



Full wwPDB X-ray Structure Validation Report

Aug 7, 2014 – 08:03 PM EDT

PDB ID : 4UNW
Title : Structure of the A_Equine_Newmarket_2_93H3 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 : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

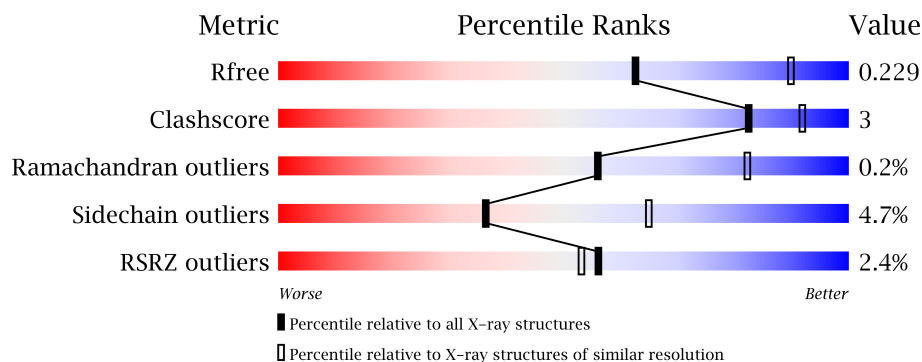
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	323	
1	C	323	
1	E	323	
2	B	173	
2	D	173	
2	F	173	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	421	-	X
4	NAG	C	611	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	E	411	-	X
4	NAG	E	421	-	X
4	NAG	E	611	-	X
4	NAG	F	201	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12914 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H3 HAEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2493	1558	440	481	14			
1	C	321	Total	C	N	O	S	0	0	0
			2501	1564	441	482	14			
1	E	321	Total	C	N	O	S	0	0	0
			2501	1564	441	482	14			

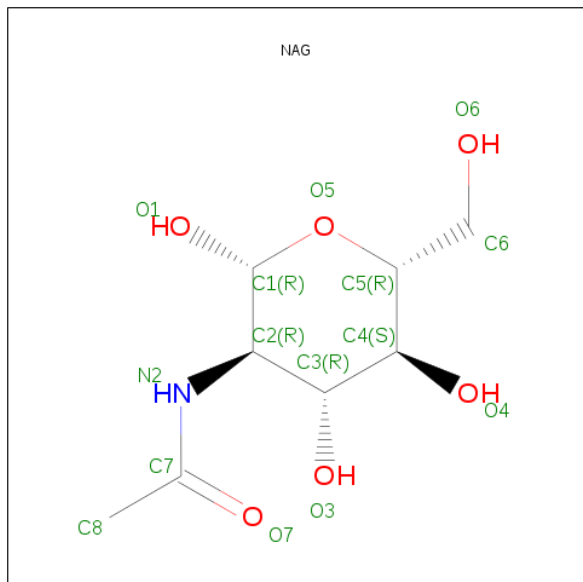
- Molecule 2 is a protein called H3 HAEMAGGLUTININ HA2 CHAIN.

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 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	C	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	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		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- 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		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

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

- 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		

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 9 is water.

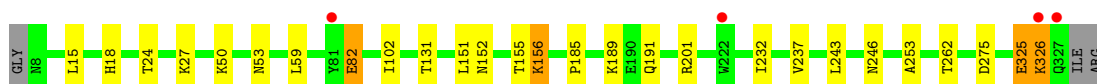
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	120	Total	O	0	0
			120	120		
9	B	124	Total	O	0	0
			124	124		
9	C	83	Total	O	0	0
			83	83		
9	D	98	Total	O	0	0
			98	98		
9	E	73	Total	O	0	0
			73	73		
9	F	64	Total	O	0	0
			64	64		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

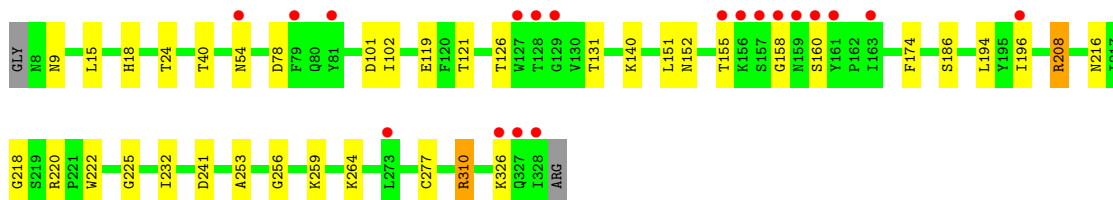
- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN

Chain A: 



