



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 06:34 AM JST

PDB ID : 6LEB
Title : Staphylococcus aureus surface protein SdrC mutant-P366H
Authors : Hang, T.; Zhang, M.; Wang, J.
Deposited on : 2019-11-25
Resolution : 1.54 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

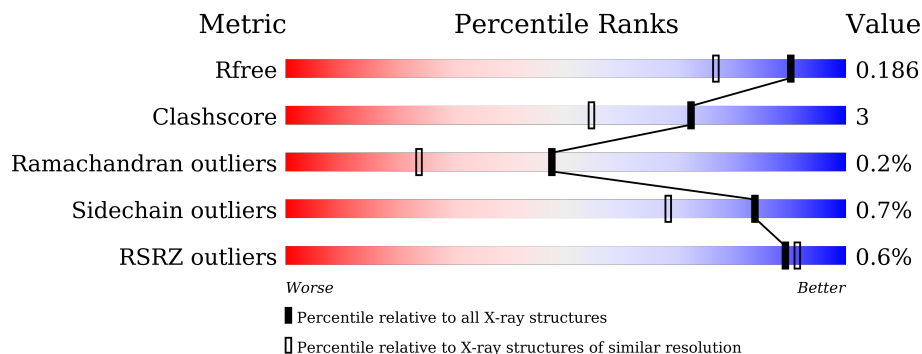
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	315	 % 89% 10% .
1	B	315	 % 89% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	504	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6248 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 Ser-Asp rich fibrinogen-binding, bone sialoprotein-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	Total	C	N	O	S	0	4	0
			2522	1565	419	536	2			
1	B	315	Total	C	N	O	S	0	9	0
			2556	1587	424	543	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	HIS	PRO	engineered mutation	UNP Q2UWK0
B	366	HIS	PRO	engineered mutation	UNP Q2UWK0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

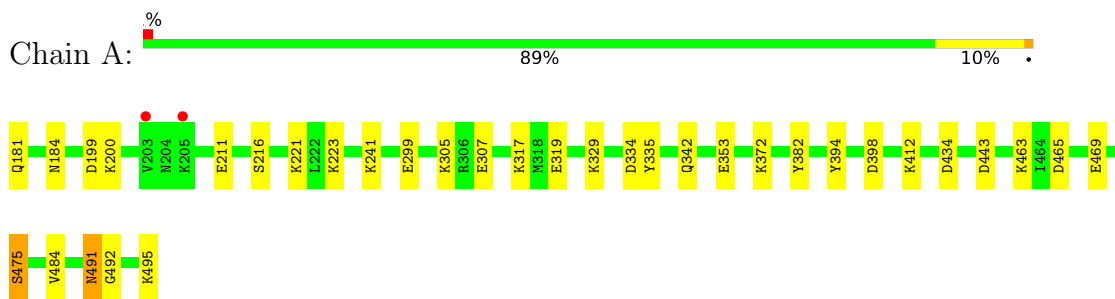
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	568	Total O 568 568	0	0
4	B	570	Total O 570 570	0	0

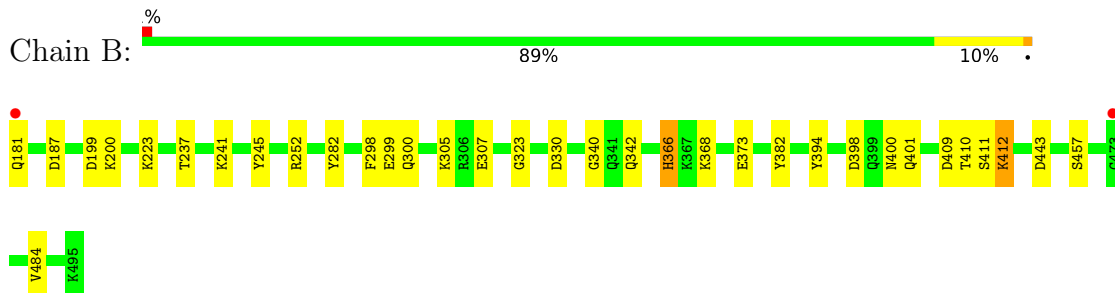
3 Residue-property plots [i](#)

