



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:48 AM GMT

PDB ID : 3CA0  
Title : Sambucus nigra agglutinin II (SNA-II), hexagonal crystal form  
Authors : Maveyraud, L.; Niwa, H.; Guillet, V.; Palmer, R.A.; Reynolds, C.D.; Mourey, L.  
Deposited on : 2008-02-19  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

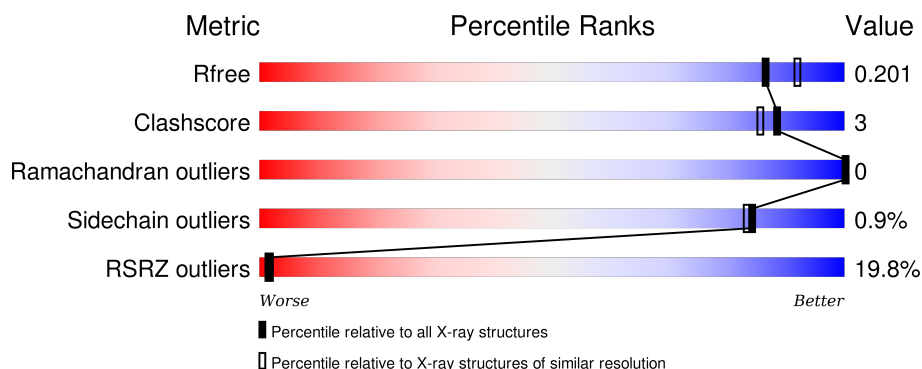
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	258	

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
2	XYP	A	264	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	267	-	-	-	X
7	ACT	A	910	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2570 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 Agglutinin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	6	0
			2026	1254	363	395	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	LEU	HIS	SEE REMARK 999	UNP P33183

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			80	45	2	33		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

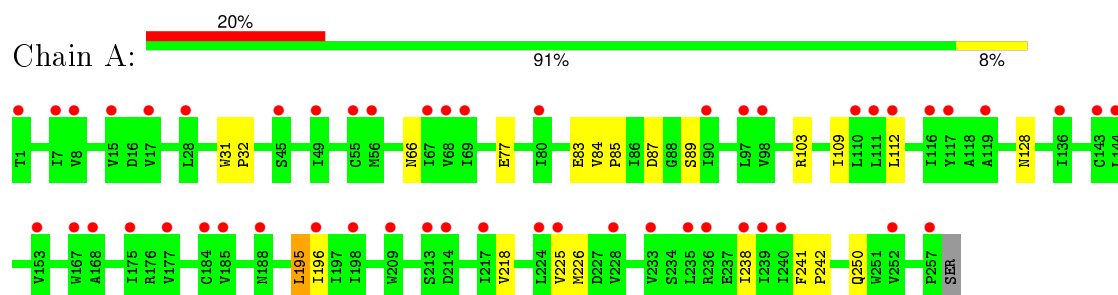
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	335	Total	O	0	0
			335	335		

### 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 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: Agglutinin II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20Å 120.20Å 177.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.91 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.95) 99.0 (19.91-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.171 , 0.194 0.181 , 0.201	Depositor DCC
$R_{free}$ test set	2762 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55058 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, BMA, NAG, FUC, ACT, MAN, 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	0.94	1/2063 (0.0%)	0.88	7/2810 (0.2%)

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
2	A	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ASN	CB-CG	6.06	1.65	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103[A]	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	A	103[B]	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	A	87	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	87	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	A	226	MET	CG-SD-CE	-5.73	91.03	100.20
1	A	195	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	112	LEU	CB-CG-CD1	-5.17	102.20	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	264	XYP	C4B,C2B,C3B