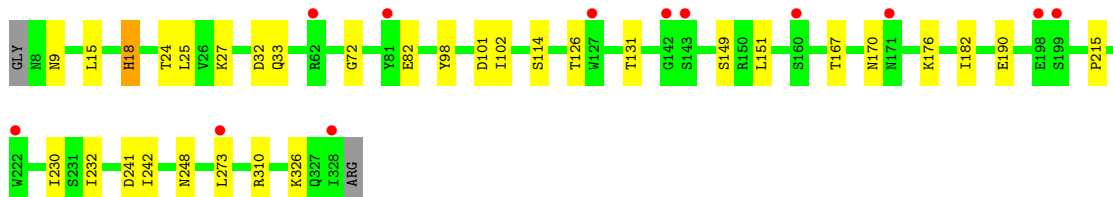
- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN

Chain C: 



- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN

Chain E: 



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain B: 



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain D: 



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.68Å 102.51Å 229.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.74 – 2.60 46.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (114.74-2.60) 99.8 (46.80-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.186 , 0.228 0.187 , 0.229	Depositor DCC
R_{free} test set	3714 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 73698 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12914	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, 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	0.42	0/2546	0.60	0/3457
1	C	0.40	0/2554	0.58	0/3468
1	E	0.39	0/2554	0.58	0/3468
2	B	0.46	0/1421	0.67	1/1910 (0.1%)
2	D	0.46	0/1421	0.67	1/1910 (0.1%)
2	F	0.45	0/1421	0.65	1/1910 (0.1%)
All	All	0.42	0/11917	0.61	3/16123 (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
8	E	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	110	LEU	CA-CB-CG	8.24	134.26	115.30
2	B	110	LEU	CA-CB-CG	7.17	131.80	115.30
2	F	110	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	E	446	NAG	C1

