



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 PM GMT

PDB ID : 4UO0  
Title : Structure of the A\_Equine\_Richmond\_07 H3 haemagglutinin  
Authors : Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogradowicz, R.W.; Martin, S.R.;  
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Deposited on : 2014-05-31  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

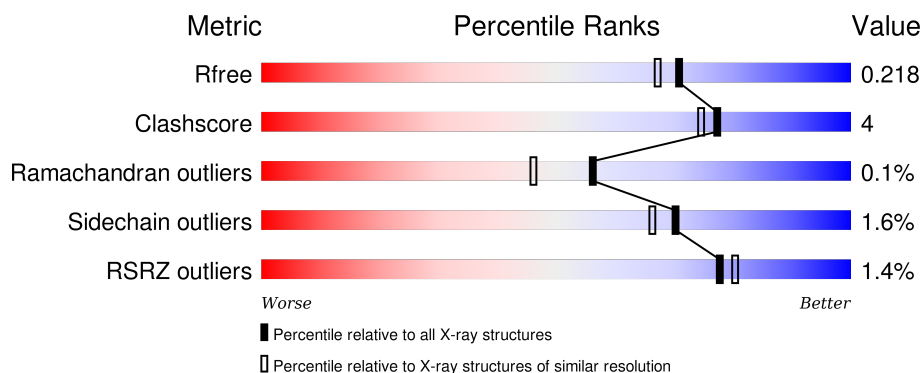
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>2%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	329	<div> <div>%</div> <div>92%</div> <div>5%</div> <div>..</div> </div>
1	E	329	<div> <div>%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
2	B	172	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
2	D	172	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	172	 % 92% 7%

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
11	FUC	C	620	X	-	-	-
12	FUC	D	200	X	-	-	X
12	NAG	D	201	-	-	-	X
12	FUC	E	600	X	-	-	-
12	FUC	F	200	X	-	-	-
12	NAG	F	201	-	-	-	X
3	NAG	A	621	X	-	-	-
3	NAG	C	441	-	-	-	X
3	NAG	E	441	-	-	-	X
4	NAG	C	422	-	-	-	X
4	MAN	C	424	-	-	-	X
5	FUC	A	600	X	-	-	-
5	NAG	A	602	-	-	-	X
8	EDO	A	1327	-	-	-	X
8	EDO	A	1328	-	-	-	X
8	EDO	B	1173	-	-	-	X
8	EDO	C	1328	-	-	-	X
8	EDO	D	1173	-	-	-	X
8	EDO	E	1327	-	-	-	X
8	EDO	F	1174	-	-	-	X
9	FUC	B	200	X	-	-	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 14213 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	8	0
			2573	1612	454	492	15			
1	C	320	Total	C	N	O	S	0	1	0
			2496	1560	441	480	15			
1	E	325	Total	C	N	O	S	0	4	0
			2548	1593	449	491	15			

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	6	0
			1428	896	242	283	7			
2	D	172	Total	C	N	O	S	0	4	0
			1421	890	245	279	7			
2	F	172	Total	C	N	O	S	0	7	0
			1437	903	245	281	8			

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

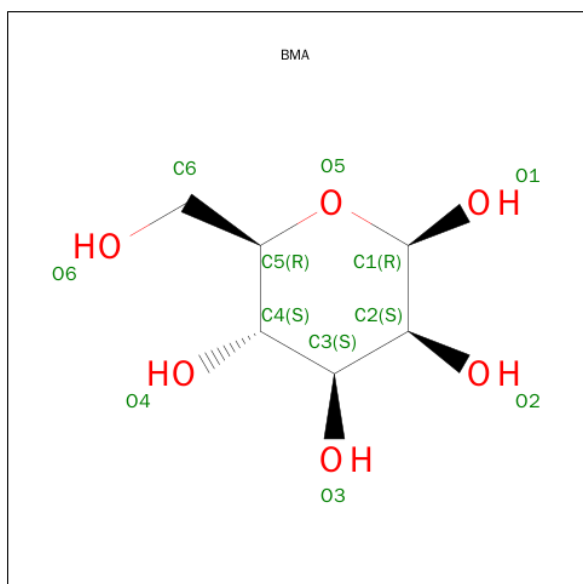
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

- 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
			49	28	2	19		

- Molecule 6 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

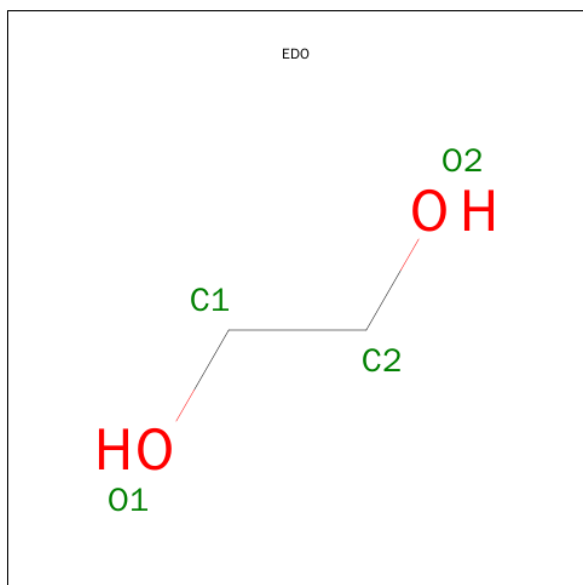


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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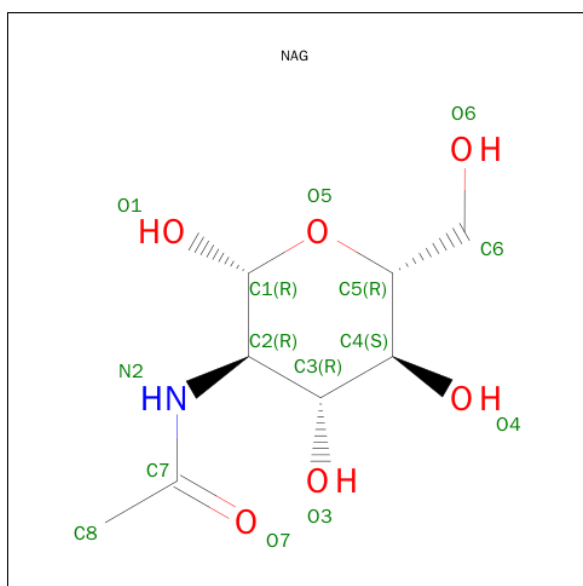
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		

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

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

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	3	Total	C	N	O	0	0
			38	22	2	14		
12	E	3	Total	C	N	O	0	0
			38	22	2	14		
12	F	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 13 is water.

