



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:40 AM BST

PDB ID : 6H3S  
Title : Schmallenberg Virus Glycoprotein Gc Head/Stalk Domains  
Authors : Hellert, J.; Aebischer, A.; Wernike, K.; Haouz, A.; Brocchi, E.; Reiche, S.; Guardado-Calvo, P.; Beer, M.; Rey, F.A.  
Deposited on : 2018-07-19  
Resolution : 2.02 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](mailto: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 : 2.13.1  
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) : 2.13.1

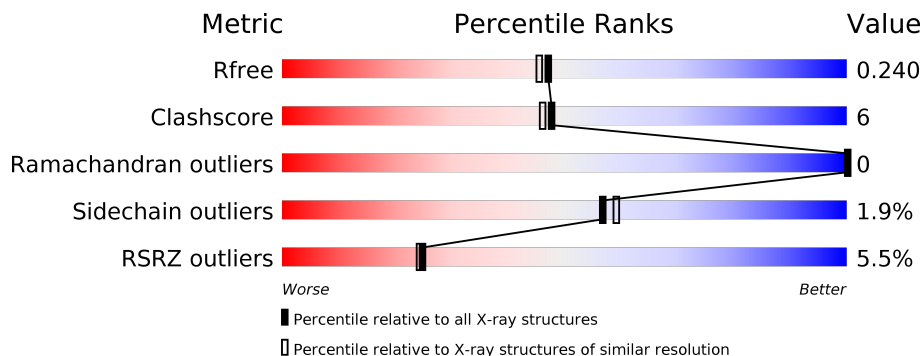
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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  $\geq 3$ , 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	421	 7% 83% 14% •
1	B	421	 3% 83% 13% ••

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6896 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	408	3237	2033	560	615	29	0	0	0
1	A	408	3237	2033	560	615	29	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	454	GLU	-	expression tag	UNP H2AM12
B	455	TRP	-	expression tag	UNP H2AM12
B	456	SER	-	expression tag	UNP H2AM12
B	457	HIS	-	expression tag	UNP H2AM12
B	458	PRO	-	expression tag	UNP H2AM12
B	459	GLN	-	expression tag	UNP H2AM12
B	460	PHE	-	expression tag	UNP H2AM12
B	461	GLU	-	expression tag	UNP H2AM12
B	462	LYS	-	expression tag	UNP H2AM12
B	463	GLY	-	expression tag	UNP H2AM12
B	464	GLY	-	expression tag	UNP H2AM12
A	454	GLU	-	expression tag	UNP H2AM12
A	455	TRP	-	expression tag	UNP H2AM12
A	456	SER	-	expression tag	UNP H2AM12
A	457	HIS	-	expression tag	UNP H2AM12
A	458	PRO	-	expression tag	UNP H2AM12
A	459	GLN	-	expression tag	UNP H2AM12
A	460	PHE	-	expression tag	UNP H2AM12
A	461	GLU	-	expression tag	UNP H2AM12
A	462	LYS	-	expression tag	UNP H2AM12
A	463	GLY	-	expression tag	UNP H2AM12
A	464	GLY	-	expression tag	UNP H2AM12

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total Cl 4 4	0	0
4	A	1	Total Cl 1 1	0	0

