wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 04:27 AM EDT

PDB ID	:	3W2D
Title	:	Crystal Structure of Staphylococcal Eenterotoxin B in complex with a novel neutralization monoclonal antibody Fab fragment
Authors	:	Liang, S.Y.; Hu, S.; Dai, J.X.; Guo, Y.J.; Lou, Z.Y.
Deposited on	:	2012-11-28
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

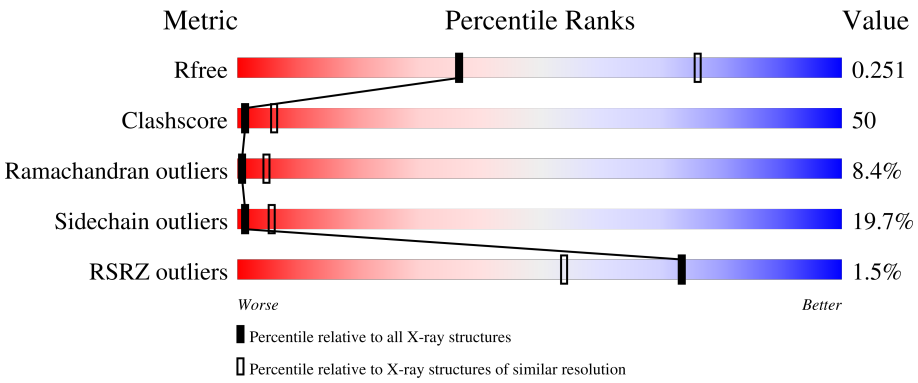
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	239	3%; 27%, 51%, 13%, •, 6%
2	L	215	30%, 47%, 22%, •
3	H	223	%; 34%, 54%, 11%, •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5393 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 Enterotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1883	1208	305	360	10	0	0	0

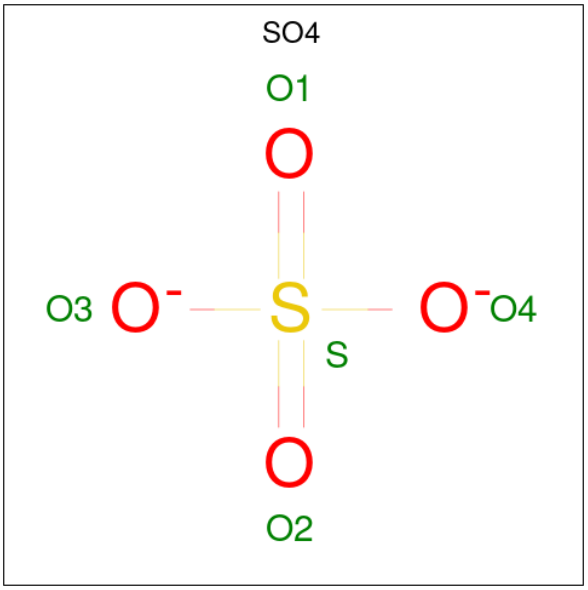
- Molecule 2 is a protein called Monoclonal Antibody 3E2 Fab figment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	215	1647	1023	273	343	8	0	0	0

- Molecule 3 is a protein called Monoclonal Antibody 3E2 Fab figment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	223	1723	1095	284	337	7	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	H	1	5	4	1	0	0

- Molecule 5 is water.

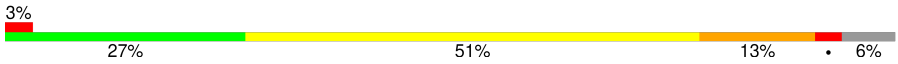
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	40	40	40	0	0
			Total	O		
5	L	47	47	47	0	0
			Total	O		
5	H	48	48	48	0	0