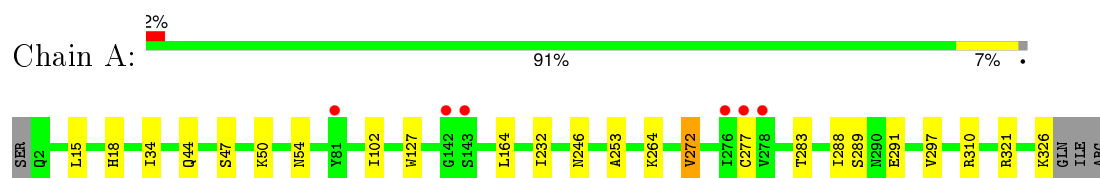
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	314	Total	O	0	0
			314	314		
13	B	191	Total	O	0	0
			191	191		
13	C	283	Total	O	0	0
			283	283		
13	D	174	Total	O	0	0
			174	174		
13	E	256	Total	O	0	0
			256	256		
13	F	134	Total	O	0	0
			134	134		



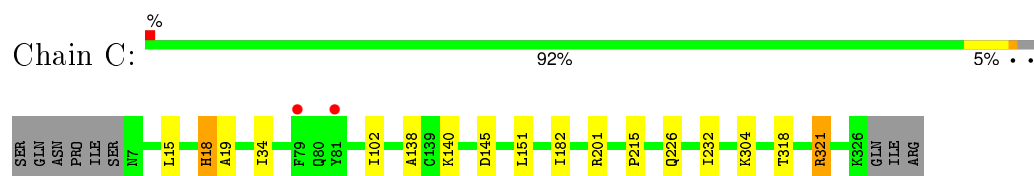
### 3 Residue-property plots [i](#)

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.

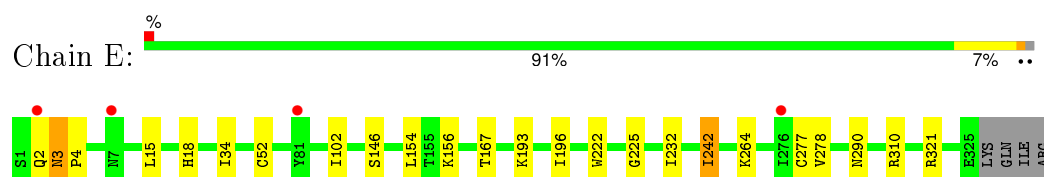
- Molecule 1: HEMAGGLUTININ



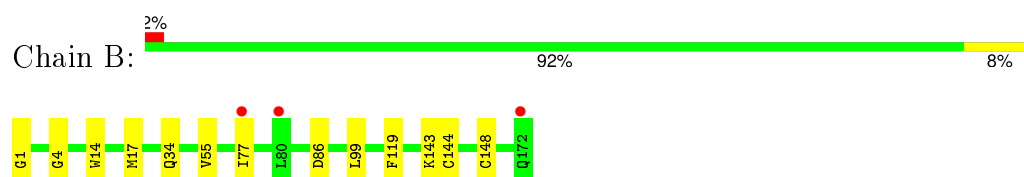
- Molecule 1: HEMAGGLUTININ



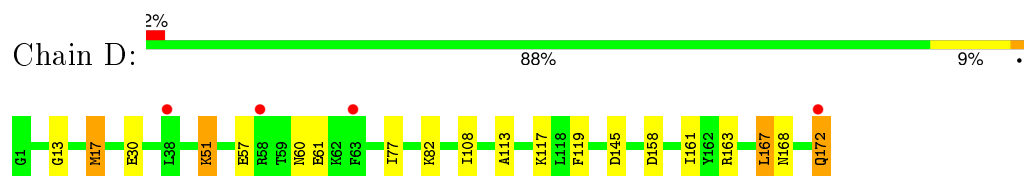
- Molecule 1: HEMAGGLUTININ



- Molecule 2: HEMAGGLUTININ

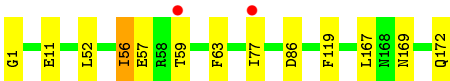


- Molecule 2: HEMAGGLUTININ



- Molecule 2: HEMAGGLUTININ





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.41Å 129.33Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.37 – 1.90 46.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (107.37-1.90) 97.3 (46.58-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.191 , 0.218 0.191 , 0.218	Depositor DCC
$R_{free}$ test set	7614 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 152146 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, MAN, BMA, NAG, EDO

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	0.39	0/2651	0.56	0/3598
1	C	0.41	0/2552	0.58	0/3464
1	E	0.39	0/2614	0.57	0/3551
2	B	0.44	0/1471	0.57	0/1978
2	D	0.42	0/1458	0.59	0/1960
2	F	0.44	0/1483	0.61	0/1994
All	All	0.41	0/12229	0.58	0/16545

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
9	B	1	0
11	C	1	0
12	D	1	0
12	E	1	0
12	F	1	0
All	All	7	0

There are no bond length outliers.

There are no bond angle outliers.

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	600	FUC	C1
3	A	621	NAG	C1

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Mol	Chain	Res	Type	Atom
9	B	200	FUC	C1
11	C	620	FUC	C1
12	D	200	FUC	C1
12	E	600	FUC	C1
12	F	200	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	2573	0	2547	16	0
1	C	2496	0	2440	14	0
1	E	2548	0	2499	16	0
2	B	1428	0	1363	25	0
2	D	1421	0	1360	19	0
2	F	1437	0	1386	19	0
3	A	112	0	100	1	0
3	C	28	0	25	0	0
3	E	112	0	100	1	0
4	A	61	0	52	2	0
4	C	122	0	104	5	0
4	E	61	0	52	0	0
5	A	49	0	43	2	0
6	A	11	0	10	0	0
7	A	39	0	34	0	0
7	C	78	0	68	1	0
8	A	8	0	12	1	0
8	B	8	0	12	0	0
8	C	8	0	12	0	0
8	D	4	0	6	0	0
8	E	8	0	12	1	0
8	F	12	0	18	0	0
9	B	24	0	22	0	0
10	C	14	0	13	0	0
10	E	14	0	13	0	0
11	C	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	38	0	34	0	0
12	E	38	0	34	0	0
12	F	38	0	34	0	0
13	A	314	0	0	4	0
13	B	191	0	0	2	0
13	C	283	0	0	0	0
13	D	174	0	0	2	0
13	E	256	0	0	1	0
13	F	134	0	0	2	0
All	All	14213	0	12466	93	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 4.

