



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:08 am BST

PDB ID : 4OWJ
Title : Crystal Structure of the *Vibrio vulnificus* Hemolysin/Cytolysin Beta-Trefoil Lectin
Authors : Kaus, K.; Olson, R.
Deposited on : 2014-02-02
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

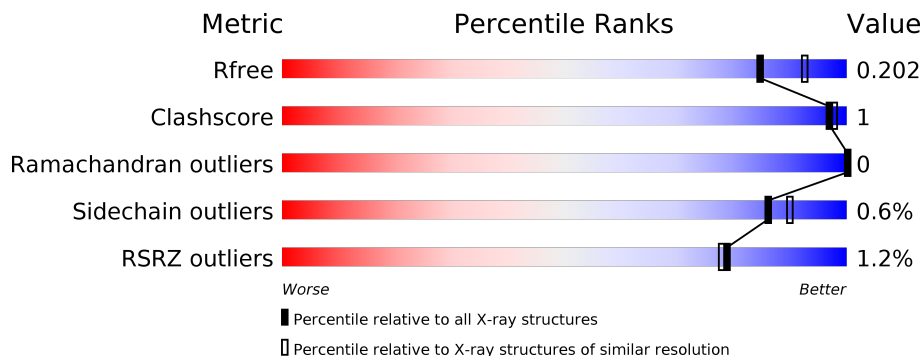
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



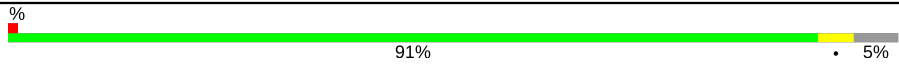
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	138	 2% 90% 5% 5%
1	B	138	 % 93% 5%
1	C	138	 % 92% 5%
1	D	138	 % 95% 5%
1	E	138	 % 91% 5%
1	F	138	 % 92% 5%

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Mol	Chain	Length	Quality of chain
1	G	138	 <p>A horizontal bar chart representing the quality of the chain. The bar is primarily green, indicating a high quality score of 91%. A small yellow segment at the end indicates a lower quality score of 5%. The bar is labeled with a '%' symbol at the start, '91%' in the middle, and '5%' at the end.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14653 atoms, of which 6631 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 Cytolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	131	1920	613	922	183	197	5	0	0	0
1	B	131	1944	621	938	186	194	5	0	0	0
1	C	131	1939	617	935	184	198	5	0	0	0
1	D	131	1926	619	927	182	193	5	0	0	0
1	E	131	1943	623	936	183	196	5	0	0	0
1	F	132	1942	619	937	186	195	5	0	0	0
1	G	131	1928	620	924	183	196	5	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

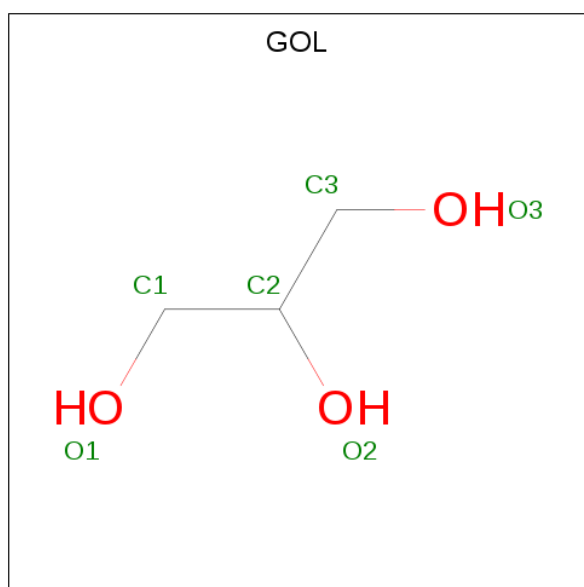
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP P19247
A	335	SER	-	expression tag	UNP P19247
A	336	ALA	-	expression tag	UNP P19247
A	337	MET	-	expression tag	UNP P19247
B	334	GLY	-	expression tag	UNP P19247
B	335	SER	-	expression tag	UNP P19247
B	336	ALA	-	expression tag	UNP P19247
B	337	MET	-	expression tag	UNP P19247
C	334	GLY	-	expression tag	UNP P19247
C	335	SER	-	expression tag	UNP P19247
C	336	ALA	-	expression tag	UNP P19247
C	337	MET	-	expression tag	UNP P19247
D	334	GLY	-	expression tag	UNP P19247
D	335	SER	-	expression tag	UNP P19247
D	336	ALA	-	expression tag	UNP P19247