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2435	15	0
1	C	2501	0	2445	17	0
1	E	2501	0	2445	12	0
2	B	1396	0	1317	13	0
2	D	1396	0	1317	16	0
2	F	1396	0	1317	12	0
3	A	56	0	50	0	0
3	C	84	0	75	1	0
3	E	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	42	0	39	0	0
4	F	14	0	13	0	0
5	A	50	0	43	1	0
6	A	61	0	52	0	0
6	C	122	0	104	1	0
6	E	61	0	52	0	0
7	B	24	0	22	0	0
7	D	24	0	22	0	0
8	E	75	0	64	1	0
9	A	120	0	0	1	0
9	B	124	0	0	2	0
9	C	83	0	0	0	0
9	D	98	0	0	2	0
9	E	73	0	0	2	0
9	F	64	0	0	1	0
All	All	12914	0	11863	74	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:107:THR:HA	2:D:110:LEU:HD13	1.57	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:102:ILE:HG12	1:C:232:ILE:HB	1.60	0.82
2:F:107:THR:HA	2:F:110:LEU:HD13	1.62	0.81
2:B:171:PHE:O	2:B:172:GLN:HB3	1.83	0.76
1:A:27:LYS:HD2	2:D:54:ARG:HH22	1.53	0.73
1:E:102:ILE:HG12	1:E:232:ILE:HB	1.73	0.70
1:C:155:THR:HG21	1:C:194:LEU:HD22	1.76	0.68
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.76	0.68
2:F:171:PHE:O	2:F:172:GLN:HB3	1.93	0.67
2:B:107:THR:HA	2:B:110:LEU:HD13	1.77	0.66
1:A:102:ILE:HG12	1:A:232:ILE:HB	1.78	0.65
1:E:27:LYS:HG2	1:E:32:ASP:O	1.98	0.64
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.80	0.64
1:A:53:ASN:HB2	9:A:2043:HOH:O	1.98	0.63
2:B:76:ARG:NE	2:D:77:ILE:HD11	2.14	0.62
5:A:433:BMA:H62	5:A:437:MAN:H5	1.82	0.61
2:D:124:ARG:HD2	9:D:2081:HOH:O	2.01	0.60
2:F:27:GLN:HG3	2:F:32:THR:HG22	1.85	0.59
1:A:27:LYS:CD	2:D:54:ARG:HH22	2.16	0.59
2:B:76:ARG:HE	2:D:77:ILE:HD11	1.70	0.57
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.05	0.55
2:F:56:ILE:O	2:F:58:ARG:HG2	2.07	0.54
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.89	0.54
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.44	0.53
2:B:158:ASP:HB3	2:B:161:ILE:HD12	1.90	0.53
1:E:167:THR:HB	1:E:242:ILE:HD11	1.91	0.52
1:C:208:ARG:HD2	1:C:241:ASP:OD2	2.09	0.52
1:C:186:SER:HA	1:C:218:GLY:O	2.10	0.51
2:D:123:ARG:NH2	9:D:2079:HOH:O	2.44	0.50
2:B:171:PHE:O	2:B:172:GLN:CB	2.56	0.49
1:A:131:THR:HG22	1:A:156:LYS:O	2.12	0.49
1:E:170:ASN:OD1	1:E:176:LYS:HE3	2.13	0.49
1:A:201:ARG:NH2	1:A:246:ASN:HB3	2.28	0.48
2:B:124:ARG:HD2	9:B:2103:HOH:O	2.14	0.48
1:E:18:HIS:HE1	9:E:2008:HOH:O	1.95	0.48
1:E:72:GLY:HA3	1:E:149:SER:OG	2.13	0.47
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.96	0.47
1:A:131:THR:HG23	1:A:155:THR:OG1	2.15	0.47
1:A:152:ASN:HB3	1:A:253:ALA:HB3	1.97	0.46
1:E:25:LEU:HD13	1:E:33:GLN:HB3	1.97	0.46
1:C:160:SER:HA	1:C:196:ILE:HG13	1.97	0.46
2:B:163:ARG:HG2	2:B:167:LEU:HD22	1.98	0.46
1:E:98:TYR:CD1	1:E:230:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:LYS:HD2	1:A:275:ASP:HB3	1.97	0.45
1:C:152:ASN:HB3	1:C:253:ALA:HB3	1.99	0.45
1:C:216:ASN:HB2	1:C:220:ARG:HH22	1.81	0.45
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.99	0.45
1:C:310:ARG:NH1	2:D:90:ASP:OD1	2.50	0.45
2:F:124:ARG:HD2	9:F:2050:HOH:O	2.17	0.45
1:C:174:PHE:CE1	1:C:259:LYS:HG3	2.52	0.44
2:D:158:ASP:HB3	2:D:161:ILE:HD12	2.00	0.44
2:B:77:ILE:HD11	2:F:76:ARG:NE	2.33	0.44
1:A:325:GLU:O	1:A:326:LYS:HB2	2.18	0.44
1:C:121:THR:O	1:C:256:GLY:HA3	2.18	0.43
8:E:442:NAG:H82	2:F:69:GLU:OE2	2.18	0.43
2:B:54:ARG:NH2	9:B:2047:HOH:O	2.51	0.43
1:C:40:THR:HG21	2:D:52:LEU:HD11	2.00	0.43
6:C:443:BMA:H3	6:C:444:MAN:H2	1.82	0.43
2:F:6:ILE:HD12	2:F:112:ASP:HA	2.00	0.42
1:C:264:LYS:HB2	2:D:63:PHE:CD1	2.54	0.42
1:E:101:ASP:HB3	9:E:2032:HOH:O	2.18	0.42
1:A:201:ARG:HH22	1:A:246:ASN:HB3	1.82	0.42
1:A:59:LEU:HD22	1:A:82:GLU:HG2	2.01	0.42
1:C:54:ASN:HD22	3:C:411:NAG:H82	1.84	0.42
2:F:167:LEU:HD12	2:F:167:LEU:HA	1.92	0.42
1:C:15:LEU:CD2	2:D:118:LEU:HG	2.50	0.42
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.42
2:B:141:TYR:O	2:B:166:ALA:HA	2.20	0.41
2:D:130:ALA:HA	2:D:139:LYS:O	2.20	0.41
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.20	0.41
2:B:163:ARG:O	2:B:167:LEU:HB2	2.21	0.41
2:F:110:LEU:HD22	2:F:111:THR:HG23	2.03	0.40
1:C:119:GLU:O	1:C:119:GLU:HG3	2.20	0.40
2:D:51:LYS:HE3	2:D:107:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/323 (98%)	300 (94%)	17 (5%)	1 (0%)	50	77
1	C	319/323 (99%)	302 (95%)	16 (5%)	1 (0%)	50	77
1	E	319/323 (99%)	302 (95%)	17 (5%)	0	100	100
2	B	170/173 (98%)	162 (95%)	7 (4%)	1 (1%)	33	63
2	D	170/173 (98%)	159 (94%)	11 (6%)	0	100	100
2	F	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
All	All	1466/1488 (98%)	1387 (95%)	76 (5%)	3 (0%)	56	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	LYS
1	C	158	GLY
2	B	57	GLU

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	281/283 (99%)	273 (97%)	8 (3%)	56	84
1	C	282/283 (100%)	269 (95%)	13 (5%)	37	66
1	E	282/283 (100%)	268 (95%)	14 (5%)	34	61
2	B	144/145 (99%)	134 (93%)	10 (7%)	22	42
2	D	144/145 (99%)	134 (93%)	10 (7%)	22	42
2	F	144/145 (99%)	139 (96%)	5 (4%)	48	77
All	All	1277/1284 (100%)	1217 (95%)	60 (5%)	36	65