All (93) 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)
2:B:77[A]:ILE:HD12	2:F:77[A]:ILE:CD1	2.03	0.88
2:B:77[A]:ILE:HD12	2:F:77[A]:ILE:HD11	1.58	0.83
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:CD1	2.57	0.82
1:E:167:THR:OG1	1:E:242:ILE:HD11	1.80	0.81
4:A:433:BMA:H62	4:A:437:MAN:H5	1.68	0.76
1:C:102:ILE:HG12	1:C:232:ILE:HB	1.67	0.74
1:E:156:LYS:HE3	1:E:193:LYS:O	1.88	0.74
2:B:77[A]:ILE:HD11	2:F:77[A]:ILE:HD13	1.73	0.71
1:C:15:LEU:CD2	2:D:119:PHE:HA	2.21	0.71
1:C:304:LYS:HG3	2:D:61:GLU:HG3	1.74	0.69
2:B:77[B]:ILE:HD11	2:D:77[B]:ILE:HD12	1.76	0.68
13:B:2079:HOH:O	2:F:86[B]:ASP:OD2	2.12	0.67
2:B:77[B]:ILE:HD13	2:D:77[B]:ILE:HD11	1.77	0.65
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:HD11	2.26	0.64
1:A:44:GLN:HG2	1:A:288[B]:ILE:HG23	1.78	0.63
1:E:34:ILE:HD11	1:E:321:ARG:HD2	1.80	0.63
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.83	0.60
2:B:77[A]:ILE:CD1	2:F:77[A]:ILE:HD13	2.29	0.60
1:E:15[B]:LEU:HD13	2:F:119:PHE:HA	1.83	0.60
1:E:156:LYS:HD3	1:E:196:ILE:HD11	1.83	0.60
1:A:44:GLN:HG2	1:A:288[B]:ILE:CG2	2.32	0.59
1:C:304:LYS:CG	2:D:61:GLU:HG3	2.33	0.58
1:C:138:ALA:HB2	1:C:226:GLN:HG2	1.85	0.58
5:A:600:FUC:H62	2:B:143:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:411:NAG:H3	3:E:412:NAG:H61	1.86	0.57
2:B:77[B]:ILE:CD1	2:D:77[B]:ILE:HD12	2.33	0.57
1:C:18:HIS:HD2	13:D:2020:HOH:O	1.87	0.57
2:D:168:ASN:O	2:D:172:GLN:HB3	2.05	0.56
1:C:34:ILE:HD11	1:C:321:ARG:HD2	1.87	0.56
2:B:14:TRP:HE3	2:B:17[B]:MET:HE2	1.72	0.55
1:A:288[B]:ILE:HD11	1:A:297:VAL:HG11	1.88	0.55
2:B:77[B]:ILE:CD1	2:D:77[B]:ILE:CD1	2.85	0.55
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.89	0.54
1:E:15[A]:LEU:HD22	2:F:119:PHE:HA	1.89	0.54
4:C:422:NAG:H62	4:C:423:BMA:H2	1.89	0.54
2:B:77[B]:ILE:HD13	2:D:77[B]:ILE:CD1	2.38	0.53
3:A:421:NAG:H82	13:A:2075:HOH:O	2.09	0.52
2:B:144:CYS:HG	2:B:148:CYS:HG	1.57	0.52
1:A:289[A]:SER:OG	1:A:291:GLU:HG2	2.10	0.52
1:E:310:ARG:NH2	2:F:86[B]:ASP:OD1	2.44	0.51
1:E:290:ASN:HB2	2:F:59:THR:HG21	1.92	0.50
1:A:283:THR:CG2	1:A:288[B]:ILE:HD13	2.41	0.50
1:A:47:SER:HA	1:A:288[A]:ILE:HG22	1.94	0.50
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.12	0.49
1:A:47:SER:HA	1:A:288[B]:ILE:HG13	1.94	0.49
13:E:2012:HOH:O	2:F:169:ASN:ND2	2.40	0.49
1:A:102:ILE:HG12	1:A:232:ILE:HB	1.95	0.49
2:F:52:LEU:HD13	2:F:56[A]:ILE:HD11	1.96	0.48
1:E:167:THR:HG1	1:E:242:ILE:HD11	1.79	0.48
1:C:19:ALA:HB2	2:D:13:GLY:HA3	1.95	0.48
2:B:4:GLY:HA3	2:D:117:LYS:HD2	1.95	0.47
2:B:17[A]:MET:HE3	2:B:34:GLN:CG	2.44	0.47
4:C:422:NAG:H5	4:C:423:BMA:O2	2.14	0.47
1:C:182:ILE:HD11	1:C:215:PRO:HG3	1.96	0.47
2:B:77[A]:ILE:HD11	2:F:77[A]:ILE:CD1	2.33	0.47
1:E:102:ILE:HG12	1:E:232:ILE:HB	1.97	0.46
2:D:158:ASP:HB3	2:D:161:ILE:HD12	1.98	0.46
2:D:17[A]:MET:HA	2:D:17[A]:MET:HE3	1.97	0.46
4:A:433:BMA:H62	4:A:437:MAN:C5	2.42	0.46
2:D:82:LYS:NZ	13:D:2108:HOH:O	2.43	0.46
2:D:113:ALA:O	2:D:117:LYS:HG3	2.16	0.46
1:A:54:ASN:HB2	1:A:277:CYS:O	2.16	0.46
1:A:164:LEU:O	1:A:246:ASN:HA	2.16	0.45
2:B:17[A]:MET:CE	2:B:34:GLN:HG2	2.45	0.45
13:A:2228:HOH:O	4:C:431:NAG:H82	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:THR:HG21	7:C:631:NAG:H61	1.97	0.45
1:E:264:LYS:HB3	2:F:63:PHE:CD2	2.52	0.45
1:C:321:ARG:HG3	1:C:321:ARG:HH11	1.82	0.44
8:A:1328:EDO:H11	13:A:2207:HOH:O	2.18	0.44
2:F:169:ASN:HA	2:F:172:GLN:HE21	1.83	0.44
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.52	0.44
2:B:17[A]:MET:HE2	2:B:34:GLN:HG2	2.00	0.43
1:E:52:CYS:HB3	1:E:277:CYS:O	2.20	0.42
2:B:17[A]:MET:CE	2:B:34:GLN:CG	2.97	0.42
1:E:264:LYS:HE3	2:F:63:PHE:CE2	2.54	0.42
5:A:600:FUC:C6	2:B:143:LYS:HD2	2.50	0.42
1:A:50:LYS:HA	1:A:272:VAL:HG13	2.02	0.42
1:E:146:SER:OG	8:E:1327:EDO:H11	2.20	0.42
1:C:140:LYS:NZ	1:C:145:ASP:OD1	2.52	0.42
4:C:422:NAG:C6	4:C:423:BMA:H2	2.50	0.41
2:D:163:ARG:HG2	2:D:167:LEU:HD22	2.01	0.41
4:C:423:BMA:H3	4:C:424:MAN:H2	1.65	0.41
1:E:3[B]:ASN:HA	1:E:4:PRO:HD2	1.86	0.41
1:A:34:ILE:HD11	1:A:321:ARG:HD3	2.02	0.41
2:F:1:GLY:HA3	13:F:2003:HOH:O	2.19	0.41
13:A:2196:HOH:O	1:C:201:ARG:NE	2.53	0.41
2:B:1:GLY:HA3	13:B:2003:HOH:O	2.21	0.41
2:B:55:VAL:HG21	2:B:99:LEU:HD11	2.03	0.41
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.56	0.40
2:D:51:LYS:HE2	2:D:51:LYS:HB2	1.96	0.40
2:F:11:GLU:HG3	13:F:2007:HOH:O	2.22	0.40
1:A:310:ARG:NH2	2:B:86[B]:ASP:OD1	2.55	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	331/329 (101%)	323 (98%)	8 (2%)	0	100	100
1	C	319/329 (97%)	309 (97%)	10 (3%)	0	100	100
1	E	327/329 (99%)	314 (96%)	10 (3%)	3 (1%)	21	9
2	B	176/172 (102%)	167 (95%)	9 (5%)	0	100	100
2	D	174/172 (101%)	166 (95%)	8 (5%)	0	100	100
2	F	177/172 (103%)	169 (96%)	8 (4%)	0	100	100
All	All	1504/1503 (100%)	1448 (96%)	53 (4%)	3 (0%)	56	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	GLN
1	E	3[A]	ASN
1	E	3[B]	ASN

