



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 PM GMT

PDB ID : 4UNX
Title : Structure of the A_Equine_Newmarket_2_93 H3 haemagglutinin in complex with 3SLN
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Deposited on : 2014-05-31
Resolution : 3.20 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

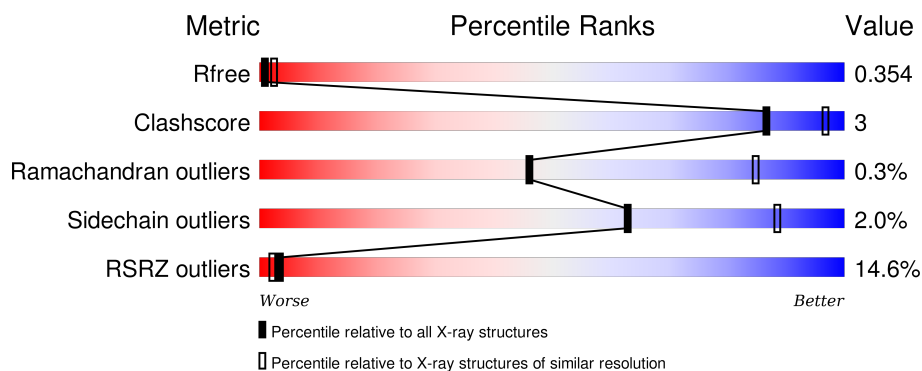
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	323	
1	C	323	
1	E	323	
2	B	173	
2	D	173	

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Mol	Chain	Length	Quality of chain
2	F	173	 % 94% 5% ..

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
4	NAG	C	411	-	-	-	X
4	NAG	E	412	X	-	-	-
7	FUC	B	202	X	-	-	-
7	FUC	D	202	X	-	-	-
7	FUC	F	202	X	-	-	-
9	SIA	E	701	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12208 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 H3 HAEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			
1	C	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			
1	E	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			

- Molecule 2 is a protein called H3 HAEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			
2	D	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			
2	F	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- 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		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	5	Total	C	N	O	0	0
			61	34	2	25		
5	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			46	25	2	19		

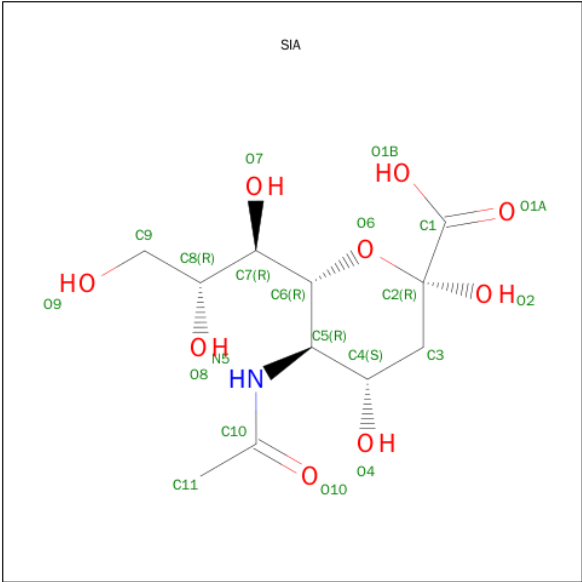
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			24	14	1	9		
7	D	2	Total	C	N	O	0	0
			24	14	1	9		
7	F	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 9 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).

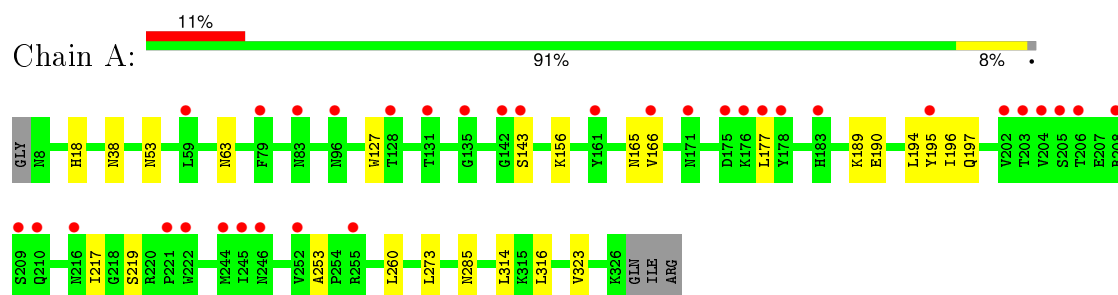



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			20	11	1	8		
9	E	1	Total	C	N	O	0	0
			20	11	1	8		

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: H3 HAEMAGGLUTININ HA1 CHAIN



Chain B:  92% 6% ..

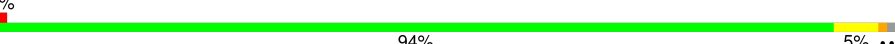


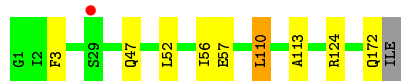
- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain D:  94% 5% ..



