



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 06:06 PM EDT

PDB ID : 8UZP
Title : Crystal Structure of the Computationally Designed Influenza Hemagglutinin Epitope Scaffold stem_mimetic_01 bound by Antibody CR9501
Authors : Harshbarger, W.; Malito, E.
Deposited on : 2023-11-16
Resolution : 2.71 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

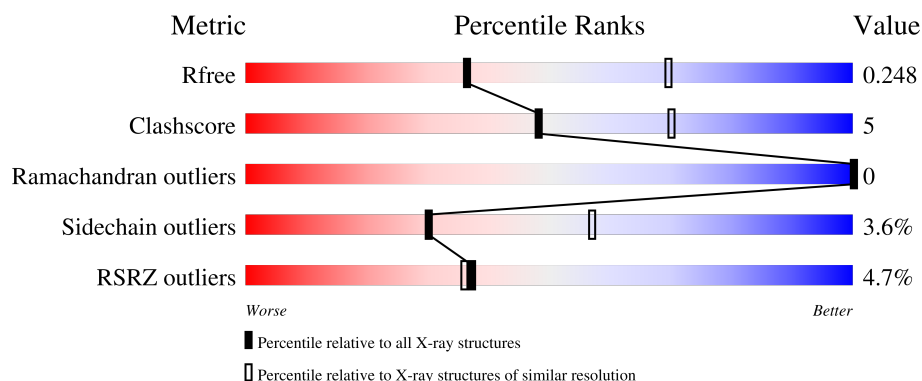
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	264	<div> <div>14%</div> <div>74%</div> <div>7%</div> <div>19%</div> </div>
1	H	264	<div> <div>68%</div> <div>13%</div> <div>19%</div> </div>
2	B	216	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
2	L	216	<div> <div>84%</div> <div>14%</div> <div>•</div> </div>
3	E	166	<div> <div>14%</div> <div>66%</div> <div>17%</div> <div>•</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	166	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8718 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 CR9114 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1592	1005	265	315	7			
1	A	214	Total	C	N	O	S	0	0	0
			1592	1005	265	315	7			

- Molecule 2 is a protein called CR9114 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1575	982	267	322	4			
2	B	212	Total	C	N	O	S	0	0	0
			1575	982	267	322	4			

- Molecule 3 is a protein called stem_mimetic_01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	143	Total	C	N	O	S	0	0	0
			1172	725	212	229	6			
3	E	144	Total	C	N	O	S	0	0	0
			1177	728	213	230	6			

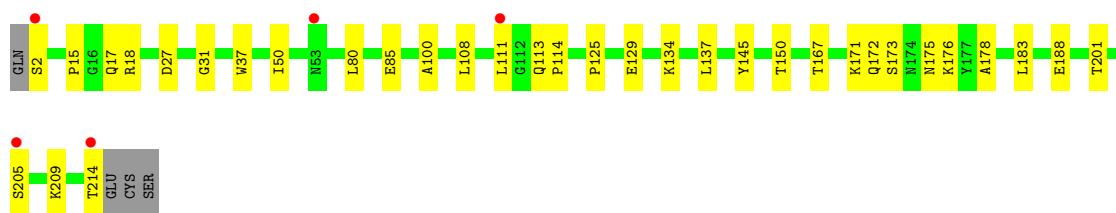
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	16	Total	O	0	0
			16	16		
4	L	8	Total	O	0	0
			8	8		
4	M	1	Total	O	0	0
			1	1		
4	E	3	Total	O	0	0
			3	3		

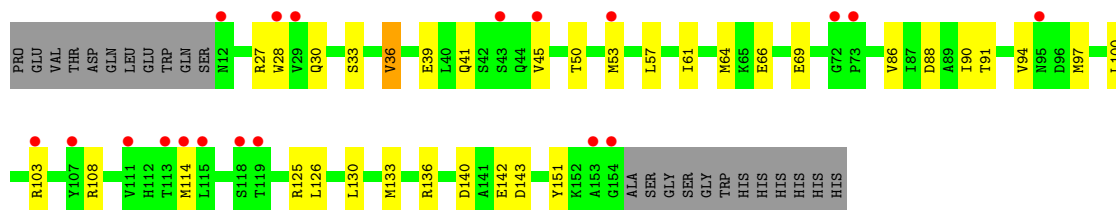
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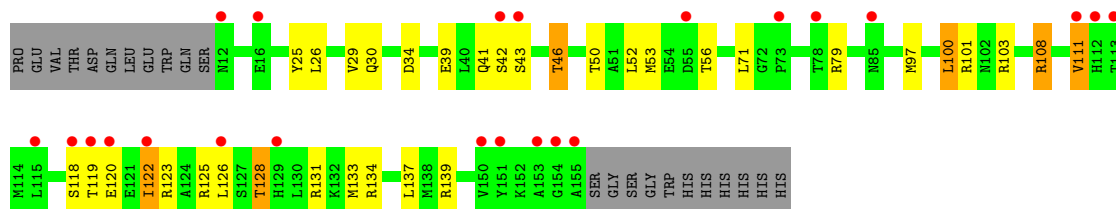
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	2	Total	O	0	0
			2	2		