### 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	296/292 (101%)	292 (99%)	4 (1%)	74	71
1	C	283/292 (97%)	280 (99%)	3 (1%)	80	79
1	E	291/292 (100%)	287 (99%)	4 (1%)	74	71
2	B	151/146 (103%)	151 (100%)	0	100	100
2	D	150/146 (103%)	142 (95%)	8 (5%)	28	16
2	F	153/146 (105%)	149 (97%)	4 (3%)	54	45
All	All	1324/1314 (101%)	1301 (98%)	23 (2%)	70	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	264	LYS

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Mol	Chain	Res	Type
1	A	272	VAL
1	A	326	LYS
1	C	18	HIS
1	C	151	LEU
1	C	321	ARG
2	D	17[A]	MET
2	D	17[B]	MET
2	D	51	LYS
2	D	57	GLU
2	D	60	ASN
2	D	108	ILE
2	D	167	LEU
2	D	172	GLN
1	E	18	HIS
1	E	154	LEU
1	E	242	ILE
1	E	278	VAL
2	F	56[A]	ILE
2	F	56[B]	ILE
2	F	57	GLU
2	F	167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	188	ASN
1	C	18	HIS
1	C	296	ASN
2	F	172	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

68 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	411	1,3	14,14,15	0.52	0	15,19,21	1.33	1 (6%)
3	NAG	A	412	3	14,14,15	0.50	0	15,19,21	1.05	1 (6%)
3	NAG	A	421	1,3	14,14,15	0.58	0	15,19,21	1.19	2 (13%)
3	NAG	A	422	3	14,14,15	0.53	0	15,19,21	0.78	0
4	NAG	A	431	1,4	14,14,15	0.63	0	15,19,21	1.04	1 (6%)
4	NAG	A	432	4	14,14,15	0.56	0	15,19,21	1.02	1 (6%)
4	BMA	A	433	4	11,11,12	0.63	0	14,15,17	2.88	5 (35%)
4	MAN	A	434	4	11,11,12	0.49	0	14,15,17	0.92	1 (7%)
4	MAN	A	437	4	11,11,12	0.59	0	14,15,17	1.49	2 (14%)
3	NAG	A	441	1,3	14,14,15	0.59	0	15,19,21	0.94	0
3	NAG	A	442	3	14,14,15	0.64	0	15,19,21	1.76	3 (20%)
5	FUC	A	600	5	10,10,11	0.63	0	14,14,16	1.24	3 (21%)
5	NAG	A	601	1,5	14,14,15	0.64	0	15,19,21	1.13	1 (6%)
5	NAG	A	602	5	14,14,15	0.55	0	15,19,21	1.27	2 (13%)
5	BMA	A	603	5	11,11,12	0.43	0	14,15,17	1.41	3 (21%)
3	NAG	A	621	1,3	14,14,15	0.59	0	15,19,21	0.97	0
3	NAG	A	622	3	14,14,15	0.56	0	15,19,21	1.38	1 (6%)
7	NAG	A	631	1,7	14,14,15	0.43	0	15,19,21	1.14	1 (6%)
7	NAG	A	632	7	14,14,15	0.50	0	15,19,21	1.00	1 (6%)
7	BMA	A	633	7	11,11,12	0.41	0	14,15,17	0.96	1 (7%)
9	FUC	B	200	9	10,10,11	0.63	0	14,14,16	1.13	0
9	NAG	B	201	9,2	14,14,15	0.53	0	15,19,21	1.68	1 (6%)
7	NAG	C	411	1,7	14,14,15	0.58	0	15,19,21	0.88	0
7	NAG	C	412	7	14,14,15	0.59	0	15,19,21	1.04	2 (13%)
7	BMA	C	413	7	11,11,12	0.67	0	14,15,17	2.49	3 (21%)
4	NAG	C	421	1,4	14,14,15	0.58	0	15,19,21	1.77	3 (20%)
4	NAG	C	422	4	14,14,15	0.72	0	15,19,21	1.16	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	C	423	4	11,11,12	0.48	0	14,15,17	0.92	0
4	MAN	C	424	4	11,11,12	0.80	0	14,15,17	1.78	2 (14%)
4	MAN	C	428	4	11,11,12	0.51	0	14,15,17	1.69	2 (14%)
4	NAG	C	431	1,4	14,14,15	0.57	0	15,19,21	0.81	0
4	NAG	C	432	4	14,14,15	0.50	0	15,19,21	1.31	2 (13%)
4	BMA	C	433	4	11,11,12	0.38	0	14,15,17	0.85	0
4	MAN	C	434	4	11,11,12	0.57	0	14,15,17	0.87	1 (7%)
4	MAN	C	437	4	11,11,12	0.59	0	14,15,17	1.31	2 (14%)
3	NAG	C	441	1,3	14,14,15	0.60	0	15,19,21	1.09	0
3	NAG	C	442	3	14,14,15	0.46	0	15,19,21	0.71	0
11	FUC	C	620	11	10,10,11	0.76	0	14,14,16	3.03	6 (42%)
11	NAG	C	621	1,11	14,14,15	0.58	0	15,19,21	1.08	1 (6%)
11	NAG	C	622	11	14,14,15	0.53	0	15,19,21	0.95	1 (6%)
11	BMA	C	623	11	11,11,12	0.56	0	14,15,17	1.46	3 (21%)
11	MAN	C	624	11	11,11,12	0.51	0	14,15,17	1.07	1 (7%)
11	MAN	C	628	11	11,11,12	0.58	0	14,15,17	2.48	3 (21%)
7	NAG	C	631	1,7	14,14,15	0.61	0	15,19,21	1.47	2 (13%)
7	NAG	C	632	7	14,14,15	0.59	0	15,19,21	1.03	2 (13%)
7	BMA	C	633	7	11,11,12	0.38	0	14,15,17	0.97	1 (7%)
12	FUC	D	200	12	10,10,11	0.76	0	14,14,16	1.55	4 (28%)
12	NAG	D	201	12,2	14,14,15	0.53	0	15,19,21	1.35	3 (20%)
12	NAG	D	202	12	14,14,15	0.51	0	15,19,21	0.97	1 (6%)
3	NAG	E	411	1,3	14,14,15	0.72	0	15,19,21	2.50	5 (33%)
3	NAG	E	412	3	14,14,15	0.45	0	15,19,21	2.09	1 (6%)
3	NAG	E	421	1,3	14,14,15	0.63	0	15,19,21	1.61	2 (13%)
3	NAG	E	422	3	14,14,15	0.51	0	15,19,21	0.86	0
4	NAG	E	431	1,4	14,14,15	0.59	0	15,19,21	1.02	1 (6%)
4	NAG	E	432	4	14,14,15	0.62	0	15,19,21	0.98	1 (6%)
4	BMA	E	433	4	11,11,12	0.38	0	14,15,17	1.16	1 (7%)
4	MAN	E	434	4	11,11,12	0.58	0	14,15,17	1.00	1 (7%)
4	MAN	E	437	4	11,11,12	0.61	0	14,15,17	1.17	1 (7%)
3	NAG	E	441	1,3	14,14,15	0.59	0	15,19,21	1.72	4 (26%)
3	NAG	E	442	3	14,14,15	0.59	0	15,19,21	2.25	3 (20%)
12	FUC	E	600	12	10,10,11	0.77	0	14,14,16	1.83	4 (28%)
12	NAG	E	601	1,12	14,14,15	0.50	0	15,19,21	1.29	1 (6%)
12	NAG	E	602	12	14,14,15	0.61	0	15,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	631	1,3	14,14,15	0.61	0	15,19,21	1.42	3 (20%)
3	NAG	E	632	3	14,14,15	0.51	0	15,19,21	0.88	0
12	FUC	F	200	12	10,10,11	0.70	0	14,14,16	0.90	0
12	NAG	F	201	12,2	14,14,15	0.55	0	15,19,21	1.52	4 (26%)
12	NAG	F	202	12	14,14,15	0.41	0	15,19,21	0.98	1 (6%)