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: Ser-Asp rich fibrinogen-binding, bone sialoprotein-binding protein



- Molecule 1: Ser-Asp rich fibrinogen-binding, bone sialoprotein-binding protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.73Å 87.13Å 63.97Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	50.00 – 1.54 48.19 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.54) 99.1 (48.19-1.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.126 , 0.177 0.138 , 0.186	Depositor DCC
R_{free} test set	5023 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3094e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, 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	1.35	5/2574 (0.2%)	1.17	9/3493 (0.3%)
1	B	1.33	6/2611 (0.2%)	1.17	10/3543 (0.3%)
All	All	1.34	11/5185 (0.2%)	1.17	19/7036 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	SER	CA-CB	5.71	1.61	1.52
1	A	211	GLU	CD-OE2	-5.66	1.19	1.25
1	B	300	GLN	CD-NE2	-5.54	1.19	1.32
1	A	216	SER	CB-OG	5.50	1.49	1.42
1	B	373	GLU	CD-OE2	5.45	1.31	1.25
1	B	457	SER	CB-OG	-5.41	1.35	1.42
1	B	245	TYR	CG-CD1	-5.25	1.32	1.39
1	A	184	ASN	CG-OD1	-5.23	1.12	1.24
1	B	323	GLY	N-CA	5.06	1.53	1.46
1	A	353	GLU	CD-OE2	5.01	1.31	1.25
1	B	382	TYR	CE1-CZ	-5.01	1.32	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	409	ASP	O-C-N	-5.89	113.27	122.70
1	A	335	TYR	CG-CD2-CE2	5.73	125.89	121.30
1	A	394	TYR	CG-CD2-CE2	5.63	125.81	121.30
1	B	409	ASP	CA-C-N	5.59	129.50	117.20
1	B	187	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	443	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	398	ASP	CB-CG-OD1	5.49	123.24	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LYS	CD-CE-NZ	5.49	124.33	111.70
1	B	298	PHE	CB-CG-CD1	5.45	124.62	120.80
1	B	443	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	329	LYS	CD-CE-NZ	-5.35	99.39	111.70
1	A	382	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	334	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	434	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	443	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	394	TYR	CB-CG-CD1	5.17	124.10	121.00
1	B	252	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	330	ASP	CB-CG-OD1	5.05	122.85	118.30

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	2522	0	2381	17	0
1	B	2556	0	2423	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	24	0	0
3	B	12	0	15	0	0
4	A	568	0	0	7	0
4	B	570	0	0	5	0
All	All	6248	0	4843	34	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 3.

All (34) 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:223:LYS:HE3	1:A:299[B]:GLU:OE2	1.40	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:VAL:HB	4:B:946:HOH:O	1.45	1.14
1:B:223:LYS:HE3	1:B:299[B]:GLU:OE2	1.80	0.81
1:A:317:LYS:HE2	1:A:319:GLU:OE2	1.94	0.68
1:A:372:LYS:NZ	1:A:469:GLU:OE2	2.28	0.67
1:B:241:LYS:HD2	4:B:987:HOH:O	1.95	0.66
1:B:400[B]:ASN:C	1:B:400[B]:ASN:HD22	1.97	0.65
1:B:412[A]:LYS:HB2	4:B:606:HOH:O	1.96	0.64
1:A:412:LYS:HB2	4:A:614:HOH:O	2.00	0.61
1:A:241:LYS:HD2	4:A:967:HOH:O	2.01	0.60
1:A:181:GLN:N	4:A:602:HOH:O	2.34	0.60
1:A:200:LYS:CD	4:A:660:HOH:O	2.50	0.59
1:A:484:VAL:O	1:A:484:VAL:HG22	2.05	0.57
1:A:491:ASN:HD22	1:A:492:GLY:H	1.55	0.55
1:B:410[B]:THR:O	1:B:412[B]:LYS:N	2.40	0.54
1:B:410[B]:THR:C	1:B:412[B]:LYS:H	2.12	0.53
1:B:410[B]:THR:C	1:B:412[B]:LYS:N	2.64	0.51
1:A:342:GLN:OE1	1:A:475:SER:OG	2.11	0.50
1:A:305:LYS:HE2	1:A:307:GLU:OE2	2.11	0.50
1:B:400[B]:ASN:HD22	1:B:401:GLN:N	2.10	0.49
1:B:199:ASP:OD1	1:B:200:LYS:HD3	2.13	0.49
1:A:200:LYS:HD2	4:A:660:HOH:O	2.13	0.49
1:A:463:LYS:HE2	1:A:465:ASP:OD1	2.12	0.49
1:A:199:ASP:HA	1:A:200:LYS:HA	1.62	0.48
1:B:305:LYS:HE2	1:B:307:GLU:OE2	2.14	0.47
1:B:366:HIS:ND1	1:B:368:LYS:HG3	2.30	0.46
1:B:412[A]:LYS:NZ	4:B:608:HOH:O	2.48	0.45
1:B:340:GLY:O	1:B:366:HIS:HD2	1.99	0.45
1:A:495:LYS:HA	4:B:613:HOH:O	2.17	0.45
1:B:366:HIS:CE1	1:B:368:LYS:HG3	2.53	0.44
1:A:200:LYS:HE3	4:A:798:HOH:O	2.17	0.44
1:A:200:LYS:HD3	4:A:660:HOH:O	2.14	0.43
1:B:342:GLN:HB3	1:B:366:HIS:NE2	2.33	0.43
1:B:237:THR:HA	1:B:282:TYR:O	2.21	0.41

