



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:49 PM GMT

PDB ID : 1F7B
Title : CRYSTAL STRUCTURE ANALYSIS OF N-ACETYLNEURAMINATE
LYASE FROM HAEMOPHILUS INFLUENZAE: CRYSTAL FORM II IN
COMPLEX WITH 4-OXO-SIALIC ACID
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Deposited on : 2000-06-26
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

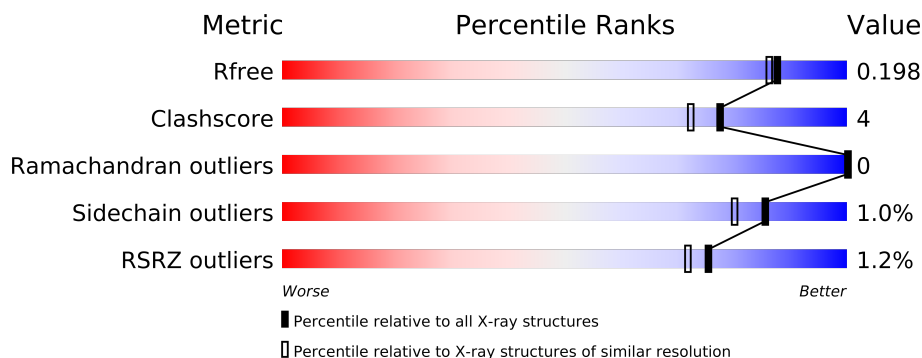
The following versions of software and data (see [references](#)) were used in the production of this report:

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))
R_{free}	66092	3513 (1.80-1.80)
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 ≥ 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	293	
1	C	293	

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	NAU	A	901	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5463 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 N-ACETYL-NEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	13	0
			2345	1515	376	443	11			
1	C	285	Total	C	N	O	S	0	14	0
			2284	1471	368	432	13			

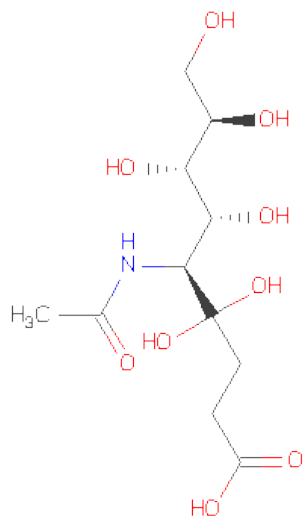
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	SER	ASN	SEE REMARK 999	UNP P44539
A	229	LYS	ALA	SEE REMARK 999	UNP P44539
A	278	ALA	GLU	SEE REMARK 999	UNP P44539
A	281	VAL	LEU	SEE REMARK 999	UNP P44539
C	131	SER	ASN	SEE REMARK 999	UNP P44539
C	229	LYS	ALA	SEE REMARK 999	UNP P44539
C	278	ALA	GLU	SEE REMARK 999	UNP P44539
C	281	VAL	LEU	SEE REMARK 999	UNP P44539

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

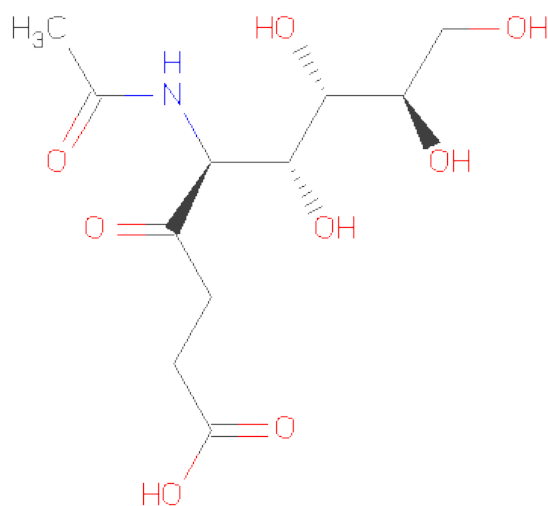
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 4,4,6,7,8,9-HEXAHYDROXY-5-METHYLCARBOXAMIDONONANOIC ACID (three-letter code: NAU) (formula: C₁₁H₂₁NO₉).



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

- Molecule 4 is 6,7,8,9-TETRAHYDROXY-5-METHYLCARBOXAMIDO-4-OXONONANOIC ACID (three-letter code: NAV) (formula: C₁₁H₁₉NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 5 is water.

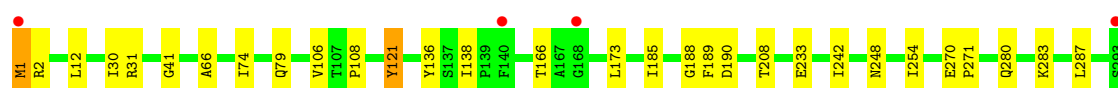
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	411	Total 411	O 411	0	0
5	C	381	Total 381	O 381	0	0

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.