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	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	412	3	-	0/6/23/26	0/1/1/1
3	NAG	A	421	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	422	3	-	0/6/23/26	0/1/1/1
4	NAG	A	431	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	432	4	-	0/6/23/26	0/1/1/1
4	BMA	A	433	4	-	0/2/19/22	0/1/1/1
4	MAN	A	434	4	-	0/2/19/22	0/1/1/1
4	MAN	A	437	4	-	0/2/19/22	0/1/1/1
3	NAG	A	441	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	442	3	-	0/6/23/26	0/1/1/1
5	FUC	A	600	5	1/1/4/5	0/0/17/20	0/1/1/1
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1
5	BMA	A	603	5	-	0/2/19/22	0/1/1/1
3	NAG	A	621	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	622	3	-	0/6/23/26	0/1/1/1
7	NAG	A	631	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	632	7	-	0/6/23/26	0/1/1/1
7	BMA	A	633	7	-	0/2/19/22	0/1/1/1
9	FUC	B	200	9	1/1/4/5	0/0/17/20	0/1/1/1
9	NAG	B	201	9,2	-	0/6/23/26	0/1/1/1
7	NAG	C	411	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	412	7	-	0/6/23/26	0/1/1/1
7	BMA	C	413	7	-	0/2/19/22	0/1/1/1
4	NAG	C	421	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	422	4	-	0/6/23/26	0/1/1/1
4	BMA	C	423	4	-	0/2/19/22	0/1/1/1
4	MAN	C	424	4	-	0/2/19/22	0/1/1/1
4	MAN	C	428	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	431	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	432	4	-	0/6/23/26	0/1/1/1
4	BMA	C	433	4	-	0/2/19/22	0/1/1/1
4	MAN	C	434	4	-	0/2/19/22	1/1/1/1
4	MAN	C	437	4	-	0/2/19/22	0/1/1/1
3	NAG	C	441	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	442	3	-	0/6/23/26	0/1/1/1
11	FUC	C	620	11	1/1/4/5	0/0/17/20	0/1/1/1
11	NAG	C	621	1,11	-	0/6/23/26	0/1/1/1
11	NAG	C	622	11	-	0/6/23/26	0/1/1/1
11	BMA	C	623	11	-	0/2/19/22	0/1/1/1
11	MAN	C	624	11	-	0/2/19/22	0/1/1/1
11	MAN	C	628	11	-	0/2/19/22	0/1/1/1
7	NAG	C	631	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	632	7	-	0/6/23/26	0/1/1/1
7	BMA	C	633	7	-	0/2/19/22	0/1/1/1
12	FUC	D	200	12	1/1/4/5	0/0/17/20	0/1/1/1
12	NAG	D	201	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	202	12	-	0/6/23/26	0/1/1/1
3	NAG	E	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	412	3	-	0/6/23/26	0/1/1/1
3	NAG	E	421	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	422	3	-	0/6/23/26	0/1/1/1
4	NAG	E	431	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	432	4	-	0/6/23/26	0/1/1/1
4	BMA	E	433	4	-	0/2/19/22	0/1/1/1
4	MAN	E	434	4	-	0/2/19/22	0/1/1/1
4	MAN	E	437	4	-	0/2/19/22	0/1/1/1
3	NAG	E	441	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	442	3	-	0/6/23/26	0/1/1/1
12	FUC	E	600	12	1/1/4/5	0/0/17/20	0/1/1/1
12	NAG	E	601	1,12	-	0/6/23/26	0/1/1/1
12	NAG	E	602	12	-	0/6/23/26	0/1/1/1
3	NAG	E	631	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	632	3	-	0/6/23/26	0/1/1/1
12	FUC	F	200	12	1/1/4/5	0/0/17/20	0/1/1/1
12	NAG	F	201	12,2	-	0/6/23/26	0/1/1/1
12	NAG	F	202	12	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	620	FUC	C1-C2-C3	-8.25	99.78	109.54
11	C	620	FUC	C1-O5-C5	-4.54	105.37	112.38
11	C	620	FUC	O5-C1-C2	-3.16	105.74	110.86
5	A	602	NAG	C2-N2-C7	-3.08	119.08	123.04
11	C	621	NAG	C2-N2-C7	-3.01	119.17	123.04
4	E	431	NAG	C2-N2-C7	-2.67	119.61	123.04
5	A	600	FUC	C1-O5-C5	-2.57	108.41	112.38
4	A	433	BMA	O5-C5-C6	-2.53	101.86	107.35
12	D	200	FUC	C1-O5-C5	-2.45	108.59	112.38
3	E	442	NAG	O7-C7-C8	-2.36	117.73	122.06
3	E	441	NAG	O3-C3-C2	-2.32	104.52	109.11
7	C	631	NAG	O6-C6-C5	-2.20	104.07	111.33
7	C	632	NAG	C2-N2-C7	-2.11	120.32	123.04
4	C	432	NAG	C6-C5-C4	-2.10	107.84	113.02
3	E	631	NAG	O4-C4-C3	-2.06	105.70	110.34
5	A	600	FUC	C1-C2-C3	-2.03	107.14	109.54
3	A	421	NAG	O4-C4-C3	-2.03	105.78	110.34
12	F	201	NAG	C3-C2-N2	-2.03	105.71	110.56
12	D	200	FUC	O5-C1-C2	-2.03	107.57	110.86
4	A	434	MAN	C1-C2-C3	-2.02	107.15	109.54