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain F:  94% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.48Å 102.25Å 228.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.19 – 3.20 52.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (114.19-3.20) 99.2 (52.18-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.319 , 0.354 0.316 , 0.354	Depositor DCC
R_{free} test set	1971 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 39307 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12208	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: BMA, NAG, SIA, GAL, FUC, 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	0.26	0/2537	0.44	0/3445
1	C	0.26	0/2537	0.44	0/3445
1	E	0.26	0/2537	0.43	0/3445
2	B	0.29	0/1421	0.47	0/1910
2	D	0.28	0/1421	0.46	0/1910
2	F	0.28	0/1421	0.45	0/1910
All	All	0.27	0/11874	0.45	0/16065

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
4	E	1	0
7	B	1	0
7	D	1	0
7	F	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	202	FUC	C1
7	D	202	FUC	C1
4	E	412	NAG	C1
7	F	202	FUC	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	2484	0	2432	18	0
1	C	2484	0	2432	11	0
1	E	2484	0	2432	15	0
2	B	1396	0	1318	7	0
2	D	1396	0	1318	8	0
2	F	1396	0	1318	6	0
3	A	28	0	26	4	0
3	C	28	0	26	3	0
3	E	14	0	13	1	0
4	A	56	0	50	4	0
4	C	56	0	50	2	0
4	E	56	0	50	5	0
5	A	61	0	52	2	0
5	E	61	0	52	1	0
6	A	46	0	40	2	0
7	B	24	0	22	1	0
7	D	24	0	22	1	0
7	F	24	0	22	0	0
8	C	50	0	43	3	0
9	C	20	0	17	0	0
9	E	20	0	17	0	0
All	All	12208	0	11752	64	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 (64) 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:E:165:ASN:HD21	4:E:431:NAG:C1	1.74	1.00
1:C:285:ASN:HD21	8:C:441:NAG:C1	1.91	0.83
2:B:154:ASN:HD22	7:B:201:NAG:C1	1.93	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ASN:ND2	4:E:431:NAG:C1	2.45	0.79
1:A:53:ASN:HD21	4:A:411:NAG:C1	1.96	0.78
1:A:38:ASN:HD21	3:A:401:NAG:C1	1.98	0.76
1:A:63:ASN:HD21	4:A:421:NAG:C1	2.00	0.73
1:C:38:ASN:HD21	3:C:401:NAG:C1	2.04	0.70
1:A:285:ASN:HD21	5:A:441:NAG:C1	2.06	0.68
1:E:274:ILE:O	4:E:411:NAG:H83	1.97	0.65
1:A:38:ASN:ND2	3:A:401:NAG:C1	2.62	0.62
1:A:165:ASN:HD21	3:A:431:NAG:C1	2.14	0.61
1:E:53:ASN:HD22	4:E:411:NAG:C1	2.16	0.58
1:A:194:LEU:HD21	6:A:701:SIA:O10	2.04	0.58
3:C:421:NAG:C1	3:C:421:NAG:C8	2.82	0.58
1:C:53:ASN:HD21	4:C:411:NAG:C1	2.17	0.58
1:A:285:ASN:ND2	5:A:441:NAG:C1	2.67	0.57
1:E:38:ASN:HD21	3:E:401:NAG:C1	2.17	0.57
1:E:53:ASN:N	1:E:53:ASN:OD1	2.37	0.57
1:C:285:ASN:ND2	8:C:441:NAG:C1	2.67	0.56
2:F:56:ILE:HG22	2:F:57:GLU:HG2	1.90	0.53
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.45	0.52
1:E:274:ILE:HD12	1:E:274:ILE:N	2.25	0.52
1:E:53:ASN:HD21	1:E:276:THR:HA	1.74	0.51
1:C:291:ASP:O	2:D:56:ILE:HG23	2.10	0.51
4:E:411:NAG:H3	4:E:412:NAG:O5	2.10	0.51
1:E:285:ASN:HD21	5:E:441:NAG:C1	2.24	0.51
1:A:165:ASN:ND2	3:A:431:NAG:C1	2.73	0.51
2:D:56:ILE:O	2:D:56:ILE:HG22	2.12	0.49
1:A:53:ASN:ND2	4:A:411:NAG:C1	2.72	0.49
1:A:219:SER:HB3	4:C:431:NAG:H82	1.94	0.49
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.95	0.49
1:E:164:LEU:HD12	1:E:251:LEU:HD23	1.94	0.49
1:A:195:TYR:O	1:A:197:GLN:N	2.46	0.48
1:C:195:TYR:O	1:C:197:GLN:N	2.47	0.48
2:D:110:LEU:C	2:D:110:LEU:HD22	2.34	0.47
2:B:134:GLY:HA2	2:D:124:ARG:HD3	1.96	0.47
1:C:285:ASN:OD1	8:C:441:NAG:H83	2.14	0.47
1:C:11:ALA:HB3	2:D:140:ILE:HB	1.97	0.47
2:F:110:LEU:HD22	2:F:110:LEU:C	2.34	0.46
6:A:701:SIA:O6	6:A:701:SIA:O8	2.33	0.46
7:D:201:NAG:H82	7:D:201:NAG:O3	2.14	0.46
1:E:54:ASN:HD22	1:E:54:ASN:N	2.14	0.46
1:E:195:TYR:O	1:E:197:GLN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:421:NAG:H83	3:C:421:NAG:C1	2.48	0.43
2:B:107:THR:HA	2:B:110:LEU:HD12	2.00	0.43
1:E:51:ILE:HB	1:E:274:ILE:HG13	2.00	0.43
2:B:158:ASP:HB3	2:B:161:ILE:HD12	2.01	0.42
1:A:189:LYS:HG3	1:A:190:GLU:N	2.33	0.42
1:A:177:LEU:HD22	1:A:260:LEU:HD21	2.00	0.42
2:F:3:PHE:CE1	2:F:113:ALA:HB2	2.55	0.42
4:A:411:NAG:C1	4:A:411:NAG:O7	2.67	0.41
2:D:134:GLY:HA2	2:F:124:ARG:HD3	2.03	0.41
1:A:217:ILE:HD12	1:A:217:ILE:N	2.36	0.41
1:E:177:LEU:HD22	1:E:260:LEU:HD21	2.03	0.41
1:C:151:LEU:HD23	1:C:252:VAL:HG11	2.03	0.40
1:E:98:TYR:CD2	1:E:230:ILE:HD12	2.57	0.40
1:C:217:ILE:HD12	1:C:217:ILE:N	2.37	0.40
2:F:47:GLN:OE1	2:F:110:LEU:HD23	2.21	0.40
1:A:316:LEU:HD23	2:B:52:LEU:HD13	2.04	0.40
1:C:109:ARG:NH1	2:D:67:GLU:OE2	2.53	0.40
2:F:52:LEU:HG	2:F:56:ILE:HD12	2.04	0.40
2:D:107:THR:HA	2:D:110:LEU:HD12	2.04	0.40
1:A:314:LEU:HB3	2:B:100:VAL:HG21	2.04	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	317/323 (98%)	295 (93%)	20 (6%)	2 (1%)	30	75
1	C	317/323 (98%)	296 (93%)	20 (6%)	1 (0%)	46	85
1	E	317/323 (98%)	294 (93%)	22 (7%)	1 (0%)	46	85
2	B	170/173 (98%)	159 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	170/173 (98%)	158 (93%)	12 (7%)	0	100	100
2	F	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
All	All	1461/1488 (98%)	1364 (93%)	93 (6%)	4 (0%)	46	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	A	196	ILE
1	C	196	ILE
1	E	196	ILE

