



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:53 AM GMT

PDB ID : 2C25  
Title : 1.8A CRYSTAL STRUCTURE OF PSATHYRELLA VELUTINA LECTIN  
IN COMPLEX WITH N-ACETYLNEURAMINIC ACID  
Authors : Cioci, G.; Mitchell, E.P.; Chazalet, V.; Gautier, C.; Oscarson, S.; Debray, H.;  
Perez, S.; Imberty, A.  
Deposited on : 2005-09-26  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

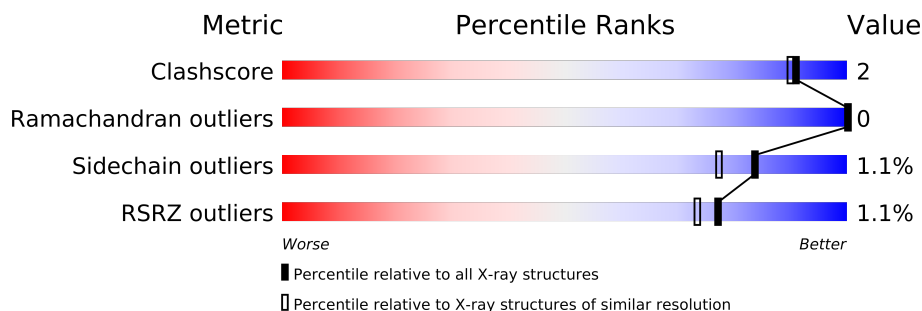
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SIA	A	601	-	X
3	SIA	A	602	-	X
3	SIA	B	600	-	X
3	SIA	B	601	-	X
4	SO4	A	701	-	X
4	SO4	B	700	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6661 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

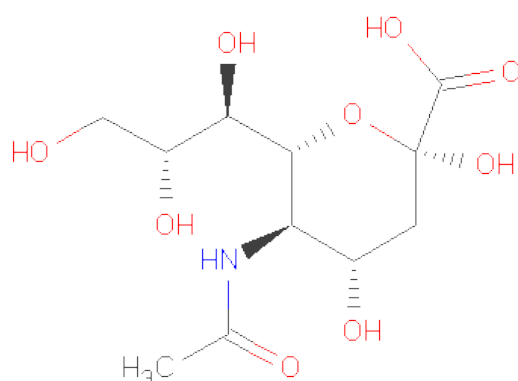
- Molecule 1 is a protein called PSATHYRELLA VELUTINA LECTIN PVL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	3	0
			3046	1934	546	557	9			
1	B	401	Total	C	N	O	S	0	1	0
			3041	1929	546	557	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total	O	0	0
			267	267		

*Continued on next page...*

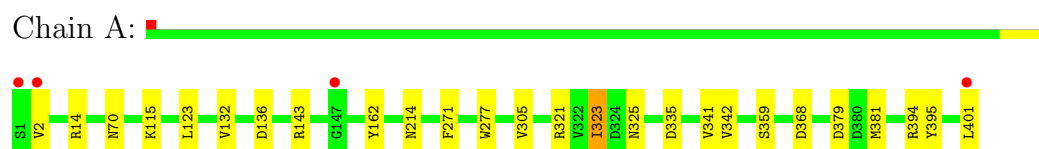
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	180	Total 180	O 180	0	0

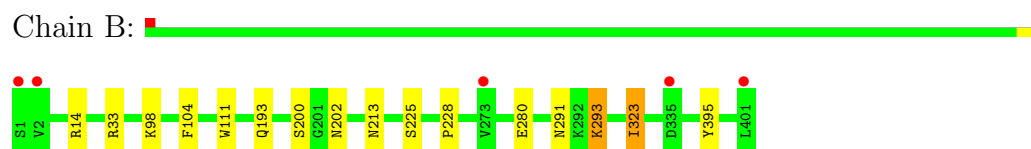
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PSATHYRELLA VELUTINA LECTIN PVL



- Molecule 1: PSATHYRELLA VELUTINA LECTIN PVL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.73Å 144.40Å 52.60Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	72.17 – 1.80 24.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.17-1.80) 99.8 (24.68-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.186 , 0.231 0.195 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.7	EDS
Estimated twinning fraction	0.018 for l,k,-h 0.047 for h,-k,-l 0.034 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 70934 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SIA, 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	0.87	0/3128	0.83	3/4245 (0.1%)
1	B	0.73	0/3113	0.80	4/4224 (0.1%)
All	All	0.80	0/6241	0.82	7/8469 (0.1%)