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	24	THR
1	A	82	GLU
1	A	151	LEU
1	A	156	LYS
1	A	189	LYS
1	A	262	THR
1	A	325	GLU
2	B	12	ASN
2	B	38	LEU
2	B	52	LEU
2	B	56	ILE
2	B	58	ARG
2	B	59	THR
2	B	77	ILE
2	B	110	LEU
2	B	167	LEU
2	B	172	GLN
1	C	9	ASN
1	C	18	HIS
1	C	24	THR
1	C	78	ASP
1	C	101	ASP
1	C	126	THR
1	C	131	THR
1	C	140	LYS
1	C	151	LEU
1	C	208	ARG
1	C	277	CYS
1	C	310	ARG
1	C	326	LYS
2	D	12	ASN
2	D	32	THR
2	D	38	LEU
2	D	52	LEU
2	D	56	ILE
2	D	58	ARG
2	D	77	ILE
2	D	110	LEU
2	D	167	LEU
2	D	172	GLN
1	E	9	ASN
1	E	18	HIS

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Mol	Chain	Res	Type
1	E	24	THR
1	E	82	GLU
1	E	114	SER
1	E	126	THR
1	E	131	THR
1	E	151	LEU
1	E	190	GLU
1	E	241	ASP
1	E	248	ASN
1	E	273	LEU
1	E	310	ARG
1	E	326	LYS
2	F	12	ASN
2	F	77	ILE
2	F	110	LEU
2	F	167	LEU
2	F	168	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	159	ASN
1	A	211	GLN
1	C	248	ASN
1	E	248	ASN
1	E	327	GLN
2	F	12	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