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	2026	0	1962	11	0
2	A	80	0	67	0	0
3	A	24	0	22	0	0
4	A	28	0	25	0	0
5	A	38	0	34	0	0
6	A	35	0	0	0	0
7	A	4	0	3	0	0
8	A	335	0	0	4	0
All	All	2570	0	2113	11	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 (11) 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:77:GLU:HG2	8:A:1082:HOH:O	1.95	0.66
1:A:250:GLN:NE2	8:A:1084:HOH:O	2.29	0.65
1:A:84:VAL:CG1	8:A:931:HOH:O	2.57	0.52
1:A:84:VAL:HG13	8:A:931:HOH:O	2.11	0.51
1:A:241:PHE:CG	1:A:242:PRO:HD2	2.47	0.50
1:A:196:ILE:HD12	1:A:238:ILE:HG22	1.95	0.48
1:A:85:PRO:HD2	1:A:89:SER:O	2.17	0.45
1:A:66:ASN:ND2	1:A:109:ILE:HD12	2.33	0.43
1:A:218:VAL:HG22	1:A:225:VAL:HG12	2.03	0.41
1:A:66:ASN:HD21	1:A:109:ILE:HD12	1.86	0.41
1:A:31:TRP:CD2	1:A:32:PRO:HD2	2.55	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	261/258 (101%)	257 (98%)	4 (2%)	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	226/223 (101%)	223 (99%)	3 (1%)	76	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83[A]	GLU
1	A	83[B]	GLU
1	A	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	164	GLN
1	A	254	GLN

### 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 ⓘ

14 carbohydrates 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	NAG	A	258	1,2	14,14,15	1.62	3 (21%)	15,19,21	1.88	5 (33%)
2	NAG	A	259	2	14,14,15	0.81	1 (7%)	15,19,21	1.04	1 (6%)
2	BMA	A	260	2	11,11,12	1.10	1 (9%)	14,15,17	1.82	4 (28%)
2	MAN	A	261	2	11,11,12	0.76	0	14,15,17	1.31	2 (14%)
2	FUC	A	262	2	10,10,11	1.05	0	14,14,16	2.12	2 (14%)
2	MAN	A	263	2	11,11,12	0.62	0	14,15,17	1.19	1 (7%)
2	XYP	A	264	2	9,9,10	1.43	2 (22%)	12,12,14	1.18	2 (16%)
3	NAG	A	265	1,3	14,14,15	0.76	1 (7%)	15,19,21	1.44	2 (13%)
3	FUC	A	266	3	10,10,11	0.72	0	14,14,16	1.51	2 (14%)
4	NAG	A	267	1,4	14,14,15	0.63	0	15,19,21	1.35	2 (13%)
4	NAG	A	268	4	14,14,15	0.55	0	15,19,21	1.61	3 (20%)
5	NAG	A	269	1,5	14,14,15	0.54	0	15,19,21	1.53	2 (13%)
5	NAG	A	270	5	14,14,15	0.60	0	15,19,21	1.29	1 (6%)
5	FUC	A	271	5	10,10,11	0.63	0	14,14,16	1.96	3 (21%)