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323[A]	ILE	CG1-CB-CG2	5.98	124.56	111.40
1	B	323[B]	ILE	CG1-CB-CG2	5.98	124.56	111.40
1	A	368	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	14	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	33	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	143	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	321	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	395	TYR	Peptide
1	B	395	TYR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3046	0	2992	20	0
1	B	3041	0	2980	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	63	0	54	1	0
3	B	42	0	36	0	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	267	0	0	5	0
5	B	180	0	0	0	0
All	All	6661	0	6062	25	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:LEU:HD11	1:A:132:VAL:HG21	1.63	0.78
1:A:381:MET:CE	1:A:394:ARG:HG2	2.16	0.74
1:A:2:VAL:HA	5:A:2004:HOH:O	1.89	0.72
1:A:335:ASP:HB2	5:A:2116:HOH:O	1.90	0.71
1:B:193:GLN:OE1	1:B:213:ASN:ND2	2.24	0.69
1:A:2:VAL:HG12	5:A:2162:HOH:O	1.95	0.65
1:A:123:LEU:HD11	1:A:132:VAL:CG2	2.26	0.65
1:A:214:ASN:ND2	3:A:601:SIA:O1A	2.32	0.61
1:A:305:VAL:HB	1:A:323[A]:ILE:HG23	1.83	0.60
1:A:401:LEU:HD12	1:A:401:LEU:N	2.16	0.60
1:A:14:ARG:HH21	1:A:401:LEU:HA	1.68	0.58
1:A:70:ASN:HB3	1:A:401:LEU:HD11	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:LEU:CD1	1:A:401:LEU:N	2.71	0.54
1:A:2:VAL:HG22	5:A:2001:HOH:O	2.09	0.52
1:A:323[A]:ILE:HD11	1:A:325:ASN:HB3	1.93	0.49
1:A:341:VAL:C	1:A:342[A]:VAL:HG13	2.36	0.46
1:B:104:PHE:HA	1:B:111:TRP:CD1	2.50	0.46
1:A:359:SER:OG	1:A:379:ASP:OD1	2.26	0.45
1:B:200:SER:HB2	1:B:202:ASN:OD1	2.16	0.45
1:A:381:MET:HE3	1:A:394:ARG:HG2	1.98	0.45
1:A:271:PHE:HA	1:A:277:TRP:CD1	2.52	0.44
1:A:2:VAL:HG23	5:A:2004:HOH:O	2.20	0.42
1:A:115:LYS:HE3	1:A:162:TYR:CZ	2.55	0.41
1:B:280:GLU:H	1:B:280:GLU:CD	2.24	0.41
1:B:291:ASN:HA	1:B:293:LYS:HZ3	1.86	0.40