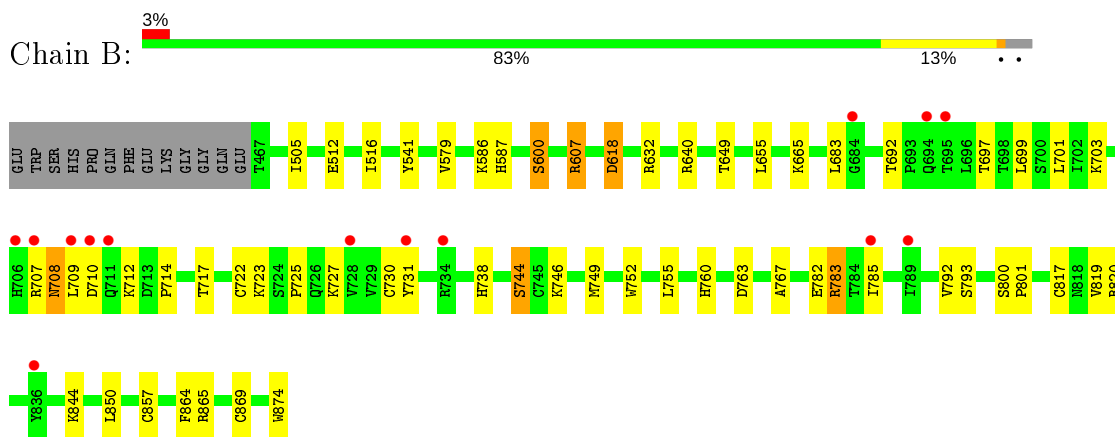
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	165	Total O 165 165	0	0
5	A	141	Total O 141 141	0	0

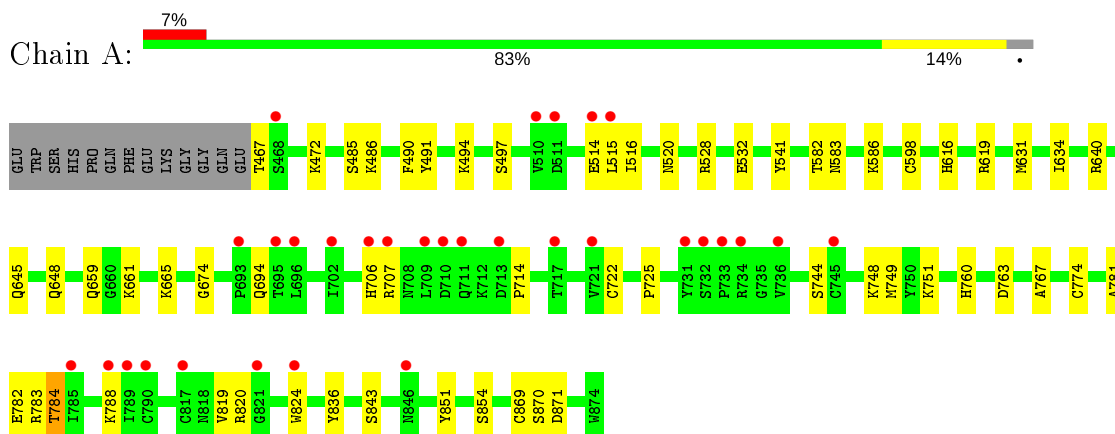
### 3 Residue-property plots [i](#)

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: Envelopment polyprotein



- Molecule 1: Envelopment polyprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.23Å 95.23Å 204.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 2.02 47.61 – 2.02	Depositor EDS
% Data completeness (in resolution range)	62.2 (47.61-2.02) 62.2 (47.61-2.02)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.209 , 0.240 0.209 , 0.240	Depositor DCC
$R_{free}$ test set	2283 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, NAG

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	0.25	0/3305	0.42	0/4473
1	B	0.27	0/3305	0.43	0/4473
All	All	0.26	0/6610	0.43	0/8946

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

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	3237	0	3194	36	0
1	B	3237	0	3194	41	0
2	A	28	0	26	2	0
2	B	28	0	26	1	0
3	A	30	0	0	1	0
3	B	25	0	0	1	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
5	A	141	0	0	5	0
5	B	165	0	0	4	0
All	All	6896	0	6440	80	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 6.

