



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:38 PM UTC

PDB ID : 6H3S / pdb_00006h3s
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

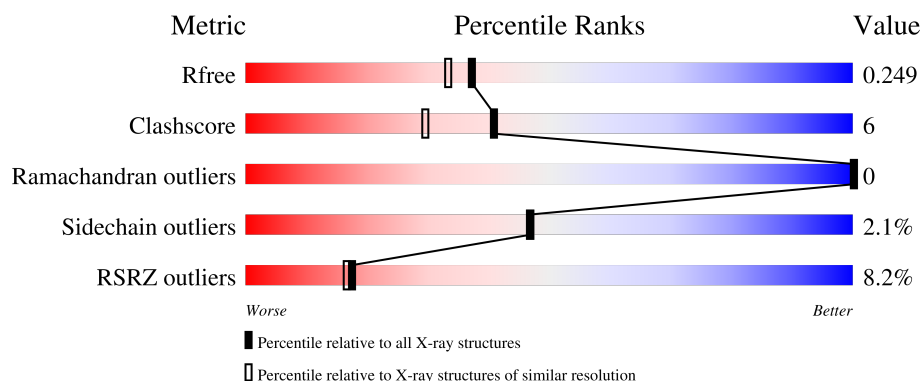
1 Overall quality at a glance

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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 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	421	12% 82% 14% ..
1	B	421	4% 82% 14% ..

2 Entry composition

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
1	B	408	Total	C	N	O	S	0	0	0
			3237	2033	560	615	29			
1	A	408	Total	C	N	O	S	0	0	0
			3237	2033	560	615	29			

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: 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

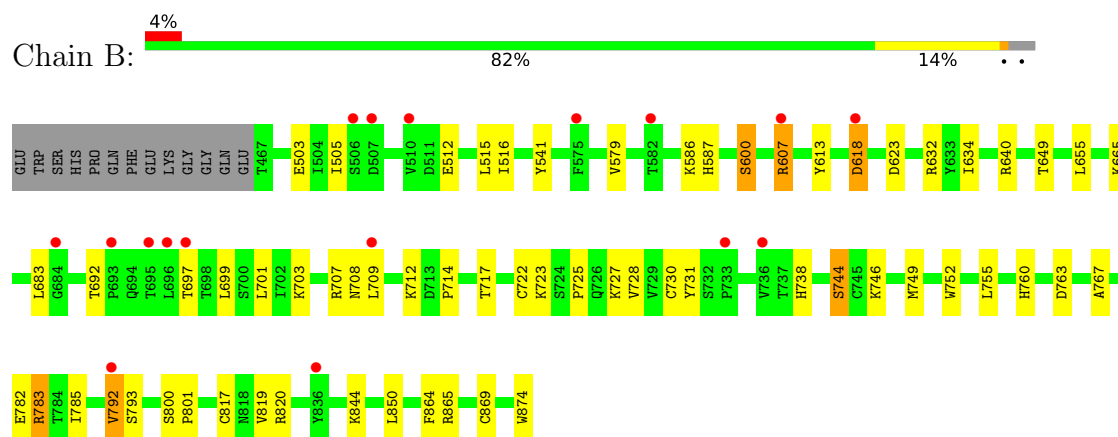
- Molecule 5 is water.

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

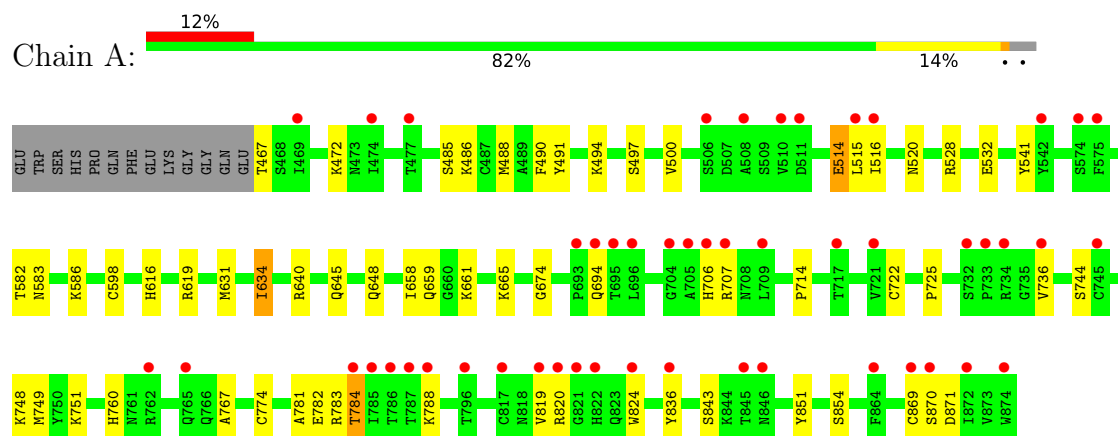
3 Residue-property plots

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 polypeptide



• Molecule 1: Envelopment polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 62.3 (47.61-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.209 , 0.240 0.220 , 0.249	Depositor DCC
R_{free} test set	2283 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage'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.*