11	C	620	FUC	O2-C2-C1	2.03	113.28	109.21
7	C	412	NAG	O5-C5-C6	2.04	111.76	107.35
5	A	601	NAG	O6-C6-C5	2.08	118.20	111.33
7	C	412	NAG	C4-C3-C2	2.10	114.50	111.23
3	E	411	NAG	O5-C5-C6	2.11	111.91	107.35
3	A	412	NAG	C2-N2-C7	2.12	125.76	123.04
3	E	441	NAG	C8-C7-N2	2.12	120.17	116.11
5	A	603	BMA	C3-C4-C5	2.14	113.93	110.20
4	E	437	MAN	C2-C3-C4	2.18	114.74	111.04
12	D	201	NAG	O6-C6-C5	2.19	118.58	111.33
12	E	600	FUC	O5-C5-C6	2.22	109.79	106.13
11	C	620	FUC	O2-C2-C3	2.22	114.58	110.12
12	F	201	NAG	O6-C6-C5	2.24	118.75	111.33
7	A	632	NAG	C4-C3-C2	2.25	114.72	111.23
11	C	623	BMA	C3-C4-C5	2.26	114.13	110.20
7	C	633	BMA	C1-C2-C3	2.26	112.22	109.54
4	C	437	MAN	C2-C3-C4	2.29	114.93	111.04
12	F	202	NAG	C1-O5-C5	2.33	115.21	112.25
12	D	202	NAG	C1-O5-C5	2.34	115.22	112.25
3	E	631	NAG	C1-O5-C5	2.35	115.23	112.25
7	C	632	NAG	C1-O5-C5	2.37	115.26	112.25
4	C	434	MAN	C1-O5-C5	2.39	115.28	112.25
7	A	633	BMA	C3-C4-C5	2.40	114.38	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	421	NAG	C3-C4-C5	2.44	114.45	110.20
4	C	421	NAG	C4-C3-C2	2.44	115.03	111.23
4	A	431	NAG	C1-O5-C5	2.45	115.36	112.25
5	A	602	NAG	C1-O5-C5	2.46	115.37	112.25
11	C	623	BMA	C1-C2-C3	2.47	112.46	109.54
3	E	411	NAG	C3-C4-C5	2.48	114.51	110.20
4	E	434	MAN	C1-C2-C3	2.49	112.49	109.54
12	D	201	NAG	C2-N2-C7	2.52	126.27	123.04
12	D	201	NAG	C1-O5-C5	2.53	115.46	112.25
12	F	201	NAG	C4-C3-C2	2.54	115.17	111.23
12	D	200	FUC	O5-C5-C6	2.57	110.39	106.13
4	C	428	MAN	C1-C2-C3	2.58	112.60	109.54
3	E	411	NAG	C2-N2-C7	2.64	126.43	123.04
5	A	600	FUC	O5-C5-C6	2.66	110.53	106.13
4	E	433	BMA	C1-C2-C3	2.69	112.72	109.54
12	D	200	FUC	C3-C4-C5	2.69	114.26	109.72
5	A	603	BMA	C2-C3-C4	2.73	115.68	111.04
5	A	603	BMA	C1-C2-C3	2.76	112.81	109.54
4	A	437	MAN	C1-C2-C3	2.79	112.84	109.54
11	C	622	NAG	C1-O5-C5	2.80	115.81	112.25
4	C	424	MAN	C2-C3-C4	2.86	115.90	111.04
11	C	624	MAN	C1-O5-C5	2.87	115.89	112.25
3	A	442	NAG	C3-C4-C5	2.89	115.23	110.20
4	A	432	NAG	C1-O5-C5	2.91	115.94	112.25
4	E	432	NAG	C1-O5-C5	2.98	116.03	112.25
12	F	201	NAG	O5-C5-C6	3.01	113.86	107.35
3	A	421	NAG	C4-C3-C2	3.07	116.00	111.23
3	E	442	NAG	C8-C7-N2	3.09	122.03	116.11
12	E	600	FUC	C2-C3-C4	3.15	116.39	111.04
4	C	437	MAN	C3-C4-C5	3.18	115.74	110.20
7	A	631	NAG	C1-O5-C5	3.21	116.32	112.25
11	C	620	FUC	O5-C5-C6	3.21	111.44	106.13
3	A	442	NAG	C4-C3-C2	3.23	116.26	111.23
12	E	600	FUC	C3-C4-C5	3.25	115.19	109.72
4	C	432	NAG	C1-O5-C5	3.29	116.42	112.25
3	E	421	NAG	C3-C4-C5	3.31	115.97	110.20
3	E	631	NAG	C4-C3-C2	3.39	116.50	111.23
7	C	631	NAG	C1-O5-C5	3.52	116.71	112.25
3	E	441	NAG	C2-N2-C7	3.53	127.58	123.04
4	C	422	NAG	O4-C4-C5	3.54	118.62	109.24
11	C	623	BMA	C1-O5-C5	3.60	116.82	112.25
3	E	441	NAG	C4-C3-C2	3.68	116.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	NAG	C2-N2-C7	3.70	127.79	123.04
4	A	433	BMA	C3-C4-C5	3.72	116.68	110.20
4	A	433	BMA	C2-C3-C4	3.93	117.72	111.04
12	E	600	FUC	C1-C2-C3	4.01	114.29	109.54
4	A	437	MAN	C1-O5-C5	4.18	117.56	112.25
3	A	622	NAG	C2-N2-C7	4.26	128.51	123.04
3	A	442	NAG	C2-N2-C7	4.26	128.51	123.04
12	E	601	NAG	C1-O5-C5	4.30	117.71	112.25
11	C	628	MAN	O5-C1-C2	4.41	118.01	110.86
3	E	421	NAG	C4-C3-C2	4.42	118.10	111.23
7	C	413	BMA	O5-C1-C2	4.43	118.04	110.86
3	E	411	NAG	C4-C3-C2	4.67	118.49	111.23
4	A	433	BMA	C1-O5-C5	5.08	118.69	112.25
11	C	628	MAN	C1-C2-C3	5.09	115.56	109.54
4	C	421	NAG	C1-O5-C5	5.12	118.74	112.25
4	C	428	MAN	C1-O5-C5	5.18	118.82	112.25
4	C	424	MAN	C1-C2-C3	5.26	115.77	109.54
7	C	413	BMA	C1-O5-C5	5.36	119.05	112.25
9	B	201	NAG	C1-O5-C5	5.47	119.19	112.25
7	C	413	BMA	C1-C2-C3	5.52	116.07	109.54
11	C	628	MAN	C1-O5-C5	5.87	119.69	112.25
4	A	433	BMA	C1-C2-C3	6.67	117.43	109.54
3	E	411	NAG	C1-O5-C5	6.77	120.84	112.25
3	E	442	NAG	C2-N2-C7	7.21	132.30	123.04
3	E	412	NAG	C1-O5-C5	7.45	121.71	112.25