All (80) 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:B:727:LYS:HB3	1:B:793:SER:O	1.55	1.04
1:A:467:THR:O	1:A:486:LYS:NZ	2.06	0.88
1:A:640:ARG:NH1	5:A:1001:HOH:O	2.10	0.83
1:B:618:ASP:OD1	1:B:618:ASP:N	2.21	0.73
1:B:727:LYS:NZ	5:B:1003:HOH:O	2.25	0.69
1:B:512:GLU:OE2	1:B:738:HIS:ND1	2.27	0.65
1:A:520:ASN:ND2	5:A:1012:HOH:O	2.31	0.63
1:A:485:SER:OG	1:A:661:LYS:NZ	2.25	0.62
1:B:874:TRP:OXT	1:A:528:ARG:NH2	2.34	0.61
1:B:516:ILE:HD11	1:B:541:TYR:CE2	2.36	0.61
1:A:616:HIS:HB3	1:A:619:ARG:HG3	1.84	0.60
2:B:902:NAG:H83	2:B:902:NAG:H3	1.85	0.59
1:B:579:VAL:HG22	1:B:586:LYS:NZ	2.17	0.59
1:A:514:GLU:HG2	1:A:784:THR:HG21	1.84	0.58
1:A:706:HIS:CD2	1:A:707:ARG:HG2	2.39	0.57
1:B:579:VAL:HG22	1:B:586:LYS:HZ2	1.70	0.56
1:B:516:ILE:HD11	1:B:541:TYR:HE2	1.70	0.55
1:A:648:GLN:NE2	5:A:1018:HOH:O	2.38	0.55
1:A:494:LYS:NZ	1:A:497:SER:O	2.35	0.55
1:B:727:LYS:HG2	1:B:793:SER:HB3	1.88	0.55
1:B:783:ARG:HD2	1:B:783:ARG:H	1.71	0.55
1:A:582:THR:O	1:A:586:LYS:NZ	2.40	0.55
1:A:751:LYS:NZ	1:A:782:GLU:OE1	2.41	0.54
1:B:717:THR:O	5:B:1002:HOH:O	2.18	0.54
1:B:819:VAL:HG12	1:B:820:ARG:HG3	1.88	0.54
1:B:709:LEU:O	1:B:712:LYS:NZ	2.31	0.54
1:A:645:GLN:NE2	1:A:694:GLN:O	2.38	0.54
1:A:725:PRO:HA	1:A:744:SER:O	2.08	0.54
1:B:655:LEU:HB3	1:B:683:LEU:HD11	1.90	0.54
1:A:714:PRO:HB3	1:A:781:ALA:HB3	1.91	0.53
1:B:665:LYS:NZ	5:B:1020:HOH:O	2.41	0.53
2:A:902:NAG:H3	2:A:902:NAG:H83	1.91	0.53
1:B:722:CYS:HB3	1:B:767:ALA:HB3	1.89	0.53
1:A:516:ILE:HD11	1:A:541:TYR:HE2	1.73	0.53
3:B:907:SO4:O4	5:B:1001:HOH:O	2.18	0.53
1:A:744:SER:HA	1:A:748:LYS:O	2.10	0.51
1:B:760:HIS:HB3	1:B:763:ASP:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD22	1:A:788:LYS:NZ	2.26	0.51
1:B:723:LYS:HD2	1:B:746:LYS:HE3	1.92	0.51
1:B:607:ARG:HD3	1:B:607:ARG:H	1.78	0.49
1:A:528:ARG:O	1:A:532:GLU:HB2	2.12	0.49
1:A:760:HIS:HD2	1:A:774:CYS:SG	2.36	0.49
1:A:824:TRP:HE3	1:A:836:TYR:CE1	2.31	0.48
1:A:819:VAL:HG12	1:A:820:ARG:HG2	1.95	0.48
1:B:699:LEU:HD11	1:B:703:LYS:HE3	1.96	0.47
1:A:486:LYS:HG2	1:A:661:LYS:HZ1	1.79	0.47
1:B:730:CYS:SG	1:B:785:ILE:HD11	2.56	0.46
1:A:583:ASN:O	1:A:586:LYS:NZ	2.48	0.46
1:A:722:CYS:HB3	1:A:767:ALA:HB3	1.98	0.46
1:B:632:ARG:NH2	1:B:640:ARG:HD3	2.31	0.46
1:B:707:ARG:HD3	1:B:792:VAL:O	2.15	0.46
1:B:697:THR:HG23	1:B:701:LEU:HD23	1.98	0.46
1:B:864:PHE:HE1	1:B:869:CYS:SG	2.38	0.46
1:A:843:SER:HA	1:A:851:TYR:HA	1.98	0.45
1:B:587:HIS:ND1	1:B:600:SER:HB2	2.32	0.45
1:B:844:LYS:HD2	1:B:850:LEU:HG	1.99	0.45
1:A:491:TYR:CZ	2:A:901:NAG:H3	2.52	0.44
1:A:870:SER:HA	1:A:871:ASP:HA	1.53	0.43
1:B:683:LEU:HD23	1:B:683:LEU:HA	1.90	0.42
1:B:727:LYS:HD2	1:B:752:TRP:CZ3	2.55	0.42
1:B:727:LYS:HB3	1:B:793:SER:C	2.34	0.42
1:A:631:MET:HA	1:A:634:ILE:HD12	2.02	0.42
1:A:659:GLN:NE2	5:A:1015:HOH:O	2.33	0.42
1:A:490:PHE:HD1	1:A:665:LYS:HD2	1.84	0.42
1:B:649:THR:HA	1:B:692:THR:HB	2.01	0.42
1:B:755:LEU:HD22	1:B:865:ARG:NH2	2.35	0.42
1:B:725:PRO:HA	1:B:744:SER:O	2.20	0.41
1:B:708:ASN:OD1	1:B:708:ASN:N	2.53	0.41
1:B:714:PRO:HA	1:B:749:MET:HB2	2.02	0.41
1:B:707:ARG:HB3	1:B:792:VAL:HB	2.02	0.41
1:B:800:SER:HB2	1:B:801:PRO:HD2	2.01	0.41
1:A:714:PRO:HA	1:A:749:MET:HB2	2.03	0.41
1:A:722:CYS:SG	1:A:725:PRO:HB3	2.61	0.41
1:A:598:CYS:O	1:A:674:GLY:HA3	2.21	0.41
1:A:472:LYS:HA	1:A:541:TYR:HD1	1.85	0.41
1:B:703:LYS:HG2	1:B:731:TYR:CE2	2.55	0.41
3:A:908:SO4:O3	5:A:1002:HOH:O	2.20	0.41
1:B:505:ILE:HG21	1:B:516:ILE:HG21	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:LYS:HD3	1:A:748:LYS:HA	1.93	0.40
1:B:782:GLU:H	1:B:782:GLU:CD	2.25	0.40