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: NAG, CL, 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	0.12	0/3305	0.35	1/4473 (0.0%)
1	B	0.14	0/3305	0.35	1/4473 (0.0%)
All	All	0.13	0/6610	0.35	2/8946 (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	B	634	ILE	N-CA-C	-7.02	105.94	112.96
1	A	634	ILE	N-CA-C	-7.02	106.21	111.90

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	3237	0	3194	38	0
1	B	3237	0	3194	43	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	84	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 (84) 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:512:GLU:OE2	1:B:738:HIS:ND1	2.27	0.65
1:B:579:VAL:HG22	1:B:586:LYS:HZ2	1.63	0.63
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: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:B:727:LYS:HG2	1:B:793:SER:HB3	1.88	0.55
1:B:783:ARG:H	1:B:783:ARG:HD2	1.71	0.55
1:A:494:LYS:NZ	1:A:497:SER:O	2.35	0.55
1:A:582:THR:O	1:A:586:LYS:NZ	2.40	0.55
1:B:727:LYS:NZ	5:B:1003:HOH:O	2.25	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:A:751:LYS:NZ	1:A:782:GLU:OE1	2.41	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:B:665:LYS:NZ	5:B:1020:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PRO:HB3	1:A:781:ALA:HB3	1.91	0.53
1:B:722:CYS:HB3	1:B:767:ALA:HB3	1.89	0.53
2:A:902:NAG:H83	2:A:902:NAG:H3	1.91	0.53
3:B:907:SO4:O4	5:B:1001:HOH:O	2.18	0.53
1:A:516:ILE:HD11	1:A:541:TYR:HE2	1.73	0.53
1:B:613:TYR:OH	1:B:623:ASP:OD2	2.24	0.53
1:B:727:LYS:HB3	1:B:793:SER:C	2.34	0.52
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
1:B:723:LYS:HD2	1:B:746:LYS:HE3	1.92	0.51
1:A:515:LEU:HD22	1:A:788:LYS:NZ	2.26	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: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:A:722:CYS:HB3	1:A:767:ALA:HB3	1.98	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:B:782:GLU:H	1:B:782:GLU:CD	2.25	0.45
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:A:488:MET:HE1	1:A:658:ILE:HG23	2.01	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:A:631:MET:HA	1:A:634:ILE:HD12	2.02	0.42
1:B:649:THR:HA	1:B:692:THR:HB	2.01	0.42
1:A:490:PHE:HD1	1:A:665:LYS:HD2	1.84	0.42
1:A:659:GLN:NE2	5:A:1015:HOH:O	2.33	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:728:VAL:HG11	1:B:749:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ASN:OD1	1:B:708:ASN:N	2.53	0.41
1:B:707:ARG:HB3	1:B:792:VAL:HB	2.02	0.41
1:B:714:PRO:HA	1:B:749:MET:HB2	2.02	0.41
1:B:800:SER:HB2	1:B:801:PRO:HD2	2.01	0.41
1:A:467:THR:C	1:A:486:LYS:NZ	2.77	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:B:703:LYS:HG2	1:B:731:TYR:CE2	2.55	0.41
1:A:472:LYS:HA	1:A:541:TYR:HD1	1.85	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
1:A:748:LYS:HD3	1:A:748:LYS:HA	1.93	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	351/421 (83%)	346 (99%)	5 (1%)	0	100	100
All	All	757/842 (90%)	747 (99%)	10 (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%)	369 (98%)	7 (2%)	50	50
1	B	376/387 (97%)	367 (98%)	9 (2%)	43	41
All	All	752/774 (97%)	736 (98%)	16 (2%)	47	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	503	GLU
1	B	515	LEU
1	B	600	SER
1	B	607	ARG
1	B	618	ASP
1	B	744	SER
1	B	783	ARG
1	B	792	VAL
1	B	817	CYS
1	A	500	VAL
1	A	514	GLU
1	A	736	VAL
1	A	783	ARG
1	A	784	THR
1	A	854	SER
1	A	869	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	520	ASN
1	B	645	GLN
1	B	810	ASN
1	A	492	GLN
1	A	567	GLN
1	A	760	HIS
1	A	764	GLN
1	A	810	ASN
1	A	846	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.24	0	6,6,6	0.11	0
3	SO4	A	908	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	905	-	4,4,4	0.26	0	6,6,6	0.18	0
2	NAG	A	901	1	14,14,15	0.25	0	17,19,21	0.47	0
3	SO4	A	905	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	A	907	-	4,4,4	0.23	0	6,6,6	0.11	0
2	NAG	B	901	1	14,14,15	0.26	0	17,19,21	0.46	0
3	SO4	B	907	-	4,4,4	0.26	0	6,6,6	0.06	0
2	NAG	B	902	1	14,14,15	0.64	1 (7%)	17,19,21	1.32	2 (11%)
3	SO4	A	906	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	A	904	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	A	903	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	B	904	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	B	903	-	4,4,4	0.25	0	6,6,6	0.13	0
2	NAG	A	902	1	14,14,15	0.41	0	17,19,21	1.45	2 (11%)

