP Q9NYZ4
A	354	SER	-	expression tag	UNP Q9NYZ4
A	355	LEU	-	expression tag	UNP Q9NYZ4
A	356	VAL	-	expression tag	UNP Q9NYZ4
A	357	PRO	-	expression tag	UNP Q9NYZ4
A	358	ARG	-	expression tag	UNP Q9NYZ4
A	359	GLY	-	expression tag	UNP Q9NYZ4
A	360	SER	-	expression tag	UNP Q9NYZ4
A	361	HIS	-	expression tag	UNP Q9NYZ4
A	362	HIS	-	expression tag	UNP Q9NYZ4
A	363	HIS	-	expression tag	UNP Q9NYZ4
A	364	HIS	-	expression tag	UNP Q9NYZ4
A	365	HIS	-	expression tag	UNP Q9NYZ4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	HIS	-	expression tag	UNP Q9NYZ4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.34Å 44.55Å 111.39Å 90.00° 111.41° 90.00°	Depositor
Resolution (Å)	42.32 – 2.87 42.32 – 2.87	Depositor EDS
% Data completeness (in resolution range)	95.3 (42.32-2.87) 95.3 (42.32-2.87)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.225 , 0.284 0.225 , 0.284	Depositor DCC
R_{free} test set	769 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtrriage
Anisotropy	0.477	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4329	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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	H	0.26	0/1650	0.47	0/2252
2	L	0.26	0/1659	0.47	0/2257
3	A	0.25	0/1127	0.44	0/1527
All	All	0.26	0/4436	0.46	0/6036

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	H	1610	0	1559	22	0
2	L	1621	0	1566	21	0
3	A	1098	0	1034	14	0
All	All	4329	0	4159	53	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 6.

All (53) 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:H:63:ASN:HB3	1:H:66:LEU:HD12	1.36	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ASN:HB3	1:H:66:LEU:CD1	1.97	0.94
3:A:38:GLN:HB2	3:A:41:LEU:HD12	1.58	0.85
3:A:57:THR:HG22	3:A:59:SER:H	1.48	0.79
2:L:83:SER:OG	2:L:84:SER:N	2.18	0.76
3:A:95:ARG:NH2	3:A:118:ASP:OD2	2.28	0.67
2:L:65:ARG:HB2	2:L:83:SER:OG	1.95	0.66
2:L:11:LEU:HD23	2:L:116:LEU:HD11	1.78	0.66
1:H:175:VAL:HG21	2:L:172:GLN:HG2	1.78	0.65
3:A:73:PRO:O	3:A:86:ARG:NH1	2.31	0.64
2:L:39:GLN:HB2	2:L:49:LEU:HD11	1.81	0.61
2:L:222:ASN:HB2	2:L:225:GLU:HG3	1.84	0.60
1:H:197:THR:HG23	1:H:198:GLN:HG3	1.83	0.59
1:H:125:PRO:HB3	1:H:151:TYR:HB3	1.85	0.59
3:A:62:VAL:HG22	3:A:102:ILE:HG22	1.86	0.57
3:A:91:GLU:O	3:A:95:ARG:NH1	2.39	0.56
1:H:216:ARG:HG2	1:H:218:GLU:HG2	1.86	0.56
2:L:104:SER:HB3	3:A:59:SER:HB3	1.88	0.56
1:H:93:VAL:HG22	1:H:114:THR:HG22	1.87	0.55
2:L:154:ARG:NH1	2:L:175:VAL:HG21	2.22	0.55
1:H:174:ALA:HB2	1:H:184:LEU:HD23	1.88	0.54
2:L:6:GLN:HG3	2:L:112:PRO:HD2	1.88	0.54
2:L:13:LEU:HD12	2:L:86:LEU:HD11	1.90	0.53
1:H:174:ALA:HA	1:H:184:LEU:HB3	1.91	0.53
2:L:50:ILE:HD11	2:L:57:LEU:HD23	1.90	0.53
2:L:83:SER:HG	2:L:84:SER:H	1.54	0.53
1:H:12:VAL:HG11	1:H:18:LEU:HG	1.92	0.52
2:L:50:ILE:CD1	2:L:57:LEU:HD23	2.40	0.52
1:H:132:PRO:HB3	1:H:143:ALA:O	2.11	0.51
2:L:33:TYR:HB3	2:L:53:SER:HA	1.91	0.51
1:H:165:LEU:HD21	1:H:188:VAL:HG21	1.93	0.50
1:H:42:ALA:HB3	1:H:45:LYS:HG3	1.95	0.49
1:H:102:TYR:CE1	3:A:53:GLN:HB2	2.49	0.47
3:A:139:LEU:HD23	3:A:139:LEU:O	2.14	0.47
3:A:36:THR:HA	3:A:149:PHE:O	2.15	0.46
1:H:169:VAL:HG12	1:H:188:VAL:HB	1.97	0.46
3:A:98:LEU:HD13	3:A:102:ILE:HD11	1.97	0.46
1:H:132:PRO:O	1:H:133:SER:HB3	2.16	0.45
2:L:99:CYS:O	2:L:111:GLY:N	2.48	0.45
2:L:63:PRO:HB2	2:L:65:ARG:HG2	1.99	0.44
1:H:216:ARG:HH21	1:H:218:GLU:HG3	1.83	0.44
2:L:37:TRP:CG	2:L:80:LEU:HD13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:LEU:HD23	1:H:195:LEU:HA	1.87	0.43
1:H:55:TRP:CD2	3:A:55:GLY:HA2	2.52	0.43
2:L:21:LEU:HD22	2:L:114:THR:HG21	2.01	0.43
3:A:115:ARG:HB2	3:A:117:ARG:HG2	2.01	0.43
1:H:203:ASN:HD22	1:H:214:ASP:CG	2.24	0.41
2:L:91:PHE:CD2	2:L:118:ILE:HG12	2.55	0.41
2:L:152:TYR:CG	2:L:153:PRO:HA	2.56	0.41
1:H:195:LEU:HD22	1:H:219:PRO:HG3	2.03	0.41
2:L:25:SER:HA	2:L:76:THR:O	2.22	0.40
3:A:99:LEU:HD11	3:A:110:SER:HB2	2.03	0.40
1:H:132:PRO:HG3	1:H:144:LEU:HB3	2.04	0.40