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	280/283 (99%)	275 (98%)	5 (2%)	66	89
1	C	280/283 (99%)	275 (98%)	5 (2%)	66	89
1	E	280/283 (99%)	273 (98%)	7 (2%)	55	86
2	B	144/145 (99%)	141 (98%)	3 (2%)	61	88
2	D	144/145 (99%)	141 (98%)	3 (2%)	61	88
2	F	144/145 (99%)	142 (99%)	2 (1%)	74	92
All	All	1272/1284 (99%)	1247 (98%)	25 (2%)	63	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	156	LYS
1	A	166	VAL
1	A	273	LEU
1	A	323	VAL
2	B	110	LEU

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Mol	Chain	Res	Type
2	B	127	ARG
2	B	172	GLN
1	C	18	HIS
1	C	156	LYS
1	C	248	ASN
1	C	273	LEU
1	C	323	VAL
2	D	110	LEU
2	D	167	LEU
2	D	172	GLN
1	E	18	HIS
1	E	54	ASN
1	E	156	LYS
1	E	165	ASN
1	E	246	ASN
1	E	273	LEU
1	E	323	VAL
2	F	110	LEU
2	F	172	GLN

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

Mol	Chain	Res	Type
1	A	54	ASN
1	A	165	ASN
2	B	154	ASN
1	C	38	ASN
1	C	54	ASN
1	C	285	ASN
1	E	38	ASN
1	E	54	ASN
1	E	165	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 ⓘ

