



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 PM GMT

PDB ID : 4UOA
Title : Structure of the A_Canine_Colorado_17864_06 H3 haemagglutinin Met29Ile mutant
Authors : Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogrodowicz, R.W.; Martin, S.R.; Walker, P.A.; Xiong, X.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-05-31
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

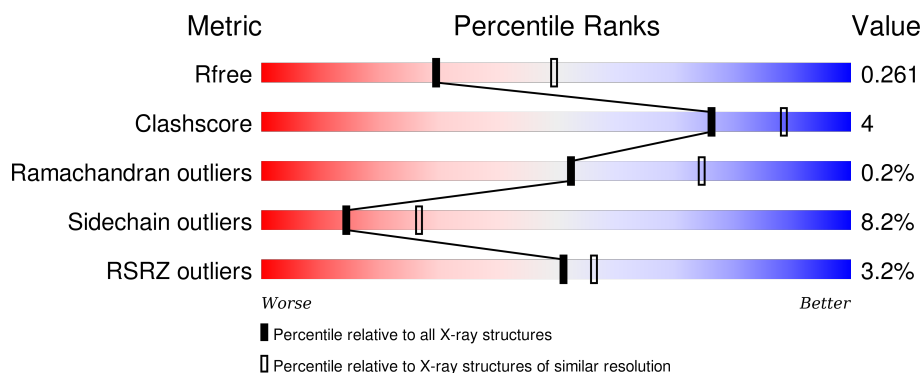
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	327	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	B	175	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>...</div> </div>

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
3	NAG	A	602	X	-	-	-
5	NAG	A	631	X	-	-	-
7	SO4	A	1327	-	-	X	-
7	SO4	A	1328	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4184 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2511	1566	445	485	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	ILE	DELETION	UNP E0UVR5
A	29	ILE	MET	ENGINEERED MUTATION	UNP E0UVR5

- Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1393	869	241	277	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	SER	-	EXPRESSION TAG	UNP E0UVR5
B	174	GLY	-	EXPRESSION TAG	UNP E0UVR5
B	175	ARG	-	EXPRESSION TAG	UNP E0UVR5
B	131	GLU	ASP	CONFLICT	UNP E0UVR5
B	161	VAL	ILE	CONFLICT	UNP E0UVR5

- 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
			28	16	2	10		

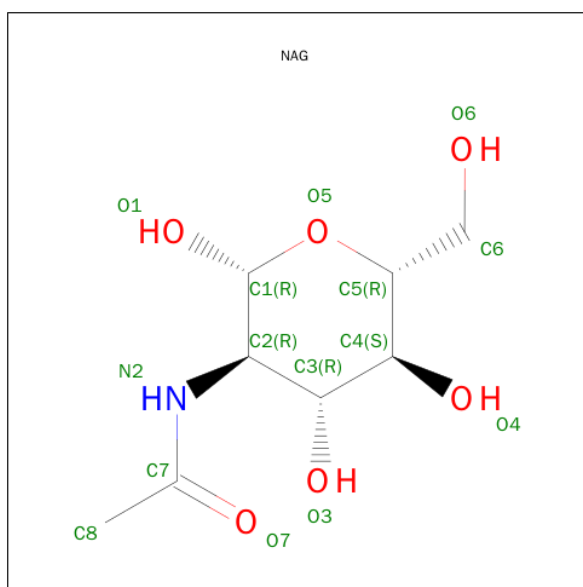
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

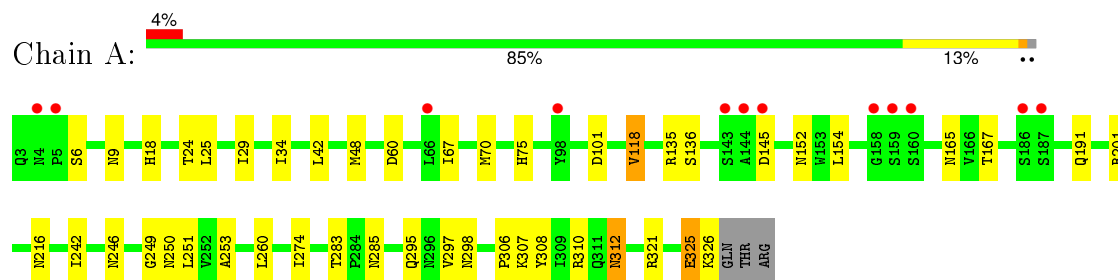
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	13	Total	O	0	0
			13	13		