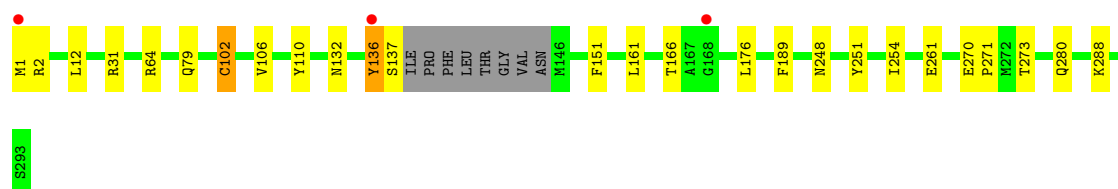
● Molecule 1: N-ACETYL-NEURAMINATE LYASE

Chain A: 



● Molecule 1: N-ACETYL-NEURAMINATE LYASE

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	65.62Å 117.99Å 80.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 14.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (15.00-1.80) 78.8 (14.95-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.210 0.163 , 0.198	Depositor DCC
R_{free} test set	2761 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54876 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5463	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: CL, NAV, NAU

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	0.46	0/2444	1.03	9/3287 (0.3%)
1	C	0.47	0/2387	1.09	12/3204 (0.4%)
All	All	0.47	0/4831	1.06	21/6491 (0.3%)

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	C	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	PRO	N-CA-CB	8.36	113.33	103.30
1	C	64	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	C	270[A]	GLU	CA-C-O	-8.26	102.75	120.10
1	C	270[B]	GLU	CA-C-O	-8.26	102.75	120.10
1	A	271	PRO	CA-N-CD	-7.68	100.75	111.50
1	A	270[A]	GLU	CA-C-O	-7.41	104.55	120.10
1	A	270[B]	GLU	CA-C-O	-7.41	104.55	120.10
1	A	2	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	C	271	PRO	N-CA-CB	7.28	112.03	103.30
1	C	271	PRO	CA-N-CD	-7.16	101.47	111.50
1	C	102[A]	CYS	CA-CB-SG	6.69	126.05	114.00
1	C	102[B]	CYS	CA-CB-SG	6.69	126.05	114.00
1	C	110	TYR	N-CA-CB	6.27	121.88	110.60
1	C	2	ARG	NE-CZ-NH2	-5.63	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	2	ARG	CD-NE-CZ	5.44	131.22	123.60
1	C	31	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	251	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	C	251	TYR	CB-CG-CD2	5.12	124.07	121.00
1	A	121	TYR	CA-CB-CG	5.06	123.01	113.40
1	A	190	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	136[B]	TYR	Mainchain