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	406/421 (96%)	401 (99%)	5 (1%)	0	100	100
1	B	406/421 (96%)	400 (98%)	6 (2%)	0	100	100
All	All	812/842 (96%)	801 (99%)	11 (1%)	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	376/387 (97%)	371 (99%)	5 (1%)	69	72
1	B	376/387 (97%)	367 (98%)	9 (2%)	49	49
All	All	752/774 (97%)	738 (98%)	14 (2%)	57	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	600	SER
1	B	607	ARG
1	B	618	ASP
1	B	708	ASN
1	B	710	ASP
1	B	744	SER
1	B	783	ARG
1	B	817	CYS
1	B	857	CYS
1	A	763	ASP
1	A	783	ARG
1	A	784	THR
1	A	854	SER
1	A	869	CYS

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	SO4	B	906	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	906	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	903	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	905	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	908	-	4,4,4	0.15	0	6,6,6	0.08	0
2	NAG	B	901	1	14,14,15	0.25	0	17,19,21	0.45	0
3	SO4	B	904	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	B	907	-	4,4,4	0.15	0	6,6,6	0.07	0
2	NAG	B	902	1	14,14,15	0.60	0	17,19,21	1.25	1 (5%)
2	NAG	A	902	1	14,14,15	0.39	0	17,19,21	1.37	2 (11%)
3	SO4	A	907	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	905	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	A	903	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	904	-	4,4,4	0.14	0	6,6,6	0.14	0
2	NAG	A	901	1	14,14,15	0.24	0	17,19,21	0.45	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	NAG	B	902	1	-	3/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	902	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	NAG	C2-N2-C7	4.39	129.15	122.90
2	B	902	NAG	C2-N2-C7	4.25	128.96	122.90
2	A	902	NAG	C1-C2-N2	2.23	114.30	110.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	NAG	C8-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	901	NAG	O7-C7-N2-C2
2	B	902	NAG	C8-C7-N2-C2
2	B	902	NAG	O7-C7-N2-C2
2	A	902	NAG	C8-C7-N2-C2
2	A	902	NAG	O7-C7-N2-C2
2	B	902	NAG	C3-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	908	SO4	1	0
3	B	907	SO4	1	0
2	B	902	NAG	1	0
2	A	902	NAG	1	0
2	A	901	NAG	1	0