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	621	NAG	C1
12	E	600	FUC	C1
12	F	200	FUC	C1
11	C	620	FUC	C1
9	B	200	FUC	C1
5	A	600	FUC	C1
12	D	200	FUC	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	434	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	421	NAG	1	0
4	A	433	BMA	2	0
4	A	437	MAN	2	0
5	A	600	FUC	2	0
4	C	422	NAG	3	0
4	C	423	BMA	4	0
4	C	424	MAN	1	0
4	C	431	NAG	1	0
7	C	631	NAG	1	0
3	E	411	NAG	1	0
3	E	412	NAG	1	0

## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
8	EDO	A	1327	-	3,3,3	0.36	0	2,2,2	0.71	0
8	EDO	A	1328	-	3,3,3	0.48	0	2,2,2	0.46	0
6	BMA	A	604	-	11,11,12	0.37	0	14,15,17	0.70	0
8	EDO	B	1173	-	3,3,3	0.40	0	2,2,2	0.59	0
8	EDO	B	1174	-	3,3,3	0.47	0	2,2,2	0.44	0
8	EDO	C	1327	-	3,3,3	0.49	0	2,2,2	0.46	0
8	EDO	C	1328	-	3,3,3	0.48	0	2,2,2	0.54	0
10	NAG	C	601	1	14,14,15	0.53	0	15,19,21	1.04	1 (6%)
8	EDO	D	1173	-	3,3,3	0.47	0	2,2,2	0.45	0
8	EDO	E	1326	-	3,3,3	0.46	0	2,2,2	0.50	0
8	EDO	E	1327	-	3,3,3	0.48	0	2,2,2	0.47	0
10	NAG	E	621	1	14,14,15	0.63	0	15,19,21	1.07	1 (6%)
8	EDO	F	1173	-	3,3,3	0.47	0	2,2,2	0.49	0
8	EDO	F	1174	-	3,3,3	0.52	0	2,2,2	0.24	0
8	EDO	F	1175	-	3,3,3	0.47	0	2,2,2	0.47	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
8	EDO	A	1327	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1328	-	-	0/1/1/1	0/0/0/0
6	BMA	A	604	-	-	0/2/19/22	0/1/1/1
8	EDO	B	1173	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1174	-	-	0/1/1/1	0/0/0/0
8	EDO	C	1327	-	-	0/1/1/1	0/0/0/0
8	EDO	C	1328	-	-	0/1/1/1	0/0/0/0
10	NAG	C	601	1	-	0/6/23/26	0/1/1/1
8	EDO	D	1173	-	-	0/1/1/1	0/0/0/0
8	EDO	E	1326	-	-	0/1/1/1	0/0/0/0
8	EDO	E	1327	-	-	0/1/1/1	0/0/0/0
10	NAG	E	621	1	-	0/6/23/26	0/1/1/1
8	EDO	F	1173	-	-	0/1/1/1	0/0/0/0
8	EDO	F	1174	-	-	0/1/1/1	0/0/0/0
8	EDO	F	1175	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	601	NAG	C1-O5-C5	2.12	114.94	112.25
10	E	621	NAG	C4-C3-C2	3.25	116.29	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1328	EDO	1	0
8	E	1327	EDO	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	325/329 (98%)	-0.01	6 (1%) 71 74	19, 29, 48, 64	0
1	C	320/329 (97%)	0.00	2 (0%) 90 91	17, 29, 48, 71	0
1	E	325/329 (98%)	-0.04	4 (1%) 81 83	18, 30, 47, 66	0
2	B	172/172 (100%)	0.06	3 (1%) 73 76	15, 26, 42, 59	0
2	D	172/172 (100%)	0.13	4 (2%) 64 67	15, 27, 44, 63	0
2	F	172/172 (100%)	0.20	2 (1%) 81 83	16, 24, 41, 61	0
All	All	1486/1503 (98%)	0.04	21 (1%) 78 80	15, 28, 47, 71	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	TYR	4.8
1	A	276	ILE	4.3
1	A	142	GLY	3.8
1	A	278	VAL	3.4
1	A	81	TYR	3.3
1	A	143	SER	3.3
2	D	58	ARG	3.3
2	F	77[A]	ILE	2.9
1	E	276	ILE	2.8
2	D	172	GLN	2.7
2	B	77[A]	ILE	2.6
2	D	38[A]	LEU	2.6
1	A	277	CYS	2.5
2	D	63	PHE	2.4
2	B	172	GLN	2.3
2	F	59	THR	2.3
1	C	79	PHE	2.3
1	E	2	GLN	2.2
1	E	81	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	7	ASN	2.0
2	B	80	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
12	NAG	F	201	14/15	0.79	0.21	13.25	54,62,68,76	0
12	FUC	D	200	10/11	0.78	0.26	8.67	62,68,71,72	0
12	NAG	D	201	14/15	0.85	0.20	8.36	56,64,69,69	0
4	MAN	C	424	11/12	0.68	0.47	4.86	84,87,90,90	0
3	NAG	C	441	14/15	0.74	0.24	3.64	52,61,65,68	0
5	NAG	A	602	14/15	0.81	0.26	3.37	58,63,71,75	0
3	NAG	E	441	14/15	0.84	0.23	3.36	52,60,68,72	0
4	NAG	C	422	14/15	0.83	0.23	2.83	65,69,73,79	0
7	NAG	C	631	14/15	0.92	0.13	1.13	28,32,35,36	0
5	NAG	A	601	14/15	0.88	0.15	0.60	43,45,55,58	0
4	NAG	E	432	14/15	0.91	0.12	0.06	41,47,53,57	0
4	NAG	A	432	14/15	0.91	0.11	-0.15	43,48,54,59	0