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	2345	0	2380	15	0
1	C	2284	0	2317	18	0
2	C	1	0	0	0	0
3	A	21	0	18	3	0
4	C	20	0	16	0	0
5	A	411	0	0	2	0
5	C	381	0	0	1	0
All	All	5463	0	4731	35	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 4.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1[A]:MET:CE	1:C:132:ASN:HD22	1.56	1.19
1:C:1[A]:MET:HE3	1:C:132:ASN:HD22	1.14	1.11
1:C:1[A]:MET:HE3	1:C:132:ASN:ND2	1.93	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1[A]:MET:CE	1:C:132:ASN:ND2	2.41	0.77
1:A:106[B]:VAL:HG12	1:A:136:TYR:CD2	2.26	0.71
1:C:261[A]:GLU:OE2	1:C:288:LYS:NZ	2.27	0.68
1:C:1[A]:MET:HE2	1:C:132:ASN:HD22	1.58	0.66
1:C:248:ASN:HD21	1:C:280:GLN:HA	1.68	0.58
1:A:248:ASN:HD21	1:A:280:GLN:HA	1.69	0.57
1:C:261[A]:GLU:OE2	1:C:288:LYS:HE2	2.06	0.56
3:A:901:NAU:HC7	3:A:901:NAU:C10	2.36	0.56
1:A:283[B]:LYS:HE2	1:A:287:LEU:HG	1.89	0.55
1:A:1:MET:HB2	5:A:1227:HOH:O	2.07	0.53
1:A:138:ILE:HA	1:A:166:THR:OG1	2.08	0.53
1:C:261[A]:GLU:OE2	1:C:288:LYS:CE	2.57	0.53
1:A:138:ILE:HA	1:A:166:THR:HG1	1.75	0.51
1:A:233:GLU:HG3	5:A:1099:HOH:O	2.13	0.48
1:C:102[A]:CYS:SG	1:C:161:LEU:CD1	3.01	0.48
1:C:151:PHE:CD2	1:C:176[A]:LEU:HD21	2.49	0.48
1:C:106:VAL:HG12	1:C:136[A]:TYR:CZ	2.49	0.47
1:C:106:VAL:HA	1:C:136[A]:TYR:CD1	2.49	0.47
1:C:102[A]:CYS:SG	1:C:161:LEU:HD11	2.54	0.47
1:C:12:LEU:HD11	1:C:254:ILE:HG21	1.99	0.45
1:C:136[B]:TYR:O	1:C:137:SER:C	2.56	0.44
3:A:901:NAU:C7	3:A:901:NAU:C10	2.95	0.44
1:A:41:GLY:HA2	1:A:74:ILE:HB	2.00	0.44
1:A:208:THR:HG21	1:A:242:ILE:HG12	2.00	0.44
1:A:108:PRO:HD3	1:A:121:TYR:CE1	2.53	0.43
1:C:136[B]:TYR:HE1	1:C:166:THR:HG21	1.83	0.43
1:A:30:ILE:HD13	1:A:66:ALA:HA	2.00	0.43
1:A:188:GLY:O	3:A:901:NAU:HC6	2.19	0.42
1:A:12:LEU:HD11	1:A:254:ILE:HG21	2.02	0.42
1:C:273:THR:HG21	5:C:1234:HOH:O	2.19	0.42
1:A:173:LEU:HD12	1:A:185:ILE:HD13	2.02	0.41
1:A:248:ASN:HB2	1:A:283[A]:LYS:HD3	2.03	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	304/293 (104%)	298 (98%)	6 (2%)	0	100	100
1	C	294/293 (100%)	289 (98%)	5 (2%)	0	100	100
All	All	598/586 (102%)	587 (98%)	11 (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	255/242 (105%)	251 (98%)	4 (2%)	75	63
1	C	249/242 (103%)	247 (99%)	2 (1%)	89	85
All	All	504/484 (104%)	498 (99%)	6 (1%)	85	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	79	GLN
1	A	189[A]	PHE
1	A	189[B]	PHE
1	C	79	GLN
1	C	189	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	ASN
1	C	51	ASN
1	C	132	ASN
1	C	248	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	NAU	A	901	1	20,20,20	2.10	6 (30%)	28,28,28	1.83	7 (25%)
4	NAV	C	902	1	19,19,19	1.35	3 (15%)	25,25,25	2.98	3 (12%)

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	NAU	A	901	1	-	1/28/30/30	0/0/0/0
4	NAV	C	902	1	-	0/27/27/27	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAU	O4B-C4	5.28	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAU	C3-C4	3.95	1.58	1.52
3	A	901	NAU	O4A-C4	2.83	1.44	1.40
4	C	902	NAV	C2-C1	-2.79	1.43	1.50
3	A	901	NAU	C2-C1	-2.63	1.43	1.50
3	A	901	NAU	C5-N2	2.56	1.49	1.45
3	A	901	NAU	C6-C5	2.53	1.57	1.53
4	C	902	NAV	O10-C10	2.13	1.27	1.23
4	C	902	NAV	O4-C4	2.12	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	902	NAV	C2-C3-C4	13.46	137.71	113.81
3	A	901	NAU	C4-C5-N2	-4.31	104.50	110.72
3	A	901	NAU	C5-N2-C10	4.16	130.20	123.74
3	A	901	NAU	C3-C4-C5	3.61	119.17	111.01
3	A	901	NAU	O4A-C4-C5	2.81	113.89	107.81
3	A	901	NAU	O4A-C4-C3	-2.60	103.15	109.90
4	C	902	NAV	O10-C10-C11	-2.26	117.63	122.04
4	C	902	NAV	C7-C6-C5	-2.22	109.99	114.25
3	A	901	NAU	C3-C2-C1	2.19	117.49	112.70
3	A	901	NAU	O1A-C1-C2	-2.04	116.01	123.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	NAU	O4B-C4-C5-C6

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, 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	293/293 (100%)	-0.62	4 (1%) 72 68	10, 15, 25, 41	0
1	C	285/293 (97%)	-0.64	3 (1%) 77 73	11, 15, 25, 37	0
All	All	578/586 (98%)	-0.63	7 (1%) 75 72	10, 15, 25, 41	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
1	C	136[A]	TYR	4.7
1	A	168	GLY	3.7
1	C	1[A]	MET	3.2
1	A	140	PHE	3.0
1	A	293	SER	2.5
1	C	168	GLY	2.5

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAU	A	901	21/21	0.22	3.21	21,26,35,37	0
4	NAV	C	902	20/20	0.18	1.24	24,28,37,37	0
2	CL	C	900	1/1	0.03	-2.80	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.