Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 06:17 PM GMT

PDB ID : 4DGR
Title : Influenza Subtype 9 Neuraminidase Benzoic Acid Inhibitor Complex
Authors : Venkatramani, L.; Johnson, E.; Kolavi, G.; Air, G.M.; Brouillette, W.; Mooers, B.H.M.
Deposited on : 2012-01-26
Resolution : 1.55 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.55 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	Percentile Ranks	Value
Rfree		0.149
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		0.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
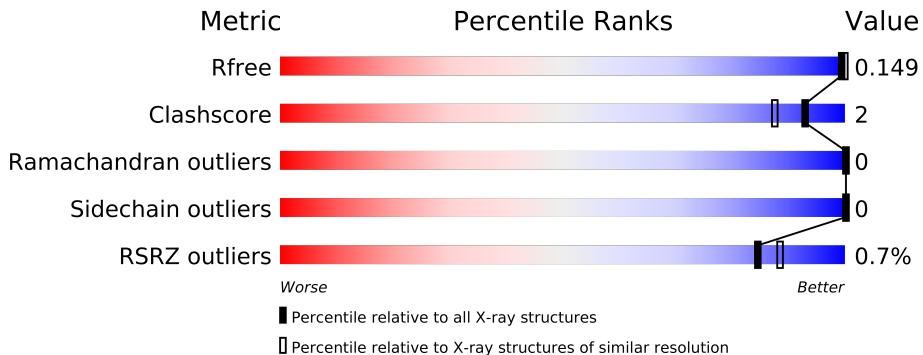
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1117 (1.58-1.54)
Clashscore	79885	1249 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

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	389	

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 7013 atoms, of which 3154 are hydrogens 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 Neuraminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	389	Total	C	H	N	O	S	15	8	0
			6088	1950	2967	548	599	24			

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	9	Total	C	H	N	O	0	0
			193	58	88	2	45		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	3	Total	C	H	N	O	0	0
			72	22	33	2	15		

- Molecule 5 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).
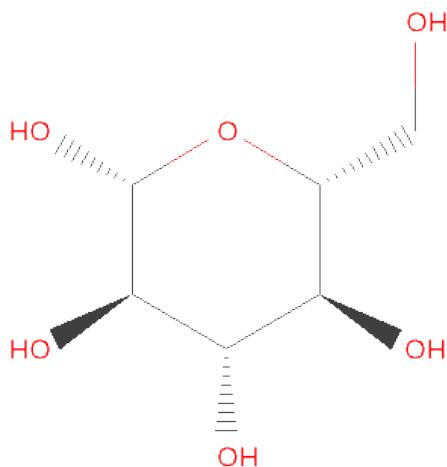
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 12	C 6	O 6	0	0
5	A	1	Total 12	C 6	O 6	0	0
5	A	1	Total 12	C 6	O 6	0	0

- Molecule 6 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).
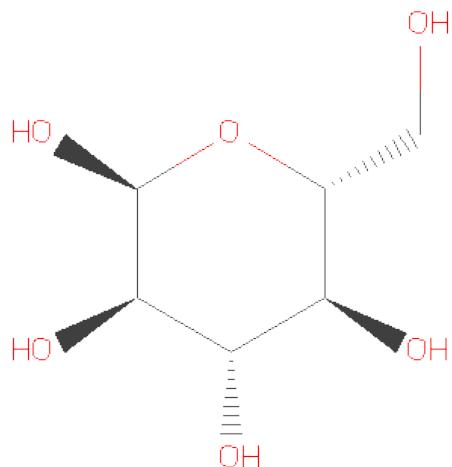
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 24	C 6	H 12	O 6	0	0