• Molecule 3: stem_mimetic_01



• Molecule 3: stem_mimetic_01



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	269.00Å 55.94Å 92.01Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	37.79 – 2.71 37.79 – 2.71	Depositor EDS
% Data completeness (in resolution range)	62.4 (37.79-2.71) 87.8 (37.79-2.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.199 , 0.246 0.203 , 0.248	Depositor DCC
R_{free} test set	35974 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8718	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	A	0.26	0/1631	0.47	0/2224
1	H	0.26	0/1631	0.47	0/2224
2	B	0.26	0/1613	0.46	0/2203
2	L	0.26	0/1613	0.46	0/2203
3	E	0.25	0/1191	0.40	0/1608
3	M	0.25	0/1186	0.40	0/1601
All	All	0.26	0/8865	0.45	0/12063

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	A	1592	0	1545	10	0
1	H	1592	0	1545	21	0
2	B	1575	0	1524	20	0
2	L	1575	0	1524	16	0
3	E	1177	0	1173	13	0
3	M	1172	0	1168	16	0
4	A	5	0	0	0	0
4	B	2	0	0	1	0
4	E	3	0	0	0	0
4	H	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	8	0	0	2	0
4	M	1	0	0	0	0
All	All	8718	0	8479	92	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 5.

The worst 5 of 92 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:91:THR:HG22	1:H:119:VAL:H	1.43	0.82
1:A:91:THR:HG22	1:A:119:VAL:H	1.44	0.79
3:M:64:MET:HG3	3:M:86:VAL:HG11	1.73	0.71
1:H:177:VAL:HB	2:L:167:THR:HG22	1.74	0.68
2:L:98:LYS:NZ	4:L:302:HOH:O	2.26	0.67

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	A	210/264 (80%)	205 (98%)	5 (2%)	0	100	100
1	H	210/264 (80%)	206 (98%)	4 (2%)	0	100	100
2	B	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
2	L	210/216 (97%)	202 (96%)	8 (4%)	0	100	100
3	E	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
3	M	141/166 (85%)	138 (98%)	3 (2%)	0	100	100
All	All	1123/1292 (87%)	1094 (97%)	29 (3%)	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	A	178/216 (82%)	176 (99%)	2 (1%)	70	87
1	H	178/216 (82%)	176 (99%)	2 (1%)	70	87
2	B	176/180 (98%)	172 (98%)	4 (2%)	45	73
2	L	176/180 (98%)	172 (98%)	4 (2%)	45	73
3	E	127/147 (86%)	112 (88%)	15 (12%)	4	10
3	M	127/147 (86%)	119 (94%)	8 (6%)	15	34
All	All	962/1086 (89%)	927 (96%)	35 (4%)	30	57

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	139	ARG
1	A	106	SER
2	B	188	GLU
3	M	142	GLU
3	M	125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	207	ASN

5.3.3 RNA ⓘ

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	A	214/264 (81%)	0.11	3 (1%) 73 73	20, 35, 65, 92	0
1	H	214/264 (81%)	-0.21	1 (0%) 87 87	14, 26, 43, 57	0
2	B	212/216 (98%)	0.20	5 (2%) 59 59	19, 39, 67, 79	0
2	L	212/216 (98%)	0.03	2 (0%) 81 80	17, 33, 56, 72	0
3	E	144/166 (86%)	1.18	23 (15%) 6 6	41, 69, 125, 163	0
3	M	143/166 (86%)	0.91	19 (13%) 8 8	28, 60, 118, 156	0
All	All	1139/1292 (88%)	0.29	53 (4%) 37 36	14, 38, 90, 163	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	155	ALA	5.5
3	E	115	LEU	4.7
3	E	153	ALA	4.4
3	E	154	GLY	4.1
3	E	42	SER	3.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.