



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2017 – 01:11 PM EDT

PDB ID : 4P2C
Title : Complex of Shiga toxin 2e with a neutralizing single-domain antibody
Authors : Lo, A.W.H.; Moonens, K.; De Kerpel, M.; Brys, L.; Pardon, E.; Remaut, H.;
De Greve, H.
Deposited on : unknown
Resolution : 2.82 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

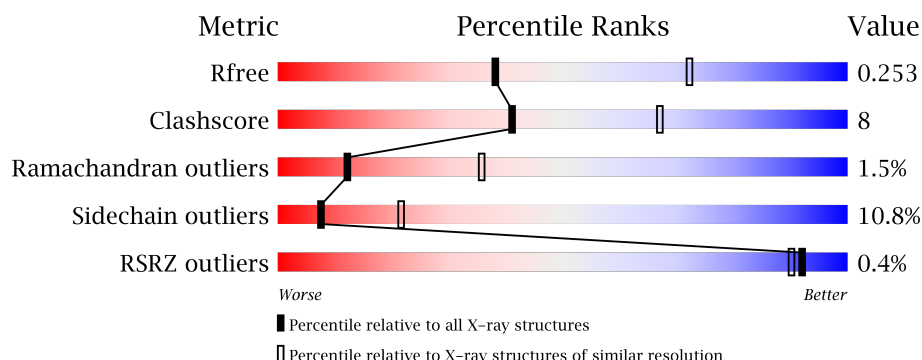
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	297	<div> <div></div> <div>62% 27% 6% 6%</div> </div>
2	B	68	<div> <div></div> <div>78% 21% .</div> </div>
2	C	68	<div> <div></div> <div>79% 19% .</div> </div>
2	D	68	<div> <div></div> <div>87% 12% .</div> </div>
2	E	68	<div> <div></div> <div>84% 15% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	68	<div><div></div><div>79%</div><div>16%</div><div></div><div></div></div>
3	G	128	<div><div>2%</div><div></div><div>70%</div><div>22%</div><div></div><div>5%</div></div>
3	H	128	<div><div></div><div>73%</div><div>18%</div><div></div><div>6%</div></div>
3	I	128	<div><div></div><div>70%</div><div>20%</div><div></div><div>6%</div></div>
3	J	128	<div><div></div><div>76%</div><div>17%</div><div>5%</div><div></div></div>
3	K	128	<div><div></div><div>73%</div><div>16%</div><div></div><div>6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9541 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 Shiga toxin 2e, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2186	1366	390	423	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	SER	TYR	engineered mutation	UNP Q7WUF4
A	167	GLN	GLU	engineered mutation	UNP Q7WUF4
A	274	THR	LYS	Variant	UNP Q7WUF4
A	291	SER	PRO	Variant	UNP Q7WUF4

- Molecule 2 is a protein called Shiga toxin 2e, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	C	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	D	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	E	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	F	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			

- Molecule 3 is a protein called Nanobody 1, Anti-F4+ETEC bacteria VHH variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	121	Total	C	N	O	S	0	0	0
			933	579	166	184	4			
3	H	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			

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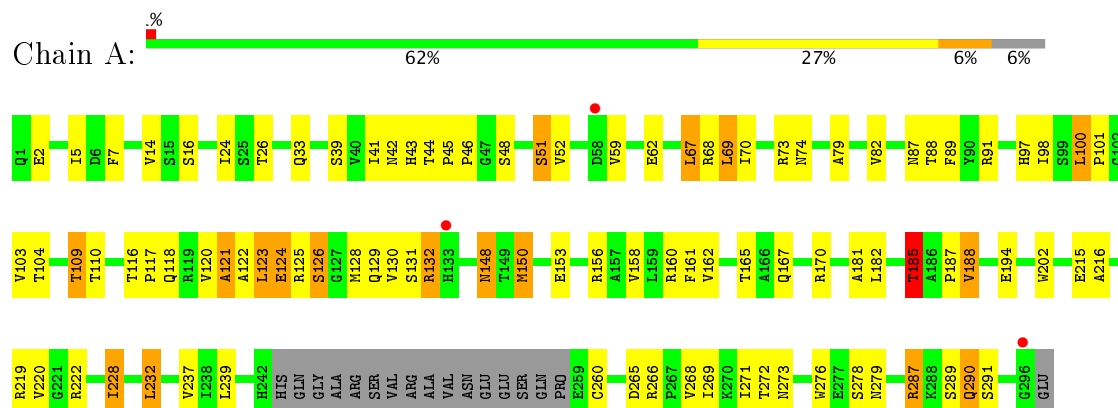
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			
3	J	127	Total	C	N	O	S	0	0	0
			990	613	183	190	4			
3	K	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			