46 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	12,14,15	0.76	0	15,19,21	1.76	3 (20%)
3	NAG	A	412	3	12,14,15	0.62	0	15,19,21	1.25	2 (13%)
5	NAG	A	431	1,5	12,14,15	0.76	1 (8%)	15,19,21	1.51	3 (20%)
5	NAG	A	432	5	12,14,15	0.58	0	15,19,21	1.11	2 (13%)
5	BMA	A	433	5	10,11,12	0.51	0	11,15,17	1.29	2 (18%)
5	MAN	A	437	5	10,11,12	0.76	0	11,15,17	1.29	2 (18%)
6	NAG	A	441	1,6	12,14,15	0.80	1 (8%)	15,19,21	1.31	2 (13%)
6	NAG	A	442	6	12,14,15	0.81	1 (8%)	15,19,21	1.30	2 (13%)
6	BMA	A	443	6	10,11,12	0.57	0	11,15,17	0.98	0
6	MAN	A	444	6	10,11,12	0.77	0	11,15,17	1.13	1 (9%)
6	MAN	A	445	6	10,11,12	0.83	0	11,15,17	1.56	2 (18%)
3	NAG	A	601	1,3	12,14,15	0.76	0	15,19,21	1.73	3 (20%)
3	NAG	A	602	3	12,14,15	0.76	0	15,19,21	1.60	2 (13%)
7	NAG	B	201	2,7	12,14,15	0.65	0	15,19,21	1.27	1 (6%)
7	FUL	B	202	7	9,10,11	0.89	0	10,14,16	0.99	1 (10%)
3	NAG	C	411	1,3	12,14,15	0.76	1 (8%)	15,19,21	1.24	2 (13%)
3	NAG	C	412	3	12,14,15	0.73	1 (8%)	15,19,21	1.21	1 (6%)
3	NAG	C	421	1,3	12,14,15	0.95	1 (8%)	15,19,21	1.36	3 (20%)
3	NAG	C	422	3	12,14,15	0.71	1 (8%)	15,19,21	0.71	0
6	NAG	C	431	1,6	12,14,15	0.72	1 (8%)	15,19,21	1.14	1 (6%)
6	NAG	C	432	6	12,14,15	0.70	1 (8%)	15,19,21	0.97	0
6	BMA	C	433	6	10,11,12	0.58	0	11,15,17	1.68	3 (27%)
6	MAN	C	434	6	10,11,12	0.84	0	11,15,17	1.25	2 (18%)
6	MAN	C	437	6	10,11,12	0.84	0	11,15,17	1.68	3 (27%)
6	NAG	C	441	1,6	12,14,15	0.78	1 (8%)	15,19,21	0.83	0
6	NAG	C	442	6	12,14,15	0.65	0	15,19,21	1.17	1 (6%)
6	BMA	C	443	6	10,11,12	0.65	0	11,15,17	0.81	0
6	MAN	C	444	6	10,11,12	0.77	0	11,15,17	0.95	1 (9%)
6	MAN	C	445	6	10,11,12	0.77	0	11,15,17	1.18	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	601	1,3	12,14,15	0.66	0	15,19,21	1.68	4 (26%)
3	NAG	C	602	3	12,14,15	0.86	1 (8%)	15,19,21	2.12	5 (33%)
7	NAG	D	201	2,7	12,14,15	0.74	0	15,19,21	2.05	4 (26%)
7	FUL	D	202	7	9,10,11	1.00	0	10,14,16	1.09	0
6	NAG	E	431	1,6	12,14,15	0.73	0	15,19,21	1.22	1 (6%)
6	NAG	E	432	6	12,14,15	0.72	0	15,19,21	1.16	1 (6%)
6	BMA	E	433	6	10,11,12	0.65	0	11,15,17	1.79	3 (27%)
6	MAN	E	434	6	10,11,12	0.85	1 (10%)	11,15,17	1.97	2 (18%)
6	MAN	E	437	6	10,11,12	0.74	0	11,15,17	1.89	3 (27%)
8	NAG	E	441	1,8	12,14,15	0.80	1 (8%)	15,19,21	1.06	2 (13%)
8	NAG	E	442	8	12,14,15	0.69	1 (8%)	15,19,21	1.03	0
8	BMA	E	443	8	10,11,12	0.72	0	11,15,17	1.92	4 (36%)
8	MAN	E	444	8	10,11,12	0.88	1 (10%)	11,15,17	2.14	2 (18%)
8	MAN	E	445	8	10,11,12	0.65	0	11,15,17	1.52	2 (18%)
8	NAG	E	446	8	12,14,15	1.01	1 (8%)	15,19,21	2.78	5 (33%)