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	402/401 (100%)	398 (99%)	4 (1%)	0	100	100
1	B	400/401 (100%)	387 (97%)	13 (3%)	0	100	100
All	All	802/802 (100%)	785 (98%)	17 (2%)	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	314/311 (101%)	311 (99%)	3 (1%)	85	80
1	B	312/311 (100%)	306 (98%)	6 (2%)	69	56
All	All	626/622 (101%)	617 (99%)	9 (1%)	84	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	323[A]	ILE
1	A	323[B]	ILE
1	B	98	LYS
1	B	225	SER
1	B	228	PRO
1	B	293	LYS
1	B	323[A]	ILE
1	B	323[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	193	GLN
1	A	213	ASN
1	B	209	GLN
1	B	213	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	SIA	A	600	-	21,21,21	2.42	3 (14%)	31,31,31	1.30	3 (9%)
3	SIA	A	601	-	21,21,21	2.24	3 (14%)	31,31,31	1.95	7 (22%)
3	SIA	A	602	-	21,21,21	2.49	3 (14%)	31,31,31	1.87	8 (25%)
4	SO4	A	700	-	4,4,4	0.74	0	6,6,6	0.52	0
4	SO4	A	701	-	4,4,4	0.16	0	6,6,6	0.48	0
4	SO4	A	702	-	4,4,4	0.71	0	6,6,6	0.33	0
3	SIA	B	600	-	21,21,21	2.45	3 (14%)	31,31,31	1.52	5 (16%)
3	SIA	B	601	-	21,21,21	2.70	4 (19%)	31,31,31	1.75	6 (19%)
4	SO4	B	700	-	4,4,4	0.19	0	6,6,6	0.46	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	SIA	A	600	-	-	0/20/38/38	0/1/1/1
3	SIA	A	601	-	-	0/20/38/38	0/1/1/1
3	SIA	A	602	-	-	0/20/38/38	0/1/1/1
4	SO4	A	700	-	-	0/0/0/0	0/0/0/0
4	SO4	A	701	-	-	0/0/0/0	0/0/0/0
4	SO4	A	702	-	-	0/0/0/0	0/0/0/0
3	SIA	B	600	-	-	0/20/38/38	0/1/1/1
3	SIA	B	601	-	-	0/20/38/38	0/1/1/1
4	SO4	B	700	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	SIA	C11-C10	-8.79	1.32	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	SIA	C11-C10	-8.46	1.32	1.50
3	B	600	SIA	C11-C10	-8.39	1.32	1.50
3	A	600	SIA	C11-C10	-8.01	1.33	1.50
3	A	601	SIA	C11-C10	-7.48	1.34	1.50
3	B	601	SIA	O2-C2	5.08	1.46	1.39
3	A	600	SIA	O10-C10	5.02	1.34	1.23
3	B	601	SIA	O10-C10	4.89	1.33	1.23
3	A	600	SIA	O2-C2	4.69	1.45	1.39
3	A	602	SIA	O10-C10	4.59	1.33	1.23
3	A	601	SIA	O10-C10	4.55	1.33	1.23
3	B	600	SIA	O2-C2	4.53	1.45	1.39
3	B	601	SIA	O6-C2	4.20	1.46	1.42
3	B	600	SIA	O10-C10	4.13	1.32	1.23
3	A	602	SIA	O2-C2	4.12	1.45	1.39
3	A	601	SIA	O2-C2	4.10	1.45	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	SIA	O1A-C1-C2	-5.58	115.73	123.48
3	B	601	SIA	C3-C2-C1	-4.88	105.38	113.58
3	A	601	SIA	O6-C6-C5	-4.54	105.27	109.55
3	A	602	SIA	O1A-C1-C2	-4.38	117.40	123.48
3	A	602	SIA	O6-C6-C7	3.90	111.36	106.34
3	A	601	SIA	O6-C2-C3	-3.81	107.97	110.22
3	B	601	SIA	O6-C2-C3	-3.75	108.00	110.22
3	B	601	SIA	O1A-C1-C2	-3.62	118.45	123.48
3	A	601	SIA	C6-C5-N5	-3.48	104.91	110.99
3	A	602	SIA	O6-C6-C5	3.48	112.83	109.55
3	B	600	SIA	C2-O6-C6	3.46	119.19	113.93
3	B	600	SIA	O1A-C1-C2	-3.45	118.69	123.48
3	A	602	SIA	C6-C5-N5	-3.21	105.38	110.99
3	B	601	SIA	O6-C6-C5	2.90	112.28	109.55
3	A	602	SIA	C7-C6-C5	-2.79	110.13	114.24
3	B	601	SIA	C8-C7-C6	-2.77	107.63	112.99
3	A	602	SIA	C2-O6-C6	2.76	118.14	113.93
3	B	600	SIA	O6-C2-C3	-2.61	108.67	110.22
3	A	600	SIA	C3-C4-C5	-2.58	107.73	110.72
3	A	601	SIA	O8-C8-C7	2.55	115.41	109.05
3	B	600	SIA	O6-C6-C5	2.51	111.92	109.55
3	A	601	SIA	O7-C7-C6	-2.50	104.03	109.45
3	A	600	SIA	O6-C2-C3	-2.41	108.79	110.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	SIA	C3-C2-C1	-2.38	109.58	113.58
3	A	602	SIA	C3-C4-C5	-2.36	107.98	110.72
3	B	600	SIA	C6-C5-N5	-2.31	106.96	110.99
3	A	601	SIA	C7-C6-C5	2.18	117.46	114.24
3	A	600	SIA	C8-C7-C6	-2.14	108.83	112.99
3	B	601	SIA	O6-C2-C1	2.03	113.49	106.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	401/401 (100%)	-0.23	4 (0%) 79 76	12, 19, 28, 39	0
1	B	401/401 (100%)	0.11	5 (1%) 75 72	15, 27, 39, 45	0
All	All	802/802 (100%)	-0.06	9 (1%) 77 73	12, 22, 36, 45	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	6.8
1	A	2	VAL	5.4
1	B	2	VAL	4.8
1	A	1	SER	4.4
1	B	401	LEU	3.2
1	B	335	ASP	2.8
1	A	401	LEU	2.7
1	A	147	GLY	2.1
1	B	273	VAL	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SIA	A	602	21/21	0.30	7.28	35,46,51,51	0
4	SO4	A	701	5/5	0.15	5.72	35,36,37,37	0
3	SIA	B	600	21/21	0.28	5.28	29,41,47,49	0
3	SIA	B	601	21/21	0.18	3.44	35,41,47,52	0
4	SO4	B	700	5/5	0.15	3.34	48,48,50,51	0
3	SIA	A	601	21/21	0.19	2.27	22,34,38,44	0
3	SIA	A	600	21/21	0.17	1.70	26,33,42,50	0
4	SO4	A	702	5/5	0.14	1.63	31,32,36,37	0
4	SO4	A	700	5/5	0.08	0.02	23,24,26,28	0
2	CA	A	500	1/1	0.04	-2.65	16,16,16,16	0
2	CA	B	500	1/1	0.03	-3.02	17,17,17,17	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.