35 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	$\# Z > 2$
4	NAG	A	411	4	14,14,15	0.51	0	15,19,21	1.20	3 (20%)
4	NAG	A	412	4	14,14,15	0.57	0	15,19,21	0.74	0
4	NAG	A	421	4	14,14,15	0.54	0	15,19,21	1.17	1 (6%)
4	NAG	A	422	4	14,14,15	0.66	0	15,19,21	2.65	4 (26%)
5	NAG	A	441	5	14,14,15	0.55	0	15,19,21	1.68	4 (26%)
5	NAG	A	442	5	14,14,15	0.53	0	15,19,21	0.71	0
5	BMA	A	443	5	11,11,12	0.31	0	14,15,17	0.57	0
5	MAN	A	444	5	11,11,12	0.61	0	14,15,17	1.11	1 (7%)
5	MAN	A	445	5	11,11,12	0.52	0	14,15,17	1.18	1 (7%)
6	SIA	A	701	6	16,20,21	0.46	0	18,28,31	0.95	2 (11%)
6	GAL	A	702	6	11,11,12	0.56	0	14,15,17	0.83	0
6	NAG	A	703	6	15,15,15	0.49	0	17,21,21	1.53	3 (17%)
7	NAG	B	201	7	14,14,15	0.51	0	15,19,21	0.82	0
7	FUC	B	202	7	10,10,11	0.79	0	14,14,16	1.84	5 (35%)
4	NAG	C	411	4	14,14,15	0.50	0	15,19,21	1.10	2 (13%)
4	NAG	C	412	4	14,14,15	0.59	0	15,19,21	1.06	2 (13%)
4	NAG	C	431	4	14,14,15	0.54	0	15,19,21	0.79	0
4	NAG	C	432	4	14,14,15	0.52	0	15,19,21	0.70	0
8	NAG	C	441	8	14,14,15	0.56	0	15,19,21	1.83	5 (33%)
8	NAG	C	442	8	14,14,15	0.36	0	15,19,21	1.88	2 (13%)
8	BMA	C	443	8	11,11,12	0.46	0	14,15,17	2.05	3 (21%)
8	MAN	C	445	8	11,11,12	0.55	0	14,15,17	1.28	2 (14%)
7	NAG	D	201	7	14,14,15	0.63	0	15,19,21	1.64	4 (26%)
7	FUC	D	202	7	10,10,11	0.59	0	14,14,16	0.77	0
4	NAG	E	411	4	14,14,15	0.67	0	15,19,21	1.52	2 (13%)
4	NAG	E	412	4	14,14,15	0.90	1 (7%)	15,19,21	1.22	2 (13%)
4	NAG	E	431	4	14,14,15	0.57	0	15,19,21	1.08	1 (6%)
4	NAG	E	432	4	14,14,15	0.48	0	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	441	5	14,14,15	0.51	0	15,19,21	1.29	2 (13%)
5	NAG	E	442	5	14,14,15	0.52	0	15,19,21	0.56	0
5	BMA	E	443	5	11,11,12	0.33	0	14,15,17	0.89	0
5	MAN	E	444	5	11,11,12	0.60	0	14,15,17	0.93	1 (7%)
5	MAN	E	445	5	11,11,12	0.52	0	14,15,17	1.22	1 (7%)
7	NAG	F	201	7	14,14,15	0.51	0	15,19,21	0.75	0
7	FUC	F	202	7	10,10,11	0.64	0	14,14,16	0.98	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
4	NAG	A	411	4	-	0/6/23/26	0/1/1/1
4	NAG	A	412	4	-	0/6/23/26	0/1/1/1
4	NAG	A	421	4	-	0/6/23/26	0/1/1/1
4	NAG	A	422	4	-	0/6/23/26	0/1/1/1
5	NAG	A	441	5	-	0/6/23/26	0/1/1/1
5	NAG	A	442	5	-	0/6/23/26	0/1/1/1
5	BMA	A	443	5	-	0/2/19/22	0/1/1/1
5	MAN	A	444	5	-	0/2/19/22	0/1/1/1
5	MAN	A	445	5	-	0/2/19/22	1/1/1/1
6	SIA	A	701	6	-	0/14/34/38	0/1/1/1
6	GAL	A	702	6	-	0/2/19/22	0/1/1/1
6	NAG	A	703	6	-	0/6/26/26	0/1/1/1
7	NAG	B	201	7	-	0/6/23/26	0/1/1/1
7	FUC	B	202	7	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	C	411	4	-	0/6/23/26	0/1/1/1
4	NAG	C	412	4	-	0/6/23/26	0/1/1/1
4	NAG	C	431	4	-	0/6/23/26	0/1/1/1
4	NAG	C	432	4	-	0/6/23/26	0/1/1/1
8	NAG	C	441	8	-	0/6/23/26	0/1/1/1
8	NAG	C	442	8	-	0/6/23/26	0/1/1/1
8	BMA	C	443	8	-	0/2/19/22	0/1/1/1
8	MAN	C	445	8	-	0/2/19/22	0/1/1/1
7	NAG	D	201	7	-	0/6/23/26	0/1/1/1
7	FUC	D	202	7	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	E	411	4	-	0/6/23/26	0/1/1/1
4	NAG	E	412	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	431	4	-	0/6/23/26	0/1/1/1
4	NAG	E	432	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	441	5	-	0/6/23/26	0/1/1/1