## 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, 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	408/421 (96%)	0.46	31 (7%) 13 13	31, 63, 116, 159	0
1	B	408/421 (96%)	0.31	14 (3%) 45 45	33, 55, 97, 136	0
All	All	816/842 (96%)	0.38	45 (5%) 25 24	31, 59, 108, 159	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	6.7
1	A	510	VAL	5.7
1	A	710	ASP	5.2
1	B	695	THR	5.2
1	A	721	VAL	4.6
1	B	710	ASP	4.3
1	A	693	PRO	4.1
1	A	702	ILE	4.0
1	B	709	LEU	3.9
1	A	788	LYS	3.6
1	A	821	GLY	3.4
1	A	732	SER	3.4
1	B	706	HIS	3.4
1	A	696	LEU	3.4
1	A	733	PRO	3.2
1	A	709	LEU	3.1
1	B	731	TYR	3.1
1	B	707	ARG	2.8
1	B	694	GLN	2.7
1	A	734	ARG	2.7
1	A	707	ARG	2.6
1	A	706	HIS	2.6
1	A	731	TYR	2.6
1	A	824	TRP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	734	ARG	2.5
1	B	789	ILE	2.4
1	A	711	GLN	2.4
1	A	511	ASP	2.4
1	B	711	GLN	2.3
1	A	817	CYS	2.3
1	A	736	VAL	2.3
1	A	785	ILE	2.3
1	A	713	ASP	2.2
1	A	790	CYS	2.2
1	A	695	THR	2.2
1	A	717	THR	2.2
1	B	684	GLY	2.2
1	A	745	CYS	2.1
1	B	785	ILE	2.1
1	A	789	ILE	2.1
1	A	468	SER	2.1
1	A	846	ASN	2.1
1	B	728	VAL	2.1
1	B	836	TYR	2.0
1	A	514	GLU	2.0

## 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 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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	902	14/15	0.81	0.17	75,88,91,93	0
2	NAG	A	902	14/15	0.85	0.16	69,81,84,84	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	909	1/1	0.86	0.13	64,64,64,64	0
3	SO4	A	908	5/5	0.86	0.18	96,96,101,103	0
4	CL	B	908	1/1	0.88	0.12	72,72,72,72	0
3	SO4	A	906	5/5	0.88	0.17	108,110,111,112	0
3	SO4	B	907	5/5	0.89	0.09	104,105,106,107	0
4	CL	A	909	1/1	0.90	0.09	101,101,101,101	0
2	NAG	B	901	14/15	0.91	0.16	58,69,74,77	0
2	NAG	A	901	14/15	0.93	0.18	62,70,73,75	0
4	CL	B	910	1/1	0.94	0.19	79,79,79,79	0
3	SO4	A	907	5/5	0.95	0.15	93,96,96,100	0
3	SO4	A	903	5/5	0.96	0.11	74,78,80,81	0
4	CL	B	911	1/1	0.97	0.11	97,97,97,97	0
3	SO4	B	903	5/5	0.97	0.13	63,67,73,74	0
3	SO4	B	904	5/5	0.97	0.11	78,79,80,82	0
3	SO4	A	905	5/5	0.97	0.11	74,77,78,81	0
3	SO4	B	906	5/5	0.97	0.09	78,80,82,83	0
3	SO4	A	904	5/5	0.98	0.14	54,55,59,62	0
3	SO4	B	905	5/5	0.98	0.16	49,50,54,58	0

## 6.5 Other polymers

There are no such residues in this entry.