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Chain	Residue	Modelled	Actual	Comment	Reference
D	337	MET	-	expression tag	UNP P19247
E	334	GLY	-	expression tag	UNP P19247
E	335	SER	-	expression tag	UNP P19247
E	336	ALA	-	expression tag	UNP P19247
E	337	MET	-	expression tag	UNP P19247
F	334	GLY	-	expression tag	UNP P19247
F	335	SER	-	expression tag	UNP P19247
F	336	ALA	-	expression tag	UNP P19247
F	337	MET	-	expression tag	UNP P19247
G	334	GLY	-	expression tag	UNP P19247
G	335	SER	-	expression tag	UNP P19247
G	336	ALA	-	expression tag	UNP P19247
G	337	MET	-	expression tag	UNP P19247

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	E	1	Total 14	C 3	H 8	O 3	0	0
2	E	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	G	1	Total 14	C 3	H 8	O 3	0	0
2	G	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	147	Total 147	O 147	0	0
3	C	118	Total 118	O 118	0	0
3	D	99	Total 99	O 99	0	0
3	E	123	Total 123	O 123	0	0
3	F	152	Total 152	O 152	0	0
3	G	153	Total 153	O 153	0	0

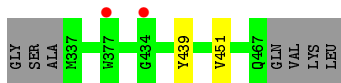
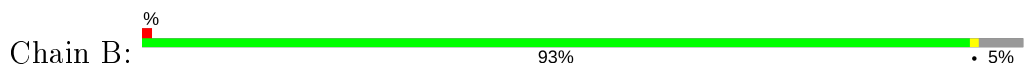
3 Residue-property plots [i](#)

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.

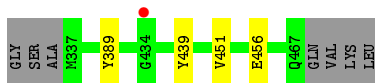
- Molecule 1: Cytolysin



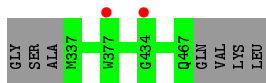
- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



- Molecule 1: Cytolysin




- Molecule 1: Cytolysin

Chain F:  92%



● Molecule 1: Cytolysin

Chain G:  % 91% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 118.21Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.07 – 2.00 48.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.07-2.00) 100.0 (48.51-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.166 , 0.200 0.171 , 0.202	Depositor DCC
R_{free} test set	4568 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14653	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.54	0/1016	0.61	0/1383
1	B	0.53	0/1026	0.64	0/1397
1	C	0.48	0/1022	0.60	0/1391
1	D	0.52	0/1019	0.59	0/1388
1	E	0.52	0/1027	0.65	0/1399
1	F	0.51	0/1023	0.68	2/1392 (0.1%)
1	G	0.54	0/1024	0.62	0/1395
All	All	0.52	0/7157	0.63	2/9745 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	390	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	F	390	ARG	NE-CZ-NH1	6.61	123.60	120.30

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	998	922	924	3	1
1	B	1006	938	935	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1004	935	937	2	0
1	D	999	927	924	0	0
1	E	1007	936	937	2	1
1	F	1005	937	938	2	0
1	G	1004	924	928	2	0
2	A	12	16	16	0	0
2	B	12	16	16	0	0
2	C	12	16	16	0	0
2	D	12	16	16	0	0
2	E	12	16	16	0	0
2	F	12	16	16	0	0
2	G	12	16	16	0	0
3	A	123	0	0	1	0
3	B	147	0	0	0	0
3	C	118	0	0	1	0
3	D	99	0	0	0	0
3	E	123	0	0	0	0
3	F	152	0	0	1	0
3	G	153	0	0	0	0
All	All	8022	6631	6635	12	1

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 1.

The worst 5 of 12 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:C:456:GLU:OE2	3:C:601:HOH:O	2.10	0.69
1:A:436:ASN:N	3:A:711:HOH:O	2.27	0.67
1:F:459:GLN:NE2	3:F:739:HOH:O	2.45	0.48
1:G:363:VAL:HG22	1:G:364:ALA:O	2.13	0.48
1:E:444:VAL:HG22	1:E:448:ASN:O	2.15	0.47

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:OD1	1:E:392:ARG:HH11[4_477]	1.57	0.03