5	NAG	E	442	5	-	0/6/23/26	0/1/1/1
5	BMA	E	443	5	-	0/2/19/22	0/1/1/1
5	MAN	E	444	5	-	0/2/19/22	0/1/1/1
5	MAN	E	445	5	-	0/2/19/22	1/1/1/1
7	NAG	F	201	7	-	0/6/23/26	0/1/1/1
7	FUC	F	202	7	1/1/4/5	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	412	NAG	C1-C2	2.87	1.56	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	202	FUC	C1-O5-C5	-3.27	107.33	112.38
8	C	442	NAG	C4-C3-C2	-3.26	106.16	111.23
4	A	422	NAG	O7-C7-C8	-3.02	116.53	122.06
8	C	441	NAG	O7-C7-C8	-2.76	117.00	122.06
5	A	441	NAG	O7-C7-C8	-2.48	117.51	122.06
7	D	201	NAG	O7-C7-C8	-2.40	117.66	122.06
6	A	703	NAG	C3-C2-N2	-2.31	105.88	110.66
4	A	411	NAG	O7-C7-C8	-2.10	118.22	122.06
4	E	412	NAG	C2-N2-C7	-2.09	120.35	123.04
7	D	201	NAG	O3-C3-C4	-2.08	105.66	110.34
6	A	701	SIA	C3-C4-C5	-2.02	109.22	111.47
8	C	441	NAG	C4-C3-C2	2.01	114.35	111.23
4	C	412	NAG	C4-C3-C2	2.02	114.37	111.23
4	C	411	NAG	C3-C4-C5	2.05	113.78	110.20
5	E	441	NAG	C4-C3-C2	2.17	114.60	111.23
8	C	443	BMA	O5-C1-C2	2.25	114.51	110.86
4	A	411	NAG	C3-C4-C5	2.25	114.12	110.20
7	B	202	FUC	O5-C5-C6	2.30	109.93	106.13
7	B	202	FUC	C3-C4-C5	2.33	113.64	109.72
4	A	411	NAG	C2-N2-C7	2.37	126.08	123.04
5	E	441	NAG	C3-C4-C5	2.38	114.35	110.20
4	C	411	NAG	C4-C3-C2	2.39	114.95	111.23
6	A	701	SIA	O6-C6-C5	2.44	112.48	108.48
8	C	445	MAN	C1-C2-C3	2.50	112.49	109.54
7	B	202	FUC	C2-C3-C4	2.52	115.33	111.04
4	E	412	NAG	C4-C3-C2	2.53	115.17	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	412	NAG	C3-C4-C5	2.60	114.73	110.20
7	D	201	NAG	C8-C7-N2	2.75	121.37	116.11
4	E	411	NAG	C3-C4-C5	2.82	115.12	110.20
5	A	444	MAN	C1-O5-C5	2.84	115.86	112.25
5	A	441	NAG	C2-N2-C7	2.86	126.72	123.04
5	E	444	MAN	C1-C2-C3	2.93	113.00	109.54
6	A	703	NAG	C3-C4-C5	3.03	115.48	110.20
4	E	431	NAG	C3-C4-C5	3.11	115.61	110.20
8	C	441	NAG	C3-C4-C5	3.17	115.72	110.20
5	A	441	NAG	C3-C4-C5	3.18	115.74	110.20
4	A	421	NAG	C3-C4-C5	3.25	115.86	110.20
5	A	441	NAG	C8-C7-N2	3.41	122.63	116.11
8	C	445	MAN	C1-O5-C5	3.44	116.61	112.25
5	E	445	MAN	C1-O5-C5	3.44	116.61	112.25
8	C	441	NAG	C8-C7-N2	3.49	122.78	116.11
8	C	441	NAG	C2-N2-C7	3.49	127.53	123.04
6	A	703	NAG	C4-C3-C2	3.51	115.29	110.43
5	A	445	MAN	C1-O5-C5	3.59	116.81	112.25
4	A	422	NAG	C3-C2-N2	3.75	119.54	110.56
7	B	202	FUC	O5-C1-C2	3.82	117.05	110.86
7	D	201	NAG	C2-N2-C7	3.89	128.03	123.04
4	E	411	NAG	C4-C3-C2	4.21	117.77	111.23
4	A	422	NAG	C8-C7-N2	4.24	124.21	116.11
8	C	443	BMA	C1-C2-C3	4.81	115.23	109.54
8	C	443	BMA	C1-O5-C5	5.17	118.81	112.25
8	C	442	NAG	C1-O5-C5	5.61	119.37	112.25
4	A	422	NAG	C2-N2-C7	7.36	132.49	123.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	412	NAG	C1
7	D	202	FUC	C1
7	B	202	FUC	C1
7	F	202	FUC	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	445	MAN	C1-C2-C3-C4-C5-O5
5	A	445	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	411	NAG	3	0
4	A	421	NAG	1	0
5	A	441	NAG	2	0
6	A	701	SIA	2	0
7	B	201	NAG	1	0
4	C	411	NAG	1	0
4	C	431	NAG	1	0
8	C	441	NAG	3	0
7	D	201	NAG	1	0
4	E	411	NAG	3	0
4	E	412	NAG	1	0
4	E	431	NAG	2	0
5	E	441	NAG	1	0