3	NAG	E	601	1,3	12,14,15	0.78	1 (8%)	15,19,21	0.79	0
3	NAG	E	602	3	12,14,15	0.64	0	15,19,21	1.14	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
5	NAG	A	431	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	432	5	-	0/6/23/26	0/1/1/1
5	BMA	A	433	5	-	0/2/19/22	0/1/1/1
5	MAN	A	437	5	-	0/2/19/22	0/1/1/1
6	NAG	A	441	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	442	6	-	0/6/23/26	0/1/1/1
6	BMA	A	443	6	-	0/2/19/22	0/1/1/1
6	MAN	A	444	6	-	0/2/19/22	0/1/1/1
6	MAN	A	445	6	-	0/2/19/22	0/1/1/1
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2,7	-	0/6/23/26	0/1/1/1
7	FUL	B	202	7	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	412	3	-	0/6/23/26	0/1/1/1
3	NAG	C	421	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	422	3	-	0/6/23/26	0/1/1/1
6	NAG	C	431	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	432	6	-	0/6/23/26	0/1/1/1
6	BMA	C	433	6	-	0/2/19/22	0/1/1/1
6	MAN	C	434	6	-	0/2/19/22	0/1/1/1
6	MAN	C	437	6	-	0/2/19/22	0/1/1/1
6	NAG	C	441	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	442	6	-	0/6/23/26	0/1/1/1
6	BMA	C	443	6	-	0/2/19/22	0/1/1/1
6	MAN	C	444	6	-	0/2/19/22	1/1/1/1
6	MAN	C	445	6	-	0/2/19/22	1/1/1/1
3	NAG	C	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	3	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2,7	-	0/6/23/26	0/1/1/1
7	FUL	D	202	7	-	0/0/17/20	0/1/1/1
6	NAG	E	431	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	432	6	-	0/6/23/26	0/1/1/1
6	BMA	E	433	6	-	0/2/19/22	0/1/1/1
6	MAN	E	434	6	-	0/2/19/22	0/1/1/1
6	MAN	E	437	6	-	0/2/19/22	0/1/1/1
8	NAG	E	441	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	442	8	-	0/6/23/26	0/1/1/1
8	BMA	E	443	8	-	0/2/19/22	0/1/1/1
8	MAN	E	444	8	-	0/2/19/22	0/1/1/1
8	MAN	E	445	8	-	0/2/19/22	0/1/1/1
8	NAG	E	446	8	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	421	NAG	O5-C5	-2.76	1.41	1.45
3	E	601	NAG	O5-C5	-2.35	1.41	1.45
6	A	442	NAG	O5-C5	-2.33	1.41	1.45
3	C	602	NAG	O5-C5	-2.29	1.41	1.45
8	E	446	NAG	O5-C5	-2.24	1.42	1.45
5	A	431	NAG	O5-C5	-2.20	1.42	1.45
8	E	441	NAG	O5-C5	-2.17	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	431	NAG	O5-C5	-2.17	1.42	1.45
6	C	441	NAG	O5-C5	-2.17	1.42	1.45
3	C	411	NAG	O5-C5	-2.16	1.42	1.45
3	C	412	NAG	O5-C5	-2.14	1.42	1.45
3	C	422	NAG	O5-C5	-2.14	1.42	1.45
6	A	441	NAG	O5-C5	-2.12	1.42	1.45
6	C	432	NAG	O5-C5	-2.09	1.42	1.45
8	E	444	MAN	O5-C5	-2.08	1.42	1.45
6	E	434	MAN	O5-C5	-2.07	1.42	1.45
8	E	442	NAG	O5-C5	-2.03	1.42	1.45