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	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	902	1	-	4/6/23/26	0/1/1/1
2	NAG	B	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	902	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	NAG	C1-C2	2.17	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	NAG	C2-N2-C7	4.67	129.15	122.90
2	B	902	NAG	C2-N2-C7	4.52	128.96	122.90
2	A	902	NAG	C1-C2-N2	2.46	114.30	110.43
2	B	902	NAG	C1-C2-N2	2.02	113.62	110.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	NAG	C8-C7-N2-C2
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	C1-C2-N2-C7
2	A	902	NAG	C1-C2-N2-C7
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
2	A	901	NAG	1	0
3	B	907	SO4	1	0
2	B	902	NAG	1	0
2	A	902	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, 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	408/421 (96%)	0.75	50 (12%) 8 7	31, 63, 116, 159	0
1	B	408/421 (96%)	0.46	17 (4%) 40 40	33, 55, 97, 136	0
All	All	816/842 (96%)	0.60	67 (8%) 17 17	31, 59, 108, 159	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	THR	3.5
1	A	508	ALA	3.4
1	A	824	TRP	3.4
1	B	510	VAL	3.1
1	B	736	VAL	3.1
1	A	864	PHE	3.0
1	A	515	LEU	3.0
1	A	510	VAL	2.9
1	A	477	THR	2.9
1	A	696	LEU	2.9
1	A	705	ALA	2.9
1	A	817	CYS	2.8
1	B	684	GLY	2.8
1	A	721	VAL	2.8
1	A	736	VAL	2.8
1	A	511	ASP	2.8
1	B	836	TYR	2.8
1	A	836	TYR	2.8
1	A	733	PRO	2.7
1	A	846	ASN	2.7
1	B	695	THR	2.7
1	A	788	LYS	2.7
1	A	786	THR	2.6
1	A	845	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	693	PRO	2.5
1	B	709	LEU	2.5
1	B	696	LEU	2.5
1	A	706	HIS	2.5
1	A	732	SER	2.4
1	A	819	VAL	2.4
1	A	785	ILE	2.4
1	A	874	TRP	2.3
1	B	506	SER	2.3
1	A	787	THR	2.3
1	A	872	ILE	2.3
1	B	733	PRO	2.3
1	B	507	ASP	2.3
1	A	765	GLN	2.2
1	A	762	ARG	2.2
1	A	709	LEU	2.2
1	A	506	SER	2.2
1	A	474	ILE	2.2
1	A	869	CYS	2.2
1	B	618	ASP	2.2
1	A	469	ILE	2.2
1	A	694	GLN	2.2
1	B	582	THR	2.2
1	A	542	TYR	2.1
1	B	693	PRO	2.1
1	A	796	THR	2.1
1	A	734	ARG	2.1
1	B	607	ARG	2.1
1	A	707	ARG	2.1
1	A	820	ARG	2.1
1	B	575	PHE	2.1
1	B	792	VAL	2.1
1	A	574	SER	2.1
1	A	870	SER	2.1
1	B	697	THR	2.1
1	A	575	PHE	2.1
1	A	745	CYS	2.0
1	A	822	HIS	2.0
1	A	695	THR	2.0
1	A	821	GLY	2.0
1	A	516	ILE	2.0
1	A	784	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	704	GLY	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 oligosaccharides 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	NAG	B	902	14/15	0.41	0.14	75,88,91,93	0
2	NAG	A	902	14/15	0.64	0.15	69,81,84,84	0
3	SO4	A	908	5/5	0.75	0.16	96,96,101,103	0
2	NAG	B	901	14/15	0.77	0.12	58,69,74,77	0
3	SO4	A	906	5/5	0.78	0.12	108,110,111,112	0
3	SO4	B	907	5/5	0.81	0.10	104,105,106,107	0
4	CL	A	909	1/1	0.81	0.14	101,101,101,101	0
2	NAG	A	901	14/15	0.82	0.10	62,70,73,75	0
4	CL	B	909	1/1	0.84	0.12	64,64,64,64	0
3	SO4	A	907	5/5	0.86	0.10	93,96,96,100	0
3	SO4	B	904	5/5	0.86	0.10	78,79,80,82	0
3	SO4	B	906	5/5	0.88	0.08	78,80,82,83	0
4	CL	B	908	1/1	0.90	0.11	72,72,72,72	0
3	SO4	A	903	5/5	0.90	0.10	74,78,80,81	0
4	CL	B	911	1/1	0.90	0.10	97,97,97,97	0
3	SO4	B	903	5/5	0.90	0.11	63,67,73,74	0
3	SO4	A	905	5/5	0.92	0.08	74,77,78,81	0
4	CL	B	910	1/1	0.92	0.09	79,79,79,79	0
3	SO4	A	904	5/5	0.96	0.06	54,55,59,62	0
3	SO4	B	905	5/5	0.96	0.08	49,50,54,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.