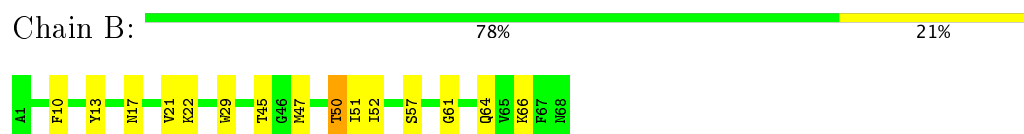
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

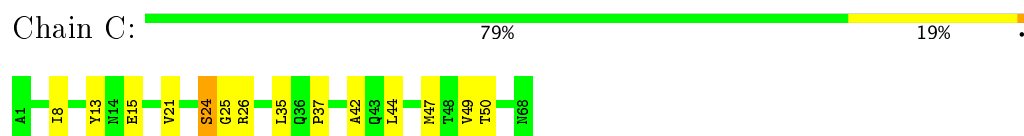
- Molecule 1: Shiga toxin 2e, subunit A



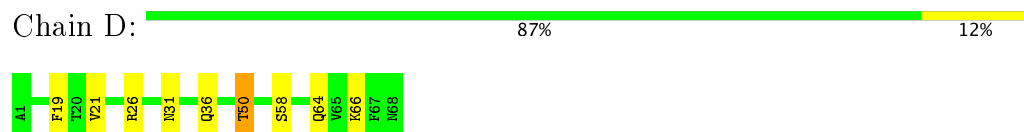
- Molecule 2: Shiga toxin 2e, subunit B



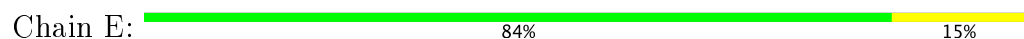
- Molecule 2: Shiga toxin 2e, subunit B



- Molecule 2: Shiga toxin 2e, subunit B



- Molecule 2: Shiga toxin 2e, subunit B





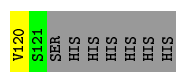
- Molecule 2: Shiga toxin 2e, subunit B

Chain F: 79% 16% •



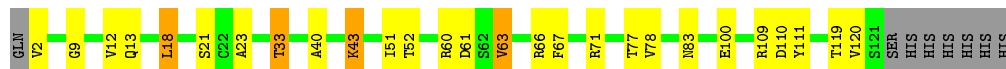
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain G: 70% 22% • 5% 2%



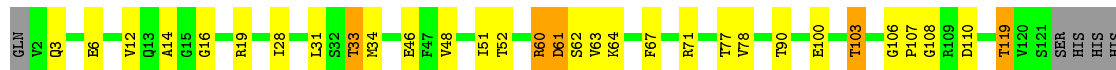
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain H: 73% 18% • 6%



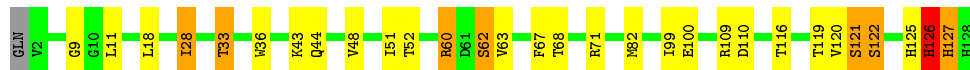
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain I: 70% 20% • 6%



- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain J: 76% 17% 5% ••



- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain K: 73% 16% •• 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	191.84Å 88.19Å 100.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.71 – 2.82 44.10 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.71-2.82) 96.9 (44.10-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1117)	Depositor
R, R_{free}	0.186 , 0.253 0.187 , 0.253	Depositor DCC
R_{free} test set	2043 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.43	0/2225	0.62	0/3025
2	B	0.50	0/542	0.64	0/732
2	C	0.52	0/542	0.67	0/732
2	D	0.55	0/542	0.68	0/732
2	E	0.47	0/542	0.60	0/732
2	F	0.50	0/542	0.65	0/732
3	G	0.45	0/951	0.63	0/1286
3	H	0.43	0/942	0.62	0/1274
3	I	0.46	0/942	0.67	0/1274
3	J	0.51	0/1014	0.69	1/1372 (0.1%)
3	K	0.49	0/942	0.68	2/1274 (0.2%)
All	All	0.47	0/9726	0.65	3/13165 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	121	SER	N-CA-C	5.73	126.47	111.00
3	K	105	TYR	N-CA-C	-5.53	96.08	111.00
3	K	78	VAL	CB-CA-C	-5.41	101.12	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	120	VAL	Peptide
3	J	126	HIS	Peptide