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	129/138 (94%)	120 (93%)	9 (7%)	0	100	100
1	B	129/138 (94%)	123 (95%)	6 (5%)	0	100	100
1	C	129/138 (94%)	123 (95%)	6 (5%)	0	100	100
1	D	129/138 (94%)	122 (95%)	7 (5%)	0	100	100
1	E	129/138 (94%)	124 (96%)	5 (4%)	0	100	100
1	F	130/138 (94%)	124 (95%)	6 (5%)	0	100	100
1	G	129/138 (94%)	124 (96%)	5 (4%)	0	100	100
All	All	904/966 (94%)	860 (95%)	44 (5%)	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	A	103/116 (89%)	102 (99%)	1 (1%)	76	81
1	B	103/116 (89%)	103 (100%)	0	100	100
1	C	105/116 (90%)	104 (99%)	1 (1%)	76	81
1	D	101/116 (87%)	101 (100%)	0	100	100
1	E	104/116 (90%)	104 (100%)	0	100	100
1	F	103/116 (89%)	102 (99%)	1 (1%)	76	81
1	G	103/116 (89%)	102 (99%)	1 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	722/812 (89%)	718 (99%)	4 (1%)	86	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	SER
1	C	389	TYR
1	F	392	ARG
1	G	389	TYR

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 ligands are 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	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.60	0	5,5,5	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	501	-	5,5,5	0.53	0	5,5,5	0.97	0
2	GOL	G	501	-	5,5,5	0.94	1 (20%)	5,5,5	1.38	1 (20%)
2	GOL	E	501	-	5,5,5	0.43	0	5,5,5	0.47	0
2	GOL	F	501	-	5,5,5	0.44	0	5,5,5	0.89	0
2	GOL	D	501	-	5,5,5	0.41	0	5,5,5	0.26	0
2	GOL	B	502	-	5,5,5	0.37	0	5,5,5	0.29	0
2	GOL	D	502	-	5,5,5	0.39	0	5,5,5	0.30	0
2	GOL	F	502	-	5,5,5	0.34	0	5,5,5	0.37	0
2	GOL	A	502	-	5,5,5	0.33	0	5,5,5	0.41	0
2	GOL	C	502	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	E	502	-	5,5,5	0.37	0	5,5,5	0.41	0
2	GOL	C	501	-	5,5,5	0.46	0	5,5,5	0.64	0
2	GOL	G	502	-	5,5,5	0.45	0	5,5,5	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	501	-	-	3/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	G	501	-	-	2/4/4/4	-
2	GOL	E	501	-	-	0/4/4/4	-
2	GOL	F	501	-	-	3/4/4/4	-
2	GOL	D	501	-	-	1/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	F	502	-	-	2/4/4/4	-
2	GOL	A	502	-	-	1/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	E	502	-	-	2/4/4/4	-
2	GOL	C	501	-	-	1/4/4/4	-
2	GOL	G	502	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	GOL	O2-C2	-2.06	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	GOL	O1-C1-C2	-2.07	100.26	110.20

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	501	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-C3
2	G	501	GOL	O1-C1-C2-C3

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	131/138 (94%)	-0.06	3 (2%) 60 59	21, 33, 61, 77	0
1	B	131/138 (94%)	-0.13	2 (1%) 73 72	24, 32, 58, 84	0
1	C	131/138 (94%)	-0.03	1 (0%) 86 85	26, 37, 62, 86	0
1	D	131/138 (94%)	-0.08	2 (1%) 73 72	24, 36, 66, 87	0
1	E	131/138 (94%)	0.03	2 (1%) 73 72	23, 31, 58, 87	0
1	F	132/138 (95%)	-0.23	0 100 100	25, 32, 50, 73	0
1	G	131/138 (94%)	-0.08	1 (0%) 86 85	21, 30, 52, 73	0
All	All	918/966 (95%)	-0.08	11 (1%) 79 78	21, 33, 60, 87	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	GLY	3.7
1	A	434	GLY	3.4
1	B	434	GLY	3.4
1	E	446	GLY	3.2
1	E	444	VAL	3.0

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 carbohydrates 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
2	GOL	A	502	6/6	0.75	0.24	66,80,85,85	0
2	GOL	B	502	6/6	0.82	0.20	69,83,85,87	0
2	GOL	F	502	6/6	0.84	0.33	63,76,77,78	0
2	GOL	D	502	6/6	0.87	0.25	63,75,78,78	0
2	GOL	D	501	6/6	0.88	0.13	43,56,62,68	0
2	GOL	G	502	6/6	0.88	0.27	57,68,71,75	0
2	GOL	C	502	6/6	0.90	0.21	61,74,77,77	0
2	GOL	F	501	6/6	0.91	0.19	41,50,57,60	0
2	GOL	C	501	6/6	0.91	0.14	43,52,59,60	0
2	GOL	A	501	6/6	0.91	0.18	37,47,57,62	0
2	GOL	E	501	6/6	0.92	0.22	31,38,49,51	0
2	GOL	B	501	6/6	0.94	0.17	37,47,54,56	0
2	GOL	E	502	6/6	0.95	0.15	59,71,75,75	0
2	GOL	G	501	6/6	0.96	0.16	31,37,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.