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	317/315 (101%)	313 (99%)	4 (1%)	0	100	100
1	B	322/315 (102%)	314 (98%)	6 (2%)	2 (1%)	25	7
All	All	639/630 (101%)	627 (98%)	10 (2%)	2 (0%)	47	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411[A]	SER
1	B	411[B]	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	A	287/283 (101%)	286 (100%)	1 (0%)	92	84
1	B	292/283 (103%)	288 (99%)	4 (1%)	67	39
All	All	579/566 (102%)	574 (99%)	5 (1%)	84	60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	ASN
1	B	181	GLN
1	B	366	HIS
1	B	412[A]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	412[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	491	ASN

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
3	GOL	B	502	-	5,5,5	0.80	0	5,5,5	1.50	1 (20%)
3	GOL	A	503	-	5,5,5	0.99	0	5,5,5	1.34	1 (20%)
3	GOL	A	504	-	5,5,5	1.82	2 (40%)	5,5,5	1.71	2 (40%)
3	GOL	A	502	-	5,5,5	0.71	0	5,5,5	1.98	1 (20%)
3	GOL	B	503	-	5,5,5	1.45	1 (20%)	5,5,5	0.50	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
3	GOL	B	502	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	GOL	O2-C2	3.46	1.53	1.43
3	B	503	GOL	O2-C2	-2.22	1.36	1.43
3	A	504	GOL	O1-C1	2.11	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	GOL	O1-C1-C2	3.43	126.63	110.20
3	A	504	GOL	C3-C2-C1	-2.88	100.49	111.70
3	B	502	GOL	O1-C1-C2	2.53	122.32	110.20
3	A	503	GOL	O2-C2-C3	-2.13	99.72	109.12
3	A	504	GOL	O2-C2-C1	2.07	118.22	109.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3

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	315/315 (100%)	-0.37	2 (0%) 89 91	9, 15, 31, 66	7 (2%)
1	B	315/315 (100%)	-0.41	2 (0%) 89 91	9, 15, 31, 62	8 (2%)
All	All	630/630 (100%)	-0.39	4 (0%) 89 91	9, 15, 31, 66	15 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	LYS	3.3
1	B	181	GLN	2.5
1	A	203	VAL	2.4
1	B	473	GLY	2.3

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
3	GOL	A	504	6/6	0.75	0.22	41,56,67,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	503	6/6	0.91	0.16	35,38,44,48	0
3	GOL	A	503	6/6	0.92	0.13	29,36,42,57	0
3	GOL	A	502	6/6	0.93	0.10	35,38,39,44	0
3	GOL	B	502	6/6	0.95	0.11	26,26,28,38	0
2	MG	A	501	1/1	0.99	0.04	20,20,20,20	0
2	MG	B	501	1/1	1.00	0.06	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.