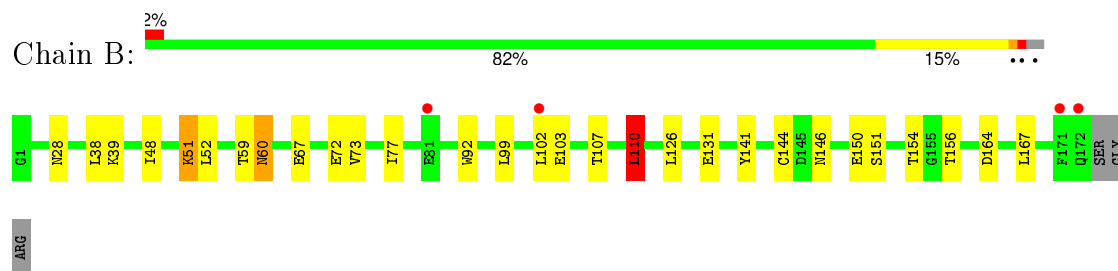
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: HA1



• Molecule 2: HA2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	99.68 Å 99.68 Å 397.21 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	132.40 – 2.50 46.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (132.40-2.50) 99.3 (46.64-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.238 , 0.265 0.238 , 0.261	Depositor DCC
R_{free} test set	1341 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26728 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4184	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.375 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: SO4, BMA, NAG, 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	0.34	0/2563	0.56	0/3477
2	B	0.42	0/1418	0.60	1/1909 (0.1%)
All	All	0.37	0/3981	0.58	1/5386 (0.0%)

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
3	A	1	0
5	A	1	0
All	All	2	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	110	LEU	CA-CB-CG	7.06	131.54	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	NAG	C1
5	A	631	NAG	C1

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	2511	0	2462	20	0
2	B	1393	0	1306	13	0
3	A	28	0	25	0	0
4	A	78	0	68	0	0
5	A	100	0	86	1	0
6	A	14	0	13	0	0
7	A	15	0	0	0	2
7	B	5	0	0	0	0
8	A	27	0	0	0	0
8	B	13	0	0	0	0
All	All	4184	0	3960	31	2

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 4.

All (31) 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:295:GLN:HB2	1:A:306:PRO:HB2	1.66	0.78
2:B:107:THR:HA	2:B:110:LEU:HD13	1.69	0.75
1:A:295:GLN:HE22	1:A:298:ASN:H	1.41	0.69
1:A:283:THR:HG22	1:A:285:ASN:H	1.59	0.67
1:A:295:GLN:HE21	1:A:297:VAL:H	1.51	0.58
2:B:60:ASN:N	2:B:60:ASN:OD1	2.36	0.57
1:A:312:ASN:H	1:A:312:ASN:HD22	1.53	0.57
1:A:167:THR:HB	1:A:242:ILE:HD11	1.87	0.56
2:B:28:ASN:HD21	2:B:146:ASN:HD22	1.54	0.54
1:A:34:ILE:HD11	1:A:321:ARG:HD2	1.89	0.54
2:B:99:LEU:O	2:B:103:GLU:HB2	2.08	0.54
1:A:295:GLN:NE2	1:A:298:ASN:H	2.08	0.52
2:B:51:LYS:HE3	2:B:103:GLU:HG3	1.89	0.52
1:A:70:MET:HA	1:A:118:VAL:CG2	2.39	0.51
2:B:151:SER:HA	2:B:154:THR:HG22	1.93	0.50
2:B:156:THR:O	2:B:156:THR:HG22	2.10	0.49
1:A:201:ARG:NH2	1:A:246:ASN:HD21	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HE2	2:B:92:TRP:CH2	2.48	0.48
2:B:28:ASN:HD21	2:B:146:ASN:ND2	2.12	0.48
2:B:48:ILE:HA	2:B:51:LYS:HD3	1.98	0.46
1:A:136:SER:O	1:A:145:ASP:HB2	2.17	0.44
1:A:295:GLN:O	1:A:308:TYR:HA	2.17	0.44
1:A:249:GLY:C	1:A:250:ASN:HD22	2.22	0.43
1:A:29:ILE:HD11	2:B:102:LEU:HB3	2.00	0.43
1:A:152:ASN:N	1:A:253:ALA:O	2.51	0.42
2:B:131:GLU:OE1	2:B:141:TYR:OH	2.33	0.42
1:A:325:GLU:H	1:A:325:GLU:CD	2.23	0.42
1:A:60:ASP:HB2	1:A:274:ILE:HD12	2.02	0.41
1:A:191:GLN:HE22	1:A:250:ASN:HD21	1.66	0.41
1:A:285:ASN:OD1	5:A:641:NAG:H2	2.21	0.41
2:B:28:ASN:HB2	2:B:144:CYS:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1327:SO4:O2	7:A:1327:SO4:O2[16_544]	0.85	1.35
7:A:1327:SO4:S	7:A:1327:SO4:O2[16_544]	2.12	0.08