- Molecule 7 is 4-[2,2-BIS(HYDROXYMETHYL)-5-OXOPYRROLIDIN-1-YL]-3-[(DIPROP YLAMINO)METHYL]BENZOICACID (three-letter code: 3LV) (formula: $C_{20}H_{30}N_2O_5$).
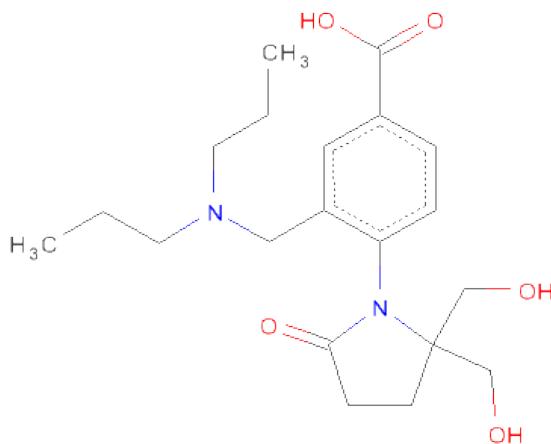
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	A	1	56	20	29	2	5	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
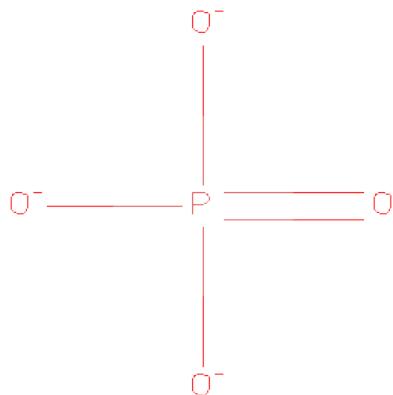
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
8	A	1	5	4	1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total Ca 2 2		0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total K 1 1		0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	448	Total O 483 483		0	35

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: Neuraminidase

Chain A:
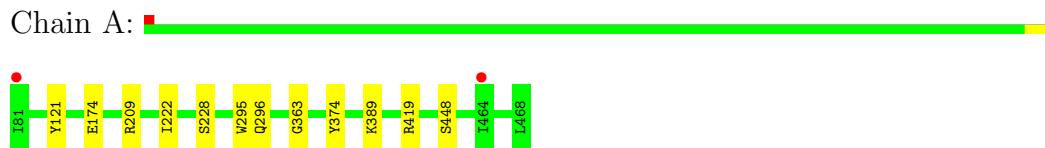
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	180.97Å 180.97Å 180.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.61 – 1.55 28.61 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.61-1.55) 99.7 (28.61-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1041)	Depositor
R, R_{free}	0.121 , 0.152 0.119 , 0.149	Depositor DCC
R_{free} test set	3682 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	0 of 72355 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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: BGC, NAG, PO4, GLC, BMA, K, CA, 3LV, MAN

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	0.43	0/3222	0.64	0/4385

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3121	2967	0	8	0
2	A	105	88	0	1	0
3	A	28	25	0	0	0
4	A	39	33	0	0	0
5	A	36	0	0	0	0
6	A	12	12	0	0	0
7	A	27	29	0	3	0
8	A	5	0	0	0	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	A	483	0	0	3	0
All	All	3859	3154	0	11	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 (11) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:419[A]:ARG:HD2	11:A:875:HOH:O	1.77	0.84
7:A:488:3LV:H12	7:A:488:3LV:C3	2.41	0.50
1:A:419[A]:ARG:HD3	1:A:448:SER:O	2.13	0.48
1:A:121:TYR:CG	1:A:228:SER:HA	2.48	0.48
1:A:222:ILE:HD12	7:A:488:3LV:H11A	1.97	0.46
7:A:488:3LV:H11A	11:A:945:HOH:O	2.18	0.42
1:A:174:GLU:OE1	1:A:209:ARG:NH1	2.50	0.42
1:A:295:TRP:CG	1:A:296:GLN:HG3	2.54	0.42
1:A:363:GLY:HA3	1:A:374:TYR:HH	1.85	0.42
1:A:389:LYS:NZ	11:A:785:HOH:O	2.54	0.41
2:A:473:MAN:H4	2:A:473:MAN:HO6	1.85	0.41

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	395/389 (102%)	378 (96%)	17 (4%)	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	349/342 (102%)	349 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	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 ⓘ