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	H	212/223 (95%)	207 (98%)	4 (2%)	1 (0%)	29	57
2	L	210/213 (99%)	202 (96%)	7 (3%)	1 (0%)	29	57
3	A	133/350 (38%)	127 (96%)	6 (4%)	0	100	100
All	All	555/786 (71%)	536 (97%)	17 (3%)	2 (0%)	34	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	83	SER
1	H	133	SER

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	H	179/186 (96%)	174 (97%)	5 (3%)	43	73
2	L	185/187 (99%)	182 (98%)	3 (2%)	62	84
3	A	118/303 (39%)	115 (98%)	3 (2%)	47	76
All	All	482/676 (71%)	471 (98%)	11 (2%)	50	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	ARG
1	H	21	SER
1	H	66	LEU
1	H	75	LYS
1	H	185	SER
2	L	67	SER
2	L	99	CYS
2	L	154	ARG
3	A	72	ARG
3	A	91	GLU
3	A	110	SER

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](#)

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	H	216/223 (96%)	0.11	5 (2%) 60 57	26, 40, 73, 100	0
2	L	212/213 (99%)	0.18	3 (1%) 75 74	27, 46, 65, 85	0
3	A	135/350 (38%)	0.21	5 (3%) 41 36	27, 41, 87, 111	0
All	All	563/786 (71%)	0.16	13 (2%) 60 57	26, 42, 72, 111	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	153	LEU	4.3
1	H	134	SER	3.6
1	H	133	SER	3.4
3	A	152	ALA	3.3
2	L	168	SER	3.0
3	A	103	TRP	3.0
3	A	139	LEU	2.9
3	A	19	GLY	2.7
1	H	163	GLY	2.6
2	L	83	SER	2.6
2	L	225	GLU	2.3
1	H	196	GLY	2.3
1	H	197	THR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.