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	322/327 (98%)	307 (95%)	14 (4%)	1 (0%)	46	68
2	B	170/175 (97%)	161 (95%)	9 (5%)	0	100	100
All	All	492/502 (98%)	468 (95%)	23 (5%)	1 (0%)	52	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER

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	285/288 (99%)	265 (93%)	20 (7%)	19	34
2	B	144/148 (97%)	129 (90%)	15 (10%)	9	16
All	All	429/436 (98%)	394 (92%)	35 (8%)	14	27

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	18	HIS
1	A	24	THR
1	A	25	LEU
1	A	42	LEU
1	A	48	MET
1	A	67	ILE
1	A	75	HIS
1	A	101	ASP
1	A	118	VAL
1	A	135	ARG
1	A	154	LEU
1	A	165	ASN
1	A	216	ASN
1	A	251	LEU
1	A	260	LEU
1	A	310	ARG
1	A	312	ASN
1	A	325	GLU
1	A	326	LYS
2	B	38	LEU
2	B	39	LYS
2	B	51	LYS

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Mol	Chain	Res	Type
2	B	52	LEU
2	B	59	THR
2	B	60	ASN
2	B	67	GLU
2	B	72	GLU
2	B	73	VAL
2	B	77	ILE
2	B	110	LEU
2	B	126	LEU
2	B	150	GLU
2	B	164	ASP
2	B	167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	183	HIS
1	A	246	ASN
1	A	250	ASN
1	A	295	GLN
1	A	312	ASN
2	B	53	ASN
2	B	65	GLN
2	B	78	GLN
2	B	95	ASN
2	B	146	ASN

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](#)

16 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	$\# Z > 2$
3	NAG	A	601	1,3	14,14,15	0.57	0	15,19,21	1.51	2 (13%)
3	NAG	A	602	3	14,14,15	0.43	0	15,19,21	0.98	1 (6%)
4	NAG	A	611	1,4	14,14,15	0.64	0	15,19,21	0.61	0
4	NAG	A	612	4	14,14,15	0.72	0	15,19,21	1.36	1 (6%)
4	BMA	A	613	4	11,11,12	0.40	0	14,15,17	1.74	3 (21%)
4	NAG	A	621	1,4	14,14,15	0.49	0	15,19,21	1.32	2 (13%)
4	NAG	A	622	4	14,14,15	0.52	0	15,19,21	0.98	0
4	BMA	A	623	4	11,11,12	0.44	0	14,15,17	1.39	2 (14%)
5	NAG	A	631	1,5	14,14,15	0.48	0	15,19,21	1.07	2 (13%)
5	NAG	A	632	5	14,14,15	0.49	0	15,19,21	0.96	0
5	BMA	A	633	5	11,11,12	0.38	0	14,15,17	0.84	0
5	MAN	A	637	5	11,11,12	0.53	0	14,15,17	1.03	1 (7%)
5	NAG	A	641	1,5	14,14,15	0.68	0	15,19,21	1.27	1 (6%)
5	NAG	A	642	5	14,14,15	0.55	0	15,19,21	1.43	2 (13%)
5	BMA	A	643	5	11,11,12	0.41	0	14,15,17	1.03	1 (7%)
5	MAN	A	647	5	11,11,12	0.64	0	14,15,17	1.61	2 (14%)

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	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	611	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	612	4	-	0/6/23/26	0/1/1/1
4	BMA	A	613	4	-	0/2/19/22	0/1/1/1
4	NAG	A	621	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	622	4	-	0/6/23/26	0/1/1/1
4	BMA	A	623	4	-	0/2/19/22	0/1/1/1
5	NAG	A	631	1,5	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	632	5	-	0/6/23/26	0/1/1/1
5	BMA	A	633	5	-	0/2/19/22	0/1/1/1
5	MAN	A	637	5	-	0/2/19/22	0/1/1/1
5	NAG	A	641	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	642	5	-	0/6/23/26	0/1/1/1
5	BMA	A	643	5	-	0/2/19/22	0/1/1/1
5	MAN	A	647	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	613	BMA	O5-C1-C2	-3.89	104.55	110.86
5	A	641	NAG	O4-C4-C3	-2.88	103.85	110.34
4	A	613	BMA	C1-C2-C3	-2.83	106.20	109.54
5	A	631	NAG	O7-C7-C8	-2.15	118.11	122.06
4	A	623	BMA	C1-C2-C3	2.10	112.02	109.54
5	A	637	MAN	C1-O5-C5	2.35	115.23	112.25
5	A	631	NAG	C8-C7-N2	2.41	120.72	116.11
5	A	647	MAN	C1-O5-C5	2.48	115.40	112.25
5	A	643	BMA	C3-C4-C5	2.69	114.88	110.20
5	A	642	NAG	C3-C4-C5	2.79	115.05	110.20
3	A	602	NAG	C1-O5-C5	2.88	115.90	112.25
3	A	601	NAG	C8-C7-N2	2.94	121.73	116.11
4	A	621	NAG	C4-C3-C2	2.98	115.87	111.23
4	A	621	NAG	C3-C4-C5	3.11	115.63	110.20
3	A	601	NAG	C2-N2-C7	3.49	127.53	123.04
5	A	642	NAG	C4-C3-C2	3.53	116.72	111.23
4	A	612	NAG	C4-C3-C2	3.55	116.74	111.23
4	A	613	BMA	C3-C4-C5	3.73	116.70	110.20
4	A	623	BMA	C1-O5-C5	4.65	118.15	112.25
5	A	647	MAN	C1-C2-C3	4.84	115.26	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	631	NAG	C1
3	A	602	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	641	NAG	1	0