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	469	1,2	12,14,15	0.64	0	15,19,21	1.11	2 (13%)
2	NAG	A	470	2	12,14,15	0.62	0	15,19,21	0.89	0
2	BMA	A	471	2	10,11,12	0.40	0	11,15,17	0.90	0
2	MAN	A	472	2	10,11,12	0.62	0	11,15,17	1.86	3 (27%)
2	MAN	A	473	2	10,11,12	0.83	0	11,15,17	1.06	1 (9%)
2	MAN	A	474	2	10,11,12	0.70	0	11,15,17	0.89	1 (9%)
2	MAN	A	475	2	10,11,12	0.93	1 (10%)	11,15,17	0.90	0
2	MAN	A	476	2	10,11,12	0.80	1 (10%)	11,15,17	0.66	0
2	MAN	A	477	2	10,11,12	0.76	0	11,15,17	0.79	0
3	NAG	A	478	1,3	12,14,15	0.81	1 (8%)	15,19,21	0.71	0
3	NAG	A	479	3	12,14,15	0.58	0	15,19,21	1.16	1 (6%)
4	NAG	A	481	1,4	12,14,15	0.87	1 (8%)	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	482	4	12,14,15	0.64	0	15,19,21	0.86	0
4	BMA	A	483	4	10,11,12	0.50	0	11,15,17	0.94	1 (9%)

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	469	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	470	2	-	0/6/23/26	0/1/1/1
2	BMA	A	471	2	-	0/2/19/22	0/1/1/1
2	MAN	A	472	2	-	0/2/19/22	0/1/1/1
2	MAN	A	473	2	-	0/2/19/22	0/1/1/1
2	MAN	A	474	2	-	0/2/19/22	0/1/1/1
2	MAN	A	475	2	-	0/2/19/22	0/1/1/1
2	MAN	A	476	2	-	0/2/19/22	0/1/1/1
2	MAN	A	477	2	-	0/2/19/22	0/1/1/1
3	NAG	A	478	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	479	3	-	0/6/23/26	0/1/1/1
4	NAG	A	481	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	482	4	-	0/6/23/26	0/1/1/1
4	BMA	A	483	4	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	475	MAN	O5-C5	-2.51	1.40	1.45
3	A	478	NAG	O5-C5	-2.32	1.41	1.45
4	A	481	NAG	O5-C5	-2.19	1.41	1.45
2	A	476	MAN	O5-C5	-2.02	1.41	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	472	MAN	O5-C5-C6	4.15	111.33	106.98
3	A	479	NAG	O5-C5-C6	3.20	110.34	106.98
2	A	469	NAG	O5-C5-C6	2.95	110.08	106.98
2	A	473	MAN	O5-C5-C6	2.79	109.91	106.98
2	A	472	MAN	C3-C4-C5	-2.67	105.43	110.20
2	A	469	NAG	O5-C5-C4	-2.39	107.62	110.65
2	A	472	MAN	C4-C3-C2	-2.21	107.53	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	483	BMA	O5-C5-C6	2.19	109.28	106.98
2	A	474	MAN	O5-C5-C6	2.19	109.28	106.98
4	A	481	NAG	C2-N2-C7	-2.18	119.42	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	#$|Z| > 2$
5	BGC	A	484	-	12,12,12	1.58	3 (25%)	17,17,17	0.98	1 (5%)
6	GLC	A	485	-	12,12,12	0.56	0	17,17,17	1.13	1 (5%)
5	BGC	A	486	-	12,12,12	1.71	4 (33%)	17,17,17	0.82	0
5	BGC	A	487	-	12,12,12	1.39	3 (25%)	17,17,17	0.72	0
7	3LV	A	488	-	28,28,28	1.56	4 (14%)	39,39,39	2.88	11 (28%)
8	PO4	A	489	-	4,4,4	0.34	0	6,6,6	0.32	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
5	BGC	A	484	-	-	0/2/22/22	0/1/1/1
6	GLC	A	485	-	-	0/2/22/22	0/1/1/1
5	BGC	A	486	-	-	0/2/22/22	0/1/1/1
5	BGC	A	487	-	-	0/2/22/22	0/1/1/1
7	3LV	A	488	-	-	0/24/40/40	0/2/2/2