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	446	NAG	C2-N2-C7	8.52	133.70	123.39
6	E	434	MAN	C4-C3-C2	5.32	116.54	110.61
8	E	444	MAN	C4-C3-C2	5.29	116.50	110.61
7	D	201	NAG	C2-N2-C7	4.93	129.36	123.39
3	C	602	NAG	C2-N2-C7	4.92	129.35	123.39
3	A	602	NAG	O5-C5-C6	4.89	112.11	106.98
3	A	411	NAG	C2-N2-C7	4.72	129.10	123.39
3	C	602	NAG	C3-C2-N2	-4.36	105.08	111.62
3	C	601	NAG	O5-C5-C6	4.27	111.47	106.98
8	E	444	MAN	O5-C5-C6	4.23	111.42	106.98
8	E	443	BMA	C3-C4-C5	3.82	117.03	110.17
8	E	445	MAN	O5-C5-C6	3.72	110.89	106.98
6	A	445	MAN	O5-C5-C6	3.71	110.87	106.98
8	E	446	NAG	O5-C5-C6	3.67	110.83	106.98
6	E	433	BMA	C4-C3-C2	3.67	114.70	110.61
8	E	443	BMA	C4-C3-C2	3.67	114.70	110.61
6	E	437	MAN	C3-C4-C5	3.59	116.62	110.17
7	D	201	NAG	C3-C2-N2	-3.53	106.32	111.62
3	A	601	NAG	C3-C4-C5	3.49	116.43	110.17
3	A	601	NAG	C4-C3-C2	3.46	118.02	110.74
6	C	433	BMA	O5-C5-C4	3.45	115.03	110.65
6	E	437	MAN	C4-C3-C2	3.44	114.44	110.61
6	C	437	MAN	C4-C3-C2	3.38	114.38	110.61
6	C	442	NAG	O5-C5-C6	3.38	110.53	106.98
6	A	442	NAG	C3-C2-N2	-3.35	106.59	111.62
3	A	412	NAG	O5-C5-C6	3.35	110.50	106.98
6	C	445	MAN	O5-C5-C6	3.26	110.41	106.98
5	A	433	BMA	O5-C5-C4	3.25	114.78	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	201	NAG	C3-C2-N2	-3.23	106.78	111.62
5	A	431	NAG	C3-C4-C5	-3.20	104.43	110.17
6	E	437	MAN	O5-C5-C4	3.13	114.63	110.65
8	E	446	NAG	C3-C2-N2	3.12	116.31	111.62
6	C	433	BMA	O5-C5-C6	2.98	110.11	106.98
3	C	602	NAG	O5-C5-C6	2.94	110.06	106.98
3	C	411	NAG	C4-C3-C2	2.90	116.84	110.74
8	E	446	NAG	C8-C7-N2	2.90	121.60	116.12
3	A	411	NAG	C3-C2-N2	2.86	115.91	111.62
3	C	421	NAG	C4-C3-C2	2.80	116.62	110.74
5	A	431	NAG	O5-C5-C6	2.79	109.91	106.98
6	C	437	MAN	C3-C4-C5	2.76	115.13	110.17
6	A	441	NAG	C2-N2-C7	2.76	126.73	123.39
5	A	437	MAN	O5-C5-C6	2.75	109.87	106.98
3	A	411	NAG	O5-C5-C4	2.74	114.14	110.65
6	E	433	BMA	C3-C4-C5	2.73	115.07	110.17
6	C	444	MAN	O5-C5-C6	2.73	109.84	106.98
3	A	412	NAG	C2-N2-C7	2.73	126.69	123.39
6	C	434	MAN	O5-C5-C6	2.70	109.82	106.98
6	E	432	NAG	O5-C5-C4	2.70	114.08	110.65
7	B	202	FUL	C3-C4-C5	2.60	114.06	109.78
6	C	437	MAN	O5-C5-C6	2.59	109.70	106.98
6	E	434	MAN	C3-C4-C5	2.59	114.81	110.17
6	E	433	BMA	O3-C3-C4	-2.58	104.58	110.36
6	A	442	NAG	O5-C5-C6	2.58	109.69	106.98
3	C	601	NAG	C3-C4-C5	-2.58	105.54	110.17
8	E	445	MAN	O5-C5-C4	2.55	113.88	110.65
6	A	441	NAG	C8-C7-N2	2.53	120.91	116.12
5	A	437	MAN	C4-C3-C2	2.51	113.41	110.61
6	A	445	MAN	C3-C4-C5	2.46	114.59	110.17
5	A	432	NAG	O5-C5-C6	2.44	109.54	106.98
3	C	601	NAG	O4-C4-C5	2.43	115.69	109.25
6	C	431	NAG	O4-C4-C3	-2.39	105.02	110.36
8	E	443	BMA	O5-C5-C4	2.38	113.67	110.65
3	C	602	NAG	C3-C4-C5	2.35	114.39	110.17
3	A	601	NAG	C2-N2-C7	-2.35	120.56	123.39
7	D	201	NAG	O6-C6-C5	2.34	119.52	111.37
8	E	441	NAG	O4-C4-C3	-2.29	105.23	110.36
3	C	602	NAG	C4-C3-C2	2.29	115.54	110.74
8	E	443	BMA	O5-C5-C6	2.28	109.37	106.98
6	E	431	NAG	O4-C4-C3	-2.27	105.29	110.36
3	C	412	NAG	C2-N2-C7	2.26	126.13	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	446	NAG	O5-C5-C4	-2.19	107.88	110.65
5	A	433	BMA	O5-C5-C6	2.19	109.27	106.98
3	E	602	NAG	O5-C5-C6	2.14	109.23	106.98
6	C	434	MAN	C4-C3-C2	2.14	112.99	110.61
3	C	421	NAG	O4-C4-C3	2.13	115.12	110.36
3	C	601	NAG	O5-C5-C4	-2.12	107.96	110.65
5	A	432	NAG	C3-C4-C5	-2.11	106.38	110.17
3	C	421	NAG	O5-C5-C6	2.11	109.19	106.98
7	D	201	NAG	C4-C3-C2	2.11	115.17	110.74
6	C	433	BMA	C4-C3-C2	-2.10	108.27	110.61
5	A	431	NAG	O4-C4-C3	-2.07	105.73	110.36
3	C	411	NAG	O4-C4-C3	-2.06	105.74	110.36
8	E	441	NAG	O5-C5-C6	2.06	109.15	106.98
3	A	602	NAG	C3-C4-C5	2.05	113.86	110.17
6	A	444	MAN	O5-C5-C6	2.03	109.11	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	E	446	NAG	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	445	MAN	C1-C2-C3-C4-C5-O5
6	C	444	MAN	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