5.6 Ligand geometry

5 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$
7	SO4	A	1327	-	4,4,4	0.38	0	6,6,6	0.13	0
7	SO4	A	1328	-	4,4,4	0.41	0	6,6,6	0.20	0
7	SO4	A	1329	-	4,4,4	0.44	0	6,6,6	0.14	0
6	NAG	A	651	1	14,14,15	0.56	0	15,19,21	1.79	4 (26%)
7	SO4	B	1173	-	4,4,4	0.54	0	6,6,6	0.38	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
7	SO4	A	1327	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1328	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1329	-	-	0/0/0/0	0/0/0/0
6	NAG	A	651	1	-	0/6/23/26	0/1/1/1
7	SO4	B	1173	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	651	NAG	O7-C7-C8	-2.18	118.05	122.06
6	A	651	NAG	O7-C7-N2	2.15	126.24	121.86
6	A	651	NAG	C3-C2-N2	3.26	118.37	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	651	NAG	C2-N2-C7	4.50	128.82	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1327	SO4	0	2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	324/327 (99%)	0.17	12 (3%) 45 50	35, 63, 85, 102	0
2	B	172/175 (98%)	0.33	4 (2%) 64 67	31, 48, 84, 108	0
All	All	496/502 (98%)	0.22	16 (3%) 51 56	31, 59, 85, 108	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	ALA	4.4
2	B	171	PHE	3.2
1	A	143	SER	2.9
1	A	158	GLY	2.9
1	A	160	SER	2.8
2	B	172	GLN	2.8
1	A	98	TYR	2.7
1	A	4	ASN	2.5
1	A	159	SER	2.4
1	A	5	PRO	2.4
2	B	81	GLU	2.4
1	A	66	LEU	2.2
2	B	102	LEU	2.2
1	A	186	SER	2.1
1	A	187	SER	2.1
1	A	145	ASP	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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	632	14/15	0.93	0.21	1.59	84,91,96,101	0
5	NAG	A	642	14/15	0.82	0.30	-	106,109,115,121	0
5	NAG	A	641	14/15	0.83	0.24	-	81,89,93,99	0
5	NAG	A	631	14/15	0.91	0.13	-	78,82,84,84	0
4	NAG	A	621	14/15	0.89	0.29	-	66,72,81,92	0
5	BMA	A	633	11/12	0.80	0.18	-	106,112,115,116	0
5	BMA	A	643	11/12	0.59	0.45	-	128,133,135,135	0
4	BMA	A	613	11/12	0.69	0.34	-	130,134,136,136	0
4	BMA	A	623	11/12	0.47	0.54	-	117,119,121,121	0
4	NAG	A	612	14/15	0.77	0.40	-	115,121,125,126	0
3	NAG	A	602	14/15	0.76	0.39	-	100,105,107,109	0
4	NAG	A	622	14/15	0.68	0.45	-	100,108,111,114	0
5	MAN	A	647	11/12	0.75	0.28	-	128,133,137,137	0
4	NAG	A	611	14/15	0.90	0.29	-	92,98,105,111	0
5	MAN	A	637	11/12	0.73	0.36	-	119,121,125,126	0
3	NAG	A	601	14/15	0.83	0.29	-	90,98,106,106	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, 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	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	A	1328	5/5	0.85	0.31	2.03	94,97,102,105	0
7	SO4	B	1173	5/5	0.93	0.20	0.09	59,65,74,78	0
7	SO4	A	1327	5/5	0.91	0.38	-	95,100,101,102	0
7	SO4	A	1329	5/5	0.88	0.19	-	93,94,99,100	0
6	NAG	A	651	14/15	0.44	0.38	-	101,103,108,108	0

6.5 Other polymers

There are no such residues in this entry.