4	NAG	C	432	14/15	0.93	0.11	-0.24	43,48,52,57	0
11	NAG	C	621	14/15	0.93	0.09	-1.22	30,35,41,45	0
4	BMA	C	433	11/12	0.81	0.15	-	62,69,74,74	0
3	NAG	A	412	14/15	0.63	0.49	-	94,100,105,105	0
12	FUC	E	600	10/11	0.74	0.28	-	71,76,79,79	0
11	MAN	C	628	11/12	0.79	0.40	-	72,74,81,85	0
12	FUC	F	200	10/11	0.80	0.37	-	74,78,80,82	0
3	NAG	C	442	14/15	0.69	0.31	-	72,77,80,80	0
11	FUC	C	620	10/11	0.89	0.16	-	49,52,54,56	0
4	BMA	C	423	11/12	0.77	0.33	-	84,86,91,97	0
12	NAG	F	202	14/15	0.69	0.34	-	82,87,91,93	0
4	MAN	A	437	11/12	0.85	0.20	-	82,85,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	B	201	14/15	0.85	0.23	-	54,61,65,68	0
4	NAG	C	431	14/15	0.92	0.12	-	38,41,42,43	0
4	NAG	A	431	14/15	0.93	0.10	-	37,40,42,43	0
7	NAG	C	412	14/15	0.73	0.35	-	82,85,89,89	0
3	NAG	A	621	14/15	0.56	0.34	-	66,72,76,82	0
3	NAG	A	422	14/15	0.65	0.50	-	84,88,94,95	0
12	NAG	E	601	14/15	0.87	0.18	-	56,60,68,72	0
4	MAN	C	428	11/12	0.50	0.56	-	94,100,104,107	0
5	BMA	A	603	11/12	0.77	0.36	-	80,86,89,92	0
7	BMA	C	413	11/12	0.56	0.30	-	90,95,101,101	0
4	MAN	C	437	11/12	0.71	0.27	-	79,80,84,85	0
7	NAG	A	632	14/15	0.74	0.26	-	70,75,80,84	0
11	MAN	C	624	11/12	0.90	0.12	-	44,49,53,54	0
11	BMA	C	623	11/12	0.84	0.19	-	49,51,62,68	0
12	NAG	D	202	14/15	0.69	0.35	-	74,80,85,85	0
3	NAG	E	631	14/15	0.90	0.13	-	41,48,52,54	0
7	BMA	A	633	11/12	0.59	0.29	-	84,87,91,93	0
7	NAG	C	632	14/15	0.90	0.12	-	38,42,44,48	0
4	NAG	C	421	14/15	0.90	0.24	-	51,57,60,62	0
3	NAG	A	622	14/15	0.74	0.39	-	83,89,93,94	0
3	NAG	E	632	14/15	0.85	0.28	-	61,67,69,69	0
3	NAG	A	421	14/15	0.85	0.20	-	62,67,74,79	0
3	NAG	E	422	14/15	0.56	0.40	-	85,89,96,97	0
12	NAG	E	602	14/15	0.71	0.19	-	70,72,77,78	0
3	NAG	A	442	14/15	0.58	0.36	-	71,79,82,84	0
9	FUC	B	200	10/11	0.86	0.35	-	72,76,79,81	0
4	NAG	E	431	14/15	0.93	0.12	-	39,42,44,44	0
5	FUC	A	600	10/11	0.84	0.30	-	59,64,68,68	0
4	MAN	E	437	11/12	0.81	0.20	-	77,80,84,85	0
4	MAN	C	434	11/12	0.75	0.27	-	70,75,81,83	0
7	BMA	C	633	11/12	0.84	0.14	-	51,54,57,60	0
7	NAG	C	411	14/15	0.78	0.30	-	65,69,74,78	0
3	NAG	A	441	14/15	0.74	0.20	-	51,62,66,71	0
3	NAG	E	421	14/15	0.73	0.29	-	61,69,74,80	0
11	NAG	C	622	14/15	0.91	0.11	-	39,45,48,49	0
7	NAG	A	631	14/15	0.84	0.20	-	48,57,61,65	0
3	NAG	E	442	14/15	0.59	0.47	-	81,84,87,90	0
3	NAG	E	412	14/15	0.59	0.39	-	95,99,101,101	0
4	BMA	E	433	11/12	0.87	0.12	-	61,67,73,75	0
4	MAN	A	434	11/12	0.66	0.22	-	79,86,93,95	0
3	NAG	E	411	14/15	0.80	0.35	-	76,82,88,90	0
4	BMA	A	433	11/12	0.76	0.12	-	64,71,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	411	14/15	0.87	0.25	-	71,75,81,89	0
4	MAN	E	434	11/12	0.80	0.25	-	78,81,84,87	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	C	1328	4/4	0.81	0.25	5.75	35,38,42,43	0
8	EDO	D	1173	4/4	0.88	0.29	3.21	51,52,52,53	0
8	EDO	F	1174	4/4	0.86	0.16	2.74	53,53,55,56	0
8	EDO	A	1327	4/4	0.88	0.14	2.70	37,37,39,40	0
8	EDO	A	1328	4/4	0.77	0.28	2.62	61,63,64,65	0
8	EDO	E	1327	4/4	0.82	0.13	2.46	48,50,52,53	0
8	EDO	B	1173	4/4	0.90	0.22	2.16	40,40,42,45	0
8	EDO	F	1173	4/4	0.85	0.20	1.59	58,59,60,61	0
8	EDO	B	1174	4/4	0.93	0.16	1.33	44,45,45,45	0
8	EDO	E	1326	4/4	0.86	0.18	1.20	54,55,57,61	0
8	EDO	F	1175	4/4	0.88	0.12	0.21	48,51,52,52	0
6	BMA	A	604	11/12	0.60	0.52	-	126,134,137,137	0
8	EDO	C	1327	4/4	0.62	0.19	-	65,65,67,67	0
10	NAG	E	621	14/15	0.71	0.51	-	68,76,80,81	0
10	NAG	C	601	14/15	0.61	0.44	-	90,93,98,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.