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	2186	0	2162	51	0
2	B	532	0	517	9	0
2	C	532	0	517	10	0
2	D	532	0	517	5	0
2	E	532	0	517	7	0
2	F	532	0	517	10	0
3	G	933	0	895	15	0
3	H	924	0	884	12	0
3	I	924	0	884	16	0
3	J	990	0	931	17	0
3	K	924	0	884	12	0
All	All	9541	0	9225	152	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 8.

The worst 5 of 152 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:181:ALA:HA	1:A:187:PRO:HD2	1.52	0.89
2:B:50:THR:HG23	2:B:66:LYS:HB3	1.58	0.82
2:E:50:THR:HG23	2:E:66:LYS:HB3	1.66	0.78
2:F:50:THR:HG23	2:F:66:LYS:HB3	1.64	0.77
2:C:24:SER:OG	2:C:25:GLY:N	2.06	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	276/297 (93%)	232 (84%)	32 (12%)	12 (4%)	3	9
2	B	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	C	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	D	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	E	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	F	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
3	G	119/128 (93%)	114 (96%)	4 (3%)	1 (1%)	22	53
3	H	118/128 (92%)	111 (94%)	7 (6%)	0	100	100
3	I	118/128 (92%)	113 (96%)	4 (3%)	1 (1%)	22	53
3	J	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	11	34
3	K	118/128 (92%)	110 (93%)	6 (5%)	2 (2%)	11	32
All	All	1204/1277 (94%)	1116 (93%)	70 (6%)	18 (2%)	12	36

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	279	ASN
1	A	290	GLN
3	I	107	PRO
3	J	122	SER

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	245/260 (94%)	214 (87%)	31 (13%)	5	15
2	B	59/59 (100%)	54 (92%)	5 (8%)	12	34
2	C	59/59 (100%)	56 (95%)	3 (5%)	28	60
2	D	59/59 (100%)	56 (95%)	3 (5%)	28	60
2	E	59/59 (100%)	56 (95%)	3 (5%)	28	60
2	F	59/59 (100%)	53 (90%)	6 (10%)	8	24
3	G	98/105 (93%)	84 (86%)	14 (14%)	4	11
3	H	97/105 (92%)	85 (88%)	12 (12%)	5	16
3	I	97/105 (92%)	84 (87%)	13 (13%)	4	13
3	J	104/105 (99%)	93 (89%)	11 (11%)	8	22
3	K	97/105 (92%)	86 (89%)	11 (11%)	7	20
All	All	1033/1080 (96%)	921 (89%)	112 (11%)	7	21

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	57	SER
3	G	104	TYR
3	K	45	ARG
3	G	21	SER
3	G	44	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	87	ASN
3	J	125	HIS

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 carbohydrates 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	280/297 (94%)	-0.03	3 (1%) 80 75	8, 50, 76, 91	0
2	B	68/68 (100%)	-0.31	0 100 100	9, 18, 29, 34	0
2	C	68/68 (100%)	-0.38	0 100 100	7, 16, 30, 36	0
2	D	68/68 (100%)	-0.54	0 100 100	6, 13, 26, 29	0
2	E	68/68 (100%)	-0.55	0 100 100	7, 13, 27, 36	0
2	F	68/68 (100%)	-0.40	0 100 100	8, 18, 30, 39	0
3	G	121/128 (94%)	0.12	2 (1%) 70 63	13, 35, 66, 75	0
3	H	120/128 (93%)	-0.22	0 100 100	10, 31, 46, 58	0
3	I	120/128 (93%)	-0.21	0 100 100	10, 29, 53, 65	0
3	J	127/128 (99%)	-0.45	0 100 100	9, 19, 35, 59	0
3	K	120/128 (93%)	-0.39	0 100 100	10, 26, 47, 68	0
All	All	1228/1277 (96%)	-0.24	5 (0%) 92 90	6, 25, 66, 91	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ASP	2.6
1	A	296	GLY	2.5
1	A	133	HIS	2.1
3	G	41	PRO	2.1
3	G	11	LEU	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 [i](#)

There are no carbohydrates 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.