6 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
4	NAG	A	421	1	12,14,15	0.63	0	15,19,21	0.77	0
4	NAG	C	611	1	12,14,15	0.58	0	15,19,21	0.87	0
4	NAG	E	411	1	12,14,15	0.62	0	15,19,21	1.69	2 (13%)
4	NAG	E	421	1	12,14,15	0.65	0	15,19,21	1.49	4 (26%)
4	NAG	E	611	1	12,14,15	0.76	1 (8%)	15,19,21	1.16	1 (6%)
4	NAG	F	201	2	12,14,15	0.86	1 (8%)	15,19,21	2.44	5 (33%)

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	421	1	-	0/6/23/26	0/1/1/1
4	NAG	C	611	1	-	0/6/23/26	0/1/1/1
4	NAG	E	411	1	-	0/6/23/26	0/1/1/1
4	NAG	E	421	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	611	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	201	NAG	O5-C5	-2.44	1.41	1.45
4	E	611	NAG	O5-C5	-2.03	1.42	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	NAG	O5-C5-C6	5.69	112.95	106.98
4	F	201	NAG	C3-C2-N2	-4.51	104.86	111.62
4	E	411	NAG	O5-C5-C4	4.39	116.23	110.65
4	E	411	NAG	C2-N2-C7	3.50	127.63	123.39
4	F	201	NAG	C2-N2-C7	3.37	127.47	123.39
4	E	421	NAG	O5-C5-C6	3.18	110.31	106.98
4	F	201	NAG	O5-C5-C4	-3.11	106.71	110.65
4	F	201	NAG	C4-C3-C2	3.05	117.15	110.74
4	E	421	NAG	C4-C3-C2	2.65	116.31	110.74
4	E	421	NAG	C3-C2-N2	-2.58	107.76	111.62
4	E	611	NAG	C2-N2-C7	2.42	126.32	123.39
4	E	421	NAG	C3-C4-C5	2.26	114.23	110.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	421	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/323 (99%)	-0.27	4 (1%) 74 75	31, 64, 92, 117	0
1	C	321/323 (99%)	0.05	19 (5%) 22 18	34, 72, 108, 126	0
1	E	321/323 (99%)	0.10	12 (3%) 39 35	38, 76, 101, 119	0
2	B	172/173 (99%)	-0.24	0 100 100	31, 44, 69, 99	0
2	D	172/173 (99%)	-0.23	0 100 100	32, 45, 69, 91	0
2	F	172/173 (99%)	-0.28	1 (0%) 86 89	32, 48, 74, 95	0
All	All	1478/1488 (99%)	-0.11	36 (2%) 56 53	31, 59, 98, 126	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	ILE	7.2
1	E	142	GLY	4.4
1	A	327	GLN	4.1
1	C	159	ASN	3.9
1	C	156	LYS	3.5
1	E	222	TRP	3.3
1	C	273	LEU	3.3
1	E	328	ILE	3.1
1	C	327	GLN	3.1
1	C	157	SER	3.0
1	E	198	GLU	3.0
1	C	196	ILE	2.9
1	C	127	TRP	2.9
1	E	81	TYR	2.8
1	C	81	TYR	2.8
1	C	160	SER	2.7
1	C	54	ASN	2.6
1	A	81	TYR	2.6
2	F	160	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	160	SER	2.6
1	C	155	THR	2.5
1	C	163	ILE	2.5
1	C	128	THR	2.4
1	C	129	GLY	2.4
1	C	161	TYR	2.4
1	A	222	TRP	2.4
1	E	199	SER	2.4
1	E	127	TRP	2.4
1	E	143	SER	2.3
1	E	273	LEU	2.3
1	E	62	ARG	2.2
1	A	326	LYS	2.2
1	E	171	ASN	2.2
1	C	158	GLY	2.2
1	C	79	PHE	2.1
1	C	326	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	C	442	14/15	0.24	19.67	95,107,119,130	0
3	NAG	C	602	14/15	0.38	17.96	115,119,122,122	0
3	NAG	C	412	14/15	0.62	14.57	131,136,143,147	0
3	NAG	A	601	14/15	0.28	12.64	70,80,88,98	0
3	NAG	C	601	14/15	0.29	11.51	78,86,99,112	0
6	MAN	C	444	11/12	0.55	11.48	151,154,165,165	0
7	FUL	D	202	10/11	0.37	9.55	101,107,109,112	0
7	NAG	D	201	14/15	0.30	6.39	93,99,105,105	0
3	NAG	A	411	14/15	0.31	5.29	97,104,113,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	E	602	14/15	0.41	5.16	83,93,98,103	0
7	FUL	B	202	10/11	0.18	3.60	95,100,107,113	0
3	NAG	E	601	14/15	0.24	2.75	68,76,80,83	0
6	NAG	A	442	14/15	0.18	2.69	72,83,94,103	0
3	NAG	C	411	14/15	0.41	2.69	108,114,123,128	0
3	NAG	C	421	14/15	0.32	1.96	133,143,152,154	0
8	NAG	E	446	14/15	0.23	1.15	116,125,130,132	0
6	NAG	A	441	14/15	0.12	0.89	59,64,68,72	0
6	NAG	E	431	14/15	0.14	0.73	99,103,106,107	0
7	NAG	B	201	14/15	0.14	0.53	77,81,91,95	0
5	NAG	A	432	14/15	0.23	0.15	93,105,113,119	0
6	NAG	E	432	14/15	0.16	-0.03	102,110,121,121	0
6	NAG	C	431	14/15	0.15	-0.09	86,88,91,92	0
6	NAG	C	432	14/15	0.16	-0.12	87,96,102,107	0
8	NAG	E	441	14/15	0.13	-0.33	71,79,84,86	0
6	MAN	C	434	11/12	0.18	-0.64	127,131,137,137	0
5	NAG	A	431	14/15	0.11	-1.24	89,92,95,96	0
6	NAG	C	441	14/15	0.11	-1.32	71,77,81,88	0
8	NAG	E	442	14/15	0.11	-1.55	89,97,105,115	0
8	MAN	E	445	11/12	0.24	-	132,136,139,141	0
6	MAN	E	434	11/12	0.20	-	139,142,151,155	0
6	MAN	E	437	11/12	0.26	-	132,140,145,146	0
6	MAN	A	445	11/12	0.19	-	82,91,94,96	0
8	BMA	E	443	11/12	0.17	-	122,128,137,140	0
3	NAG	A	602	14/15	0.37	-	103,116,124,125	0
6	BMA	C	433	11/12	0.20	-	111,116,119,125	0
5	BMA	A	433	11/12	0.29	-	125,132,138,140	0
6	MAN	C	445	11/12	0.18	-	107,114,121,121	0
6	BMA	A	443	11/12	0.27	-	99,112,123,128	0
8	MAN	E	444	11/12	0.51	-	141,144,151,152	0
5	MAN	A	437	11/12	0.27	-	138,144,154,154	0
3	NAG	C	422	14/15	0.48	-	152,159,164,169	0
6	BMA	C	443	11/12	0.40	-	123,137,143,148	0
6	BMA	E	433	11/12	0.16	-	125,130,135,139	0
6	MAN	A	444	11/12	0.33	-	130,131,133,136	0
3	NAG	A	412	14/15	0.40	-	120,126,134,134	0
6	MAN	C	437	11/12	0.30	-	118,124,128,130	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	E	411	14/15	0.42	7.83	112,125,129,130	0
4	NAG	E	611	14/15	0.35	6.50	101,117,122,123	0
4	NAG	F	201	14/15	0.31	5.02	101,108,111,113	0
4	NAG	C	611	14/15	0.43	4.46	109,120,125,128	0
4	NAG	A	421	14/15	0.33	2.93	97,104,109,113	0
4	NAG	E	421	14/15	0.45	2.15	115,124,130,134	0

6.5 Other polymers ⓘ

There are no such residues in this entry.