5.6 Ligand geometry ⓘ

7 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	$\# Z > 2$
3	NAG	A	401	-	14,14,15	0.63	0	15,19,21	1.32	2 (13%)
3	NAG	A	431	-	14,14,15	0.47	0	15,19,21	0.97	0
3	NAG	C	401	-	14,14,15	0.45	0	15,19,21	1.35	2 (13%)
3	NAG	C	421	-	14,14,15	0.53	0	15,19,21	1.89	3 (20%)
9	SIA	C	701	-	16,20,21	0.24	0	18,28,31	0.89	1 (5%)
3	NAG	E	401	-	14,14,15	0.54	0	15,19,21	0.80	0
9	SIA	E	701	-	16,20,21	0.24	0	18,28,31	1.04	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
3	NAG	A	401	-	-	0/6/23/26	0/1/1/1
3	NAG	A	431	-	-	0/6/23/26	0/1/1/1
3	NAG	C	401	-	-	0/6/23/26	0/1/1/1
3	NAG	C	421	-	-	0/6/23/26	0/1/1/1
9	SIA	C	701	-	-	0/14/34/38	0/1/1/1
3	NAG	E	401	-	-	0/6/23/26	0/1/1/1
9	SIA	E	701	-	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	421	NAG	O7-C7-C8	-2.83	116.88	122.06
9	E	701	SIA	C7-C6-C5	-2.28	110.87	114.32
9	C	701	SIA	O6-C6-C5	2.46	112.51	108.48
3	C	401	NAG	C3-C4-C5	2.53	114.61	110.20
3	A	401	NAG	C3-C4-C5	2.75	114.99	110.20
3	A	401	NAG	C4-C3-C2	2.97	115.85	111.23
9	E	701	SIA	O6-C6-C5	3.05	113.47	108.48
3	C	421	NAG	C8-C7-N2	3.63	123.06	116.11
3	C	401	NAG	C1-O5-C5	3.90	117.20	112.25
3	C	421	NAG	C2-N2-C7	5.18	129.69	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	2	0
3	A	431	NAG	2	0
3	C	401	NAG	1	0
3	C	421	NAG	2	0
3	E	401	NAG	1	0