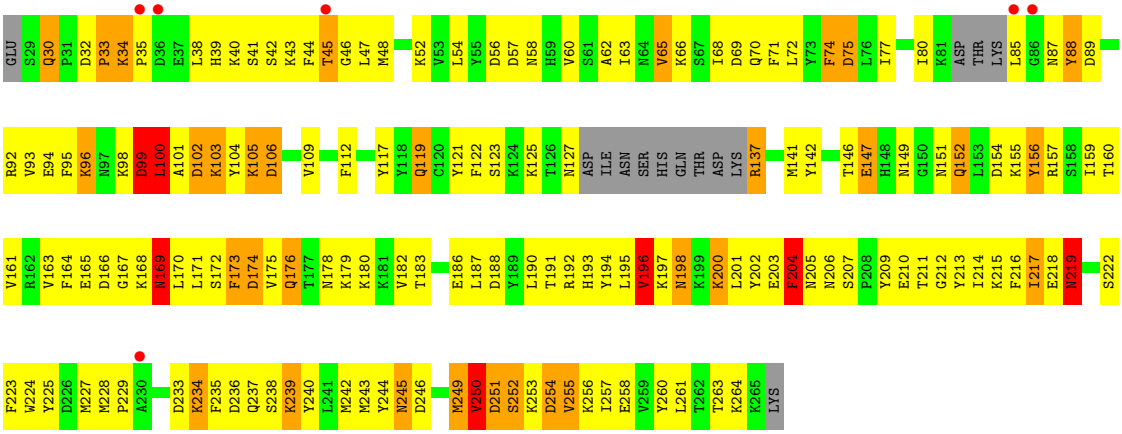
3 Residue-property plots (i)

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: Enterotoxin type B

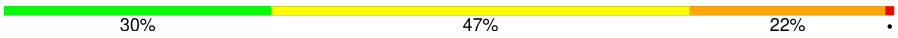
Chain A:

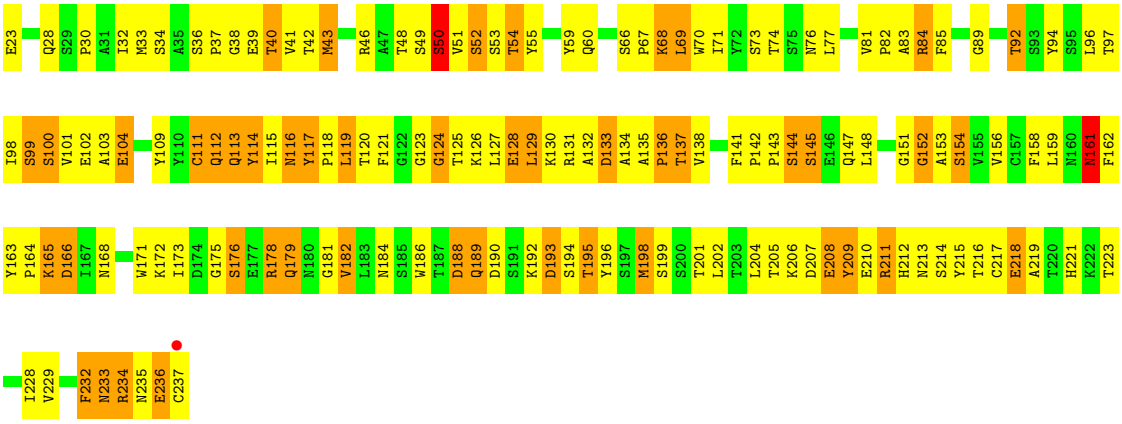




- Molecule 2: Monoclonal Antibody 3E2 Fab figment light chain

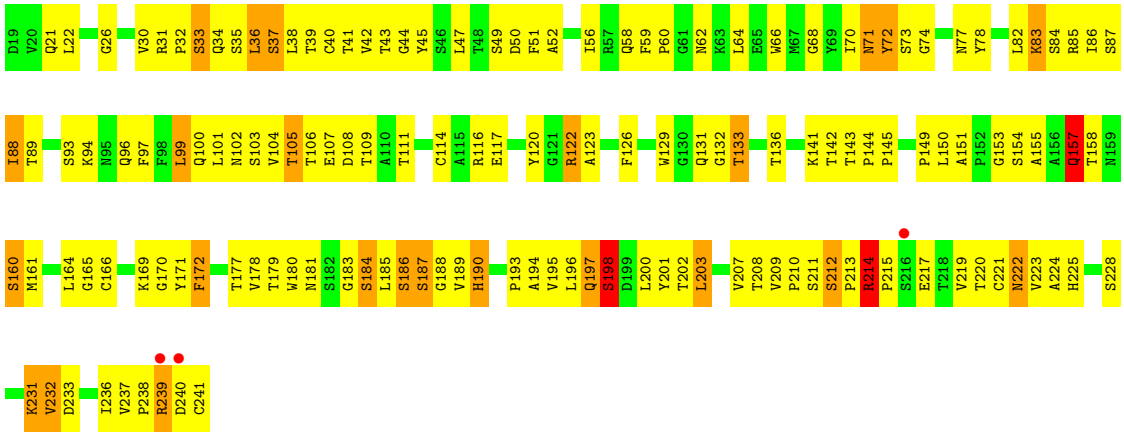
Chain L:





- Molecule 3: Monoclonal Antibody 3E2 Fab figment heavy chain

Chain H:


D19 V20 Q21 L22 G26 V30 R31 P32 S33 Q34 S35 L36 S37 L38 T39 C40 T41 V42 T43 G44 Y45 S46 L47 T48 S49 D50 F51 A52 I56 R57 Q58 F59 P60 G61 N62 K63 L64 E65 W66 M67 G68 Y69 I70 N71 Y72 S73 G74 N77 Y78 L82 K83 S84 R85 I86 S87
I88 T89 S93 K94 N95 Q96 F97 F98 L99 Q100 L101 N102 S103 V104 T105 T106 E107 D108 T109 A110 T111 C114 A115 R116 E117 Y120 G121 R122 A123 F126 W129 G130 Q131 G132 T133 T136 K141 T142 T143 P144 P145 P149 L150 A151 P152 G153 S154 A155 A156 Q157 T158 N159
S160 M161 L164 G165 C166 K169 G170 Y171 F172 T177 V178 T179 W180 N181 S182 G183 S184 L185 S186 S187 G188 V189 H190 P193 A194 V195 L196 Q197 S198 D199 L200 Y201 T202 L203 V207 T208 V209 P210 S211 S212 P213 R214 P215 S216 E217 T218 V219 T220 C221 N222 V223 A224 H225 S228
K231 V232 D233 I236 V237 P238 R239 D240 C241

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	40.56Å 109.31Å 86.22Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	36.44 – 3.10 36.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.44-3.10) 92.4 (36.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.196 , 0.261 0.192 , 0.251	Depositor DCC
R_{free} test set	674 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5393	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4

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	0.57	0/1925	0.71	0/2586
2	L	0.56	0/1685	0.79	0/2292
3	H	0.57	0/1773	0.73	0/2430
All	All	0.57	0/5383	0.74	0/7308

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	1883	0	1831	179	0
2	L	1647	0	1564	215	0
3	H	1723	0	1662	141	0
4	H	5	0	0	0	0
5	A	40	0	0	1	0
5	H	48	0	0	2	0
5	L	47	0	0	4	0
All	All	5393	0	5057	518	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 50.

The worst 5 of 518 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:A:207:SER:O	1:A:264:LYS:NZ	1.85	1.10
2:L:172:LYS:HD2	2:L:216:THR:HG22	1.34	1.08
1:A:234:LYS:HD3	1:A:235:PHE:H	1.19	1.06
3:H:181:ASN:O	3:H:184:SER:OG	1.73	1.04
2:L:55:TYR:CD1	2:L:115:ILE:HD11	1.94	1.01

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	219/239 (92%)	158 (72%)	41 (19%)	20 (9%)	1 4
2	L	213/215 (99%)	161 (76%)	30 (14%)	22 (10%)	0 3
3	H	221/223 (99%)	177 (80%)	31 (14%)	13 (6%)	1 10
All	All	653/677 (96%)	496 (76%)	102 (16%)	55 (8%)	1 5

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	99	ASP
1	A	100	LEU
1	A	169	ASN
1	A	245	ASN

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	211/225 (94%)	166 (79%)	45 (21%)	1 4
2	L	188/188 (100%)	153 (81%)	35 (19%)	1 7
3	H	195/195 (100%)	158 (81%)	37 (19%)	1 6
All	All	594/608 (98%)	477 (80%)	117 (20%)	1 6

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	104	GLU
3	H	214	ARG
2	L	188	ASP
3	H	212	SER
3	H	157	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	113	GLN
2	L	116	ASN
3	H	197	GLN
2	L	233	ASN
3	H	157	GLN

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)

1 ligand is 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	$\#\|Z\| > 2$
4	SO4	H	301	-	4,4,4	0.40	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	225/239 (94%)	-0.15	6 (2%)	54	31	18, 45, 69, 85	0
2	L	215/215 (100%)	-0.16	1 (0%)	91	81	13, 40, 80, 103	0
3	H	223/223 (100%)	-0.25	3 (1%)	77	59	13, 32, 96, 117	0
All	All	663/677 (97%)	-0.19	10 (1%)	73	54	13, 40, 84, 117	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	4.1
1	A	86	GLY	2.8
1	A	45	THR	2.6
1	A	36	ASP	2.4
2	L	237	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

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(Å^2)	Q<0.9
4	SO4	H	301	5/5	0.98	0.13	30,31,38,44	0

6.5 Other polymers (i)

There are no such residues in this entry.