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	258	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	259	2	-	0/6/23/26	0/1/1/1
2	BMA	A	260	2	-	0/2/19/22	0/1/1/1
2	MAN	A	261	2	-	0/2/19/22	0/1/1/1
2	FUC	A	262	2	-	0/0/17/20	0/1/1/1
2	MAN	A	263	2	-	0/2/19/22	0/1/1/1
2	XYP	A	264	2	3/3/3/4	0/0/14/17	0/1/1/1
3	NAG	A	265	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	266	3	-	0/0/17/20	0/1/1/1
4	NAG	A	267	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	268	4	-	0/6/23/26	0/1/1/1
5	NAG	A	269	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	270	5	-	0/6/23/26	0/1/1/1
5	FUC	A	271	5	-	0/0/17/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	264	XYP	O5B-C5B	-2.89	1.37	1.42
2	A	260	BMA	O5-C1	-2.56	1.39	1.43
2	A	259	NAG	O5-C1	-2.54	1.39	1.43
3	A	265	NAG	O5-C1	-2.25	1.40	1.43
2	A	264	XYP	C4B-C3B	2.43	1.55	1.52
2	A	258	NAG	C4-C3	2.44	1.58	1.52
2	A	258	NAG	C8-C7	3.00	1.56	1.50
2	A	258	NAG	C2-N2	3.19	1.52	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	262	FUC	C1-C2-C3	-6.50	101.85	109.54
2	A	258	NAG	O4-C4-C3	-4.07	101.17	110.34
5	A	269	NAG	C4-C3-C2	-3.87	105.21	111.23
2	A	260	BMA	C1-C2-C3	-3.29	105.65	109.54
2	A	260	BMA	C3-C4-C5	-3.28	104.48	110.20
2	A	260	BMA	O3-C3-C4	-3.20	103.14	110.34
2	A	258	NAG	C3-C4-C5	-2.83	105.27	110.20
4	A	267	NAG	O3-C3-C2	-2.82	103.54	109.11
5	A	271	FUC	C1-C2-C3	-2.74	106.31	109.54
2	A	262	FUC	O2-C2-C3	-2.67	104.75	110.12
2	A	258	NAG	O3-C3-C4	-2.59	104.50	110.34
2	A	261	MAN	C2-C3-C4	-2.52	106.76	111.04
2	A	259	NAG	O3-C3-C2	-2.44	104.29	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	268	NAG	O7-C7-C8	-2.28	117.89	122.06
4	A	268	NAG	C3-C2-N2	-2.26	105.15	110.56
2	A	260	BMA	C6-C5-C4	-2.18	107.63	113.02
3	A	265	NAG	C4-C3-C2	-2.09	107.98	111.23
2	A	264	XYP	O3B-C3B-C2B	2.02	113.64	110.00
2	A	258	NAG	O5-C5-C6	2.14	111.98	107.35
4	A	267	NAG	O3-C3-C4	2.16	115.20	110.34
2	A	258	NAG	C3-C2-N2	2.27	116.00	110.56
2	A	264	XYP	O4B-C4B-C5B	2.36	113.93	109.21
2	A	263	MAN	C1-O5-C5	2.48	115.39	112.25
2	A	261	MAN	O3-C3-C4	2.56	116.11	110.34
3	A	266	FUC	O5-C5-C4	2.80	114.38	109.53
3	A	265	NAG	O3-C3-C2	2.96	114.98	109.11
5	A	271	FUC	O5-C5-C4	3.04	114.79	109.53
5	A	270	NAG	C2-N2-C7	3.28	127.26	123.04
5	A	269	NAG	C1-O5-C5	3.52	116.72	112.25
3	A	266	FUC	C1-O5-C5	3.54	117.84	112.38
4	A	268	NAG	C1-O5-C5	4.29	117.70	112.25
5	A	271	FUC	C1-O5-C5	4.91	119.97	112.38

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	264	XYP	C4B
2	A	264	XYP	C2B
2	A	264	XYP	C3B

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

8 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	$\# Z  > 2$
6	SO4	A	901	-	4,4,4	0.57	0	6,6,6	0.62	0
6	SO4	A	902	-	4,4,4	0.35	0	6,6,6	0.56	0
6	SO4	A	903	-	4,4,4	0.75	0	6,6,6	0.56	0
6	SO4	A	904	-	4,4,4	0.21	0	6,6,6	0.25	0
6	SO4	A	905	-	4,4,4	0.08	0	6,6,6	0.29	0
6	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.44	0
6	SO4	A	907	-	4,4,4	0.16	0	6,6,6	0.63	0
7	ACT	A	910	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-

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
6	SO4	A	901	-	-	0/0/0/0	0/0/0/0
6	SO4	A	902	-	-	0/0/0/0	0/0/0/0
6	SO4	A	903	-	-	0/0/0/0	0/0/0/0
6	SO4	A	904	-	-	0/0/0/0	0/0/0/0
6	SO4	A	905	-	-	0/0/0/0	0/0/0/0
6	SO4	A	906	-	-	0/0/0/0	0/0/0/0
6	SO4	A	907	-	-	0/0/0/0	0/0/0/0
7	ACT	A	910	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	910	ACT	CH3-C	2.21	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