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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PO4	A	489	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	488	3LV	C5-N5	4.33	1.48	1.43
7	A	488	3LV	C17-C18	-3.86	1.50	1.54
7	A	488	3LV	C15-N5	3.52	1.41	1.37
5	A	484	BGC	O3-C3	-2.73	1.36	1.43
5	A	486	BGC	O5-C5	-2.63	1.37	1.44
7	A	488	3LV	C20-C18	-2.57	1.49	1.53
5	A	486	BGC	O5-C1	-2.56	1.38	1.43
5	A	487	BGC	O5-C5	-2.35	1.38	1.44
5	A	487	BGC	O5-C1	-2.33	1.38	1.43
5	A	486	BGC	O3-C3	-2.32	1.37	1.43
5	A	484	BGC	O5-C1	-2.21	1.38	1.43
5	A	487	BGC	O2-C2	-2.17	1.37	1.43
5	A	484	BGC	O5-C5	-2.14	1.39	1.44
5	A	486	BGC	O4-C4	-2.11	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	488	3LV	C5-N5-C15	14.96	136.29	122.23
7	A	488	3LV	C16-C15-N5	3.83	111.04	107.75
7	A	488	3LV	O15-C15-N5	-3.47	122.39	124.94
7	A	488	3LV	C18-N5-C15	-3.23	107.56	112.53
7	A	488	3LV	C18-N5-C5	-2.94	116.14	122.38
5	A	484	BGC	C1-C2-C3	-2.93	105.89	110.53
7	A	488	3LV	C7-C2-C3	2.47	122.35	119.24
7	A	488	3LV	O20-C20-C18	2.39	117.23	110.96
7	A	488	3LV	C4-C5-N5	-2.37	116.94	120.78
6	A	485	GLC	C6-C5-C4	-2.34	107.34	113.00
7	A	488	3LV	C17-C18-N5	2.09	104.95	102.19
7	A	488	3LV	C4-C8-N8	2.08	116.58	112.79
7	A	488	3LV	C6-C5-C4	2.06	122.81	119.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	389/389 (100%)	-0.42	2 (0%)	88	91	8, 12, 20, 38	5 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ILE	7.5
1	A	464	ILE	3.3

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 ⓘ

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(Å^2)	Q<0.9
2	MAN	A	477	11/12	0.25	-	39,46,54,55	0
2	NAG	A	469	14/15	0.09	-	13,17,27,27	0
4	BMA	A	483	11/12	0.47	-	64,68,82,82	0
3	NAG	A	478	14/15	0.12	-	17,23,28,31	0
4	NAG	A	481	14/15	0.18	-	27,38,44,45	0
2	MAN	A	474	11/12	0.03	-	15,17,19,21	0
3	NAG	A	479	14/15	0.26	-	31,40,47,49	0
2	MAN	A	475	11/12	0.13	-	22,29,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	A	472	11/12	0.05	-	15,18,25,29	0
2	MAN	A	476	11/12	0.23	-	32,37,44,46	0
2	BMA	A	471	11/12	0.05	-	14,17,21,21	0
2	MAN	A	473	11/12	0.04	-	17,19,23,26	0
2	NAG	A	470	14/15	0.08	-	13,17,24,29	0
4	NAG	A	482	14/15	0.29	-	49,58,68,70	0

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. 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(Å^2)	Q<0.9
8	PO4	A	489	5/5	0.07	-	23,23,24,25	5
5	BGC	A	484	12/12	0.24	-	18,26,28,29	12
9	CA	A	491	1/1	0.05	-	19,19,19,19	1
9	CA	A	490	1/1	0.02	-	15,15,15,15	0
5	BGC	A	487	12/12	0.26	-	11,21,23,24	12
6	GLC	A	485	12/12	0.12	-	19,23,30,33	24
7	3LV	A	488	27/27	0.15	-	8,13,34,34	56
10	K	A	492	1/1	0.03	-	33,33,33,33	1
5	BGC	A	486	12/12	0.21	-	29,30,34,36	12

6.5 Other polymers (i)

There are no such residues in this entry.