



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GDI
Title : A subtype N10 neuraminidase-like protein of A/little yellow-shouldered bat/
Guatemala/164/2009
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2012-07-31
Resolution : 1.95 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

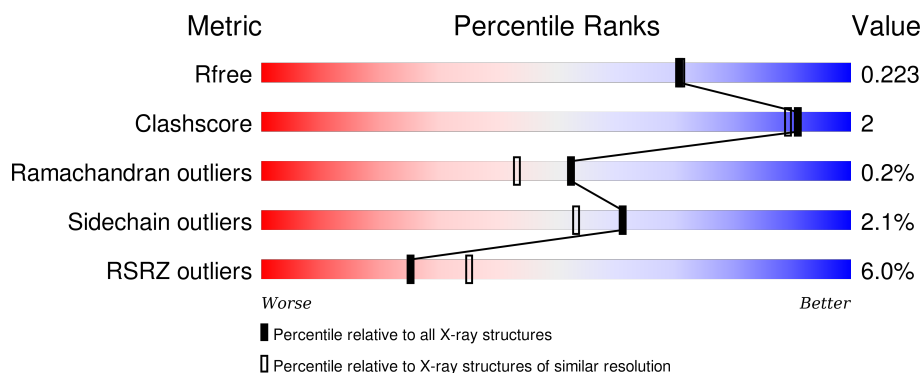
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



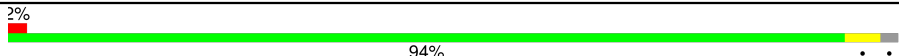
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	373	<div> <div>3%</div> <div>93%</div> <div>5%</div> </div>
1	B	373	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	C	373	<div> <div>10%</div> <div>87%</div> <div>11%</div> </div>
1	D	373	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	E	373	<div> <div>6%</div> <div>89%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	373	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	505	-	-	-	X
5	GOL	A	512	-	-	-	X
5	GOL	B	511	-	-	-	X
5	GOL	D	508	-	-	-	X
5	GOL	E	511	-	-	-	X
5	GOL	E	512	-	-	-	X
5	GOL	F	512	-	-	-	X
5	GOL	F	515	-	-	-	X
6	NO3	A	513	-	X	-	X
6	NO3	A	514	-	X	-	X
6	NO3	B	513	-	X	-	-
6	NO3	B	514	-	X	-	-
6	NO3	B	515	-	X	-	-
6	NO3	B	516	-	X	-	X
6	NO3	B	517	-	X	-	X
6	NO3	C	510	-	X	-	X
6	NO3	C	511	-	X	-	X
6	NO3	D	509	-	X	-	-
6	NO3	D	510	-	X	-	X
6	NO3	F	516	-	X	-	-
6	NO3	F	517	-	X	-	-
6	NO3	F	518	-	X	-	X
9	FUC	D	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36150 atoms, of which 16780 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 Neuraminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	B	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	C	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	D	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	E	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	F	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	EXPRESSION TAG	UNP H6QM85
A	78	SER	-	EXPRESSION TAG	UNP H6QM85
A	79	PRO	-	EXPRESSION TAG	UNP H6QM85
A	80	SER	-	EXPRESSION TAG	UNP H6QM85
A	81	ARG	-	EXPRESSION TAG	UNP H6QM85
B	77	GLY	-	EXPRESSION TAG	UNP H6QM85
B	78	SER	-	EXPRESSION TAG	UNP H6QM85
B	79	PRO	-	EXPRESSION TAG	UNP H6QM85
B	80	SER	-	EXPRESSION TAG	UNP H6QM85
B	81	ARG	-	EXPRESSION TAG	UNP H6QM85
C	77	GLY	-	EXPRESSION TAG	UNP H6QM85
C	78	SER	-	EXPRESSION TAG	UNP H6QM85
C	79	PRO	-	EXPRESSION TAG	UNP H6QM85
C	80	SER	-	EXPRESSION TAG	UNP H6QM85
C	81	ARG	-	EXPRESSION TAG	UNP H6QM85
D	77	GLY	-	EXPRESSION TAG	UNP H6QM85
D	78	SER	-	EXPRESSION TAG	UNP H6QM85