### 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	257/258 (99%)	1.25	51 (19%) ⓘ ⓘ	49, 53, 61, 68	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	5.8
1	A	144	LEU	4.9
1	A	257	PRO	4.4
1	A	185	VAL	4.3
1	A	15	VAL	3.9
1	A	184	CYS	3.9
1	A	196	ILE	3.7
1	A	28	LEU	3.5
1	A	167	TRP	3.4
1	A	175	ILE	3.4
1	A	236	ARG	3.4
1	A	238	ILE	3.3
1	A	17	VAL	3.2
1	A	177	VAL	3.2
1	A	98	VAL	3.1
1	A	153	VAL	3.1
1	A	49	ILE	3.0
1	A	198	ILE	3.0
1	A	45	SER	3.0
1	A	69	ILE	3.0
1	A	240	ILE	2.9
1	A	224	LEU	2.8
1	A	111	LEU	2.8
1	A	7	ILE	2.7
1	A	228	VAL	2.7
1	A	225	VAL	2.7
1	A	56	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	ILE	2.6
1	A	213	SER	2.5
1	A	233	VAL	2.5
1	A	55	CYS	2.4
1	A	217	ILE	2.4
1	A	214	ASP	2.4
1	A	68	VAL	2.4
1	A	112	LEU	2.3
1	A	235	LEU	2.3
1	A	119	ALA	2.3
1	A	252	VAL	2.2
1	A	90	ILE	2.2
1	A	209	TRP	2.2
1	A	136	ILE	2.2
1	A	239	ILE	2.2
1	A	8	VAL	2.2
1	A	168	ALA	2.1
1	A	67	ILE	2.1
1	A	188	ASN	2.0
1	A	116	ILE	2.0
1	A	97	LEU	2.0
1	A	110	LEU	2.0
1	A	117	TYR	2.0
1	A	143	CYS	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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	267	14/15	0.68	0.35	2.88	46,56,64,73	0
2	NAG	A	258	14/15	0.93	0.20	0.97	34,38,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	259	14/15	0.95	0.14	-1.77	38,42,47,47	0
2	XYP	A	264	9/10	0.93	0.10	-2.19	38,43,45,46	0
5	NAG	A	270	14/15	0.52	0.68	-	105,107,108,109	0
5	FUC	A	271	10/11	0.36	0.62	-	106,108,109,110	0
2	MAN	A	263	11/12	0.73	0.43	-	64,68,75,78	0
2	FUC	A	262	10/11	0.85	0.26	-	43,46,50,53	0
2	MAN	A	261	11/12	0.56	0.57	-	79,83,85,86	0
5	NAG	A	269	14/15	0.72	0.46	-	85,92,100,101	0
4	NAG	A	268	14/15	0.55	0.53	-	79,81,86,86	0
2	BMA	A	260	11/12	0.91	0.25	-	47,56,63,68	0
3	FUC	A	266	10/11	0.62	0.47	-	86,92,94,94	0
3	NAG	A	265	14/15	0.88	0.33	-	58,65,76,79	0

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACT	A	910	4/4	0.88	0.23	2.56	44,45,45,46	0
6	SO4	A	901	5/5	0.99	0.14	-1.81	37,37,44,48	0
6	SO4	A	906	5/5	0.96	0.43	-	74,77,78,80	0
6	SO4	A	902	5/5	0.95	0.41	-	58,59,65,68	0
6	SO4	A	903	5/5	0.86	0.47	-	53,71,75,76	0
6	SO4	A	907	5/5	0.90	0.26	-	44,49,55,57	5
6	SO4	A	904	5/5	0.88	0.42	-	90,92,92,94	0
6	SO4	A	905	5/5	0.72	0.49	-	111,113,115,115	0

## 6.5 Other polymers

There are no such residues in this entry.