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	319/323 (98%)	0.81	34 (10%) 8 4	73, 109, 145, 155	0
1	C	319/323 (98%)	1.06	55 (17%) 2 1	91, 120, 162, 175	0
1	E	319/323 (98%)	1.88	121 (37%) 0 0	108, 150, 173, 186	0
2	B	172/173 (99%)	0.32	2 (1%) 81 69	64, 79, 108, 121	0
2	D	172/173 (99%)	0.25	2 (1%) 81 69	64, 76, 108, 122	0
2	F	172/173 (99%)	0.22	1 (0%) 90 84	68, 86, 110, 124	0
All	All	1473/1488 (98%)	0.90	215 (14%) 3 2	64, 108, 163, 186	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	58	VAL	9.3
1	E	243	LEU	8.3
1	E	59	LEU	7.5
1	E	179	ILE	7.2
1	C	200	GLY	6.8
1	E	222	TRP	6.7
1	C	199	SER	6.0
1	C	161	TYR	5.9
1	C	157	SER	5.8
1	E	218	GLY	5.7
1	E	127	TRP	5.6
1	E	143	SER	5.4
1	E	151	LEU	5.4
1	C	187	SER	5.3
1	E	199	SER	5.2
1	A	245	ILE	5.1
1	E	159	ASN	5.1
1	A	206	THR	5.1
1	C	158	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	198	GLU	4.9
1	E	147	PHE	4.9
1	E	223	VAL	4.8
1	A	210	GLN	4.8
1	E	155	THR	4.8
1	E	272	ALA	4.7
1	E	126	THR	4.7
1	C	154	LEU	4.7
1	E	47	SER	4.7
1	E	60	ASP	4.5
1	C	159	ASN	4.5
1	E	136	SER	4.4
1	E	79	PHE	4.4
1	E	273	LEU	4.4
1	E	191	GLN	4.3
1	C	135	GLY	4.3
1	E	160	SER	4.2
1	E	194	LEU	4.2
1	E	66	LEU	4.2
1	E	245	ILE	4.2
1	E	162	PRO	4.1
1	C	70	MET	4.1
1	E	82	GLU	4.1
1	E	71	LEU	4.1
1	E	244	MET	4.0
1	E	144	ALA	4.0
1	E	140	LYS	4.0
1	E	224	ARG	4.0
1	E	135	GLY	3.9
1	E	288	ILE	3.9
1	E	94	PHE	3.9
1	A	246	ASN	3.8
1	E	96	ASN	3.8
1	E	86	LEU	3.7
1	A	205	SER	3.7
1	A	161	TYR	3.7
1	C	155	THR	3.7
1	E	56	TYR	3.7
1	E	275	ASP	3.7
1	A	222	TRP	3.7
1	E	142	GLY	3.6
1	E	189	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	219	SER	3.6
1	A	142	GLY	3.6
1	E	118	LEU	3.6
1	E	138	ALA	3.6
1	E	83	ASN	3.6
1	E	197	GLN	3.5
1	E	161	TYR	3.5
1	E	200	GLY	3.5
1	E	256	GLY	3.5
1	E	166	VAL	3.5
1	E	282	ILE	3.5
1	A	244	MET	3.4
1	C	224	ARG	3.4
1	A	195	TYR	3.4
1	E	221	PRO	3.4
1	E	241	ASP	3.3
1	E	234	TRP	3.3
1	C	128	THR	3.3
1	A	79	PHE	3.3
1	A	83	ASN	3.2
1	E	48	ILE	3.2
1	E	61	GLY	3.2
1	C	218	GLY	3.2
1	E	128	THR	3.2
1	C	251	LEU	3.2
1	C	145	ASP	3.1
1	E	246	ASN	3.1
1	C	162	PRO	3.1
1	C	229	ARG	3.1
1	E	52	CYS	3.1
1	C	118	LEU	3.1
1	C	130	VAL	3.1
1	E	74	PRO	3.1
1	C	156	LYS	3.0
1	E	78	ASP	3.0
1	E	167	THR	3.0
1	C	194	LEU	3.0
1	E	75	HIS	3.0
1	E	190	GLU	3.0
1	A	204	VAL	3.0
1	A	175	ASP	3.0
1	E	70	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	176	LYS	2.9
1	E	177	LEU	2.9
1	E	125	PHE	2.9
1	C	225	GLY	2.9
1	C	132	GLN	2.9
1	E	57	ARG	2.9
1	E	239	PRO	2.9
1	E	88	ILE	2.9
1	E	201	ARG	2.9
1	A	183	HIS	2.9
1	E	85	ASP	2.8
1	E	156	LYS	2.8
1	E	164	LEU	2.8
1	A	221	PRO	2.8
1	E	214	ILE	2.8
1	E	152	ASN	2.8
1	E	95	SER	2.8
1	C	153	TRP	2.8
1	E	281	CYS	2.8
1	A	216	ASN	2.8
2	D	1	GLY	2.7
1	A	208	ARG	2.7
1	A	209	SER	2.7
1	E	188	ASN	2.7
1	A	255	ARG	2.7
1	C	212	THR	2.7
1	A	178	TYR	2.7
1	E	208	ARG	2.7
1	E	87	PHE	2.7
1	A	59	LEU	2.6
1	E	122	ALA	2.6
1	E	163	ILE	2.6
1	E	225	GLY	2.6
1	A	96	ASN	2.6
1	C	79	PHE	2.6
1	C	131	THR	2.5
1	C	213	VAL	2.5
1	E	302	TYR	2.5
1	C	232	ILE	2.5
1	C	144	ALA	2.5
1	C	48	ILE	2.5
1	E	184	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	VAL	2.5
1	E	98	TYR	2.5
1	A	143	SER	2.5
1	C	160	SER	2.5
1	E	228	GLY	2.5
1	C	192	THR	2.5
1	E	99	PRO	2.5
2	B	61	GLU	2.5
1	E	54	ASN	2.5
1	C	196	ILE	2.5
1	A	128	THR	2.5
1	E	248	ASN	2.5
1	C	183	HIS	2.5
1	E	49	GLY	2.4
1	E	271	ASP	2.4
1	C	61	GLY	2.4
1	E	252	VAL	2.4
1	A	171	ASN	2.4
1	C	142	GLY	2.4
1	C	54	ASN	2.4
1	E	187	SER	2.4
1	E	124	GLY	2.4
1	A	177	LEU	2.3
1	E	183	HIS	2.3
1	C	197	GLN	2.3
1	E	77	ASP	2.3
1	C	127	TRP	2.3
1	C	217	ILE	2.3
1	C	163	ILE	2.3
1	E	68	ASP	2.3
1	E	251	LEU	2.3
1	E	93	ALA	2.3
1	A	131	THR	2.2
1	E	213	VAL	2.2
2	F	29	SER	2.2
1	A	166	VAL	2.2
1	E	133	ASN	2.2
1	E	173	ASN	2.2
1	C	214	ILE	2.2
1	E	270	SER	2.2
1	C	78	ASP	2.2
1	A	202	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	277	CYS	2.2
2	B	81	GLU	2.2
1	E	110	SER	2.2
1	A	135	GLY	2.2
1	E	181	GLY	2.2
1	E	285	ASN	2.2
1	C	276	THR	2.1
1	E	137	GLY	2.1
1	C	146	SER	2.1
1	C	98	TYR	2.1
1	E	51	ILE	2.1
2	D	2	ILE	2.1
1	E	193	LYS	2.1
1	C	188	ASN	2.1
1	C	228	GLY	2.1
1	E	274	ILE	2.1
1	A	203	THR	2.1
1	C	246	ASN	2.1
1	E	259	LYS	2.1
1	C	253	ALA	2.1
1	C	193	LYS	2.1
1	E	180	TRP	2.1
1	E	157	SER	2.1
1	E	145	ASP	2.1
1	E	92	SER	2.0
1	E	65	THR	2.0
1	C	248	ASN	2.0
1	E	286	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](#)