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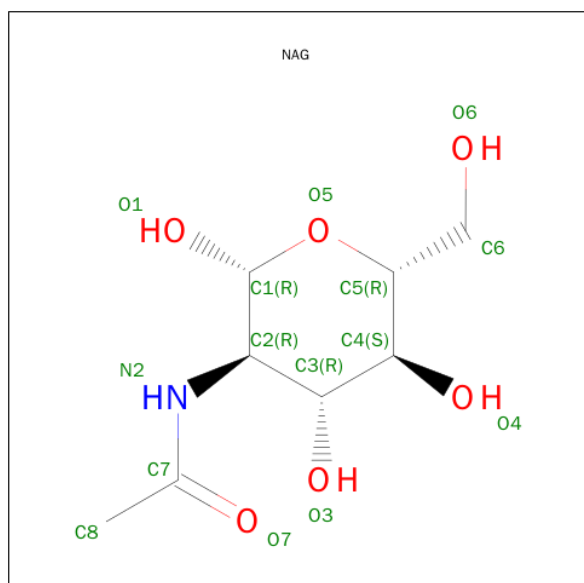
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Chain	Residue	Modelled	Actual	Comment	Reference
D	79	PRO	-	EXPRESSION TAG	UNP H6QM85
D	80	SER	-	EXPRESSION TAG	UNP H6QM85
D	81	ARG	-	EXPRESSION TAG	UNP H6QM85
E	77	GLY	-	EXPRESSION TAG	UNP H6QM85
E	78	SER	-	EXPRESSION TAG	UNP H6QM85
E	79	PRO	-	EXPRESSION TAG	UNP H6QM85
E	80	SER	-	EXPRESSION TAG	UNP H6QM85
E	81	ARG	-	EXPRESSION TAG	UNP H6QM85
F	77	GLY	-	EXPRESSION TAG	UNP H6QM85
F	78	SER	-	EXPRESSION TAG	UNP H6QM85
F	79	PRO	-	EXPRESSION TAG	UNP H6QM85
F	80	SER	-	EXPRESSION TAG	UNP H6QM85
F	81	ARG	-	EXPRESSION TAG	UNP H6QM85

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			59	34	2	23		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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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	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	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	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

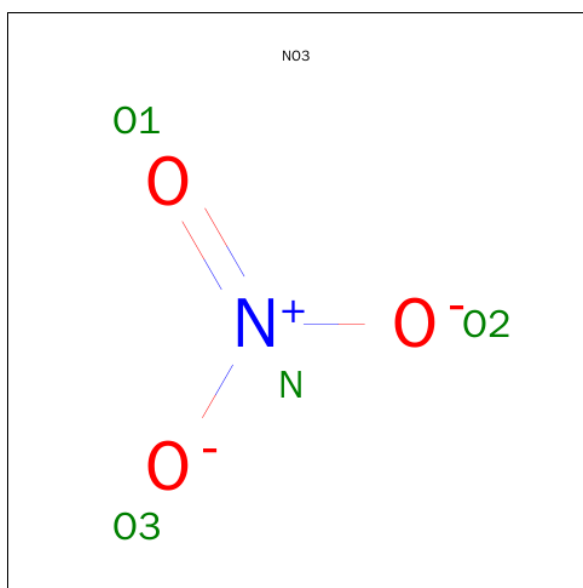
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	A	1	Total	Ca	0	0
			1	1		
4	F	2	Total	Ca	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	6	Total	C	N	O	0	0
			70	40	2	28		

- 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
			48	28	2	18		
8	E	4	Total	C	N	O	0	0
			48	28	2	18		
8	F	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

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

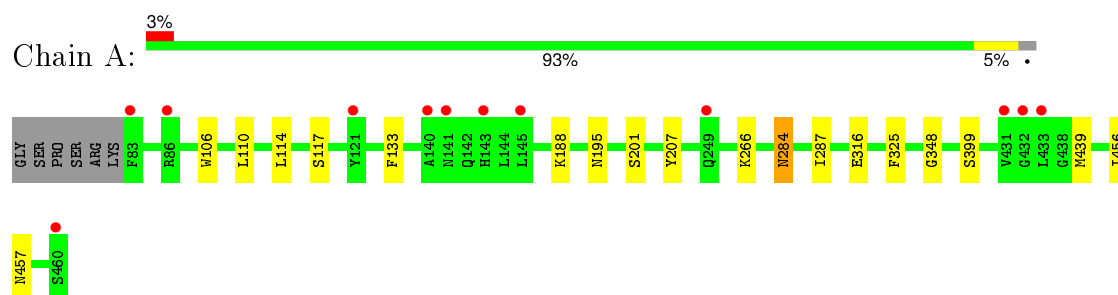
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	247	Total 247	O 247	0	0
12	B	246	Total 246	O 246	0	0
12	C	176	Total 176	O 176	0	0
12	D	213	Total 213	O 213	0	0
12	E	207	Total 207	O 207	0	0
12	F	319	Total 319	O 319	0	0

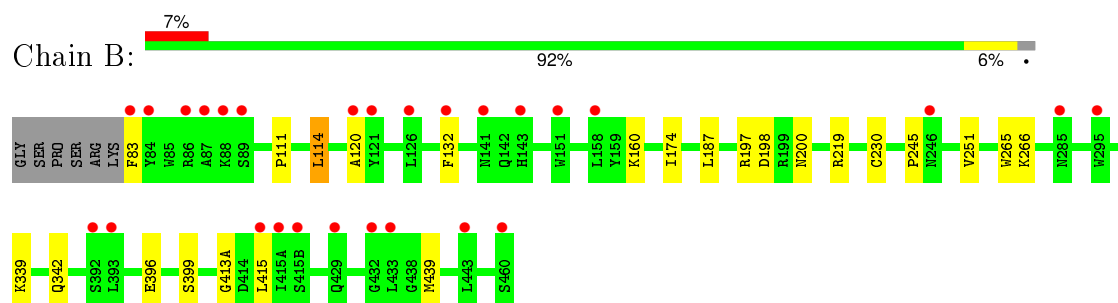
3 Residue-property plots [i](#)

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.

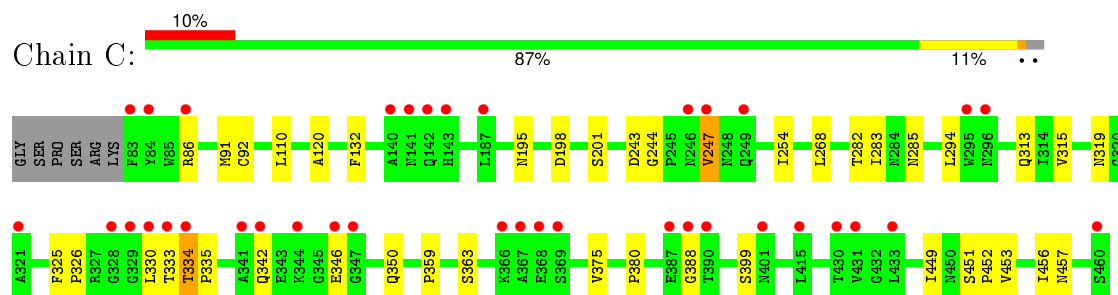
• Molecule 1: Neuraminidase



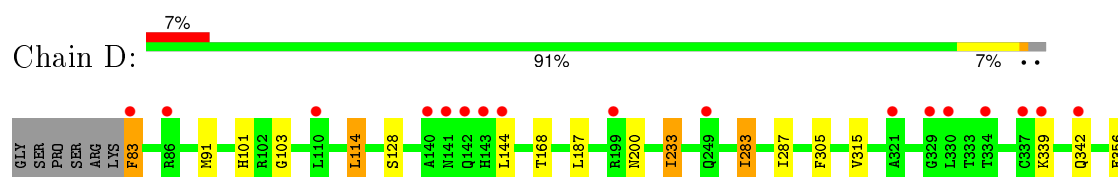
• Molecule 1: Neuraminidase

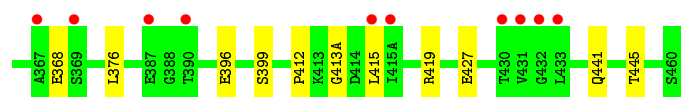


• Molecule 1: Neuraminidase