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(\AA^2)	Q<0.9
4	NAG	C	411	14/15	0.52	0.44	1.24	120,125,130,133	0
4	NAG	E	432	14/15	0.65	0.35	-0.42	164,170,175,176	0
4	NAG	C	432	14/15	0.73	0.35	-0.59	133,141,146,147	0
8	NAG	C	441	14/15	0.87	0.25	-0.69	112,116,119,120	0
5	NAG	E	441	14/15	0.85	0.26	-1.24	132,133,136,137	0
6	SIA	A	701	20/21	0.81	0.22	-1.31	125,129,132,133	0
7	NAG	B	201	14/15	0.89	0.20	-	93,98,105,106	0
4	NAG	E	431	14/15	0.76	0.25	-	165,167,169,169	0
4	NAG	E	411	14/15	0.56	0.56	-	159,163,167,167	0
7	FUC	D	202	10/11	0.79	0.28	-	83,88,92,94	0
5	NAG	A	441	14/15	0.91	0.18	-	84,87,89,90	0
8	NAG	C	442	14/15	0.71	0.36	-	118,121,125,128	0
4	NAG	A	422	14/15	0.43	0.59	-	125,130,136,137	0
4	NAG	C	412	14/15	0.49	0.45	-	134,140,143,145	0
5	BMA	A	443	11/12	0.69	0.33	-	96,99,102,103	0
6	GAL	A	702	11/12	0.87	0.17	-	130,133,135,135	0
5	MAN	A	445	11/12	0.72	0.23	-	92,95,99,99	0
4	NAG	C	431	14/15	0.85	0.21	-	135,138,142,143	0
5	MAN	E	444	11/12	0.44	0.70	-	143,147,149,151	0
6	NAG	A	703	15/15	0.64	0.38	-	137,142,148,148	0
4	NAG	A	411	14/15	0.61	0.33	-	109,112,118,118	0
5	NAG	E	442	14/15	0.74	0.29	-	130,134,138,138	0
5	BMA	E	443	11/12	0.73	0.30	-	135,138,142,143	0
4	NAG	A	421	14/15	0.82	0.47	-	114,116,121,122	0
4	NAG	E	412	14/15	0.58	0.71	-	170,174,179,179	0
5	NAG	A	442	14/15	0.80	0.29	-	89,91,94,95	0
8	BMA	C	443	11/12	0.54	0.45	-	128,131,137,139	0
5	MAN	E	445	11/12	0.61	0.34	-	130,133,136,138	0
8	MAN	C	445	11/12	0.62	0.34	-	122,127,134,135	0
7	FUC	B	202	10/11	0.78	0.35	-	90,98,102,103	0
5	MAN	A	444	11/12	0.51	0.49	-	102,104,106,107	0
7	FUC	F	202	10/11	0.56	0.56	-	96,101,103,104	0
4	NAG	A	412	14/15	0.63	0.56	-	121,126,129,129	0
7	NAG	F	201	14/15	0.74	0.40	-	99,102,107,108	0
7	NAG	D	201	14/15	0.78	0.27	-	85,91,99,102	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(\AA^2)	Q<0.9
9	SIA	E	701	20/21	0.49	0.60	0.90	164,170,175,175	0
9	SIA	C	701	20/21	0.60	0.37	-0.47	151,156,161,162	0
3	NAG	E	401	14/15	0.79	0.27	-	127,130,134,137	0
3	NAG	A	401	14/15	0.79	0.27	-	77,79,81,82	0
3	NAG	C	401	14/15	0.85	0.24	-	93,96,97,98	0
3	NAG	A	431	14/15	0.68	0.33	-	157,161,164,167	0
3	NAG	C	421	14/15	0.49	0.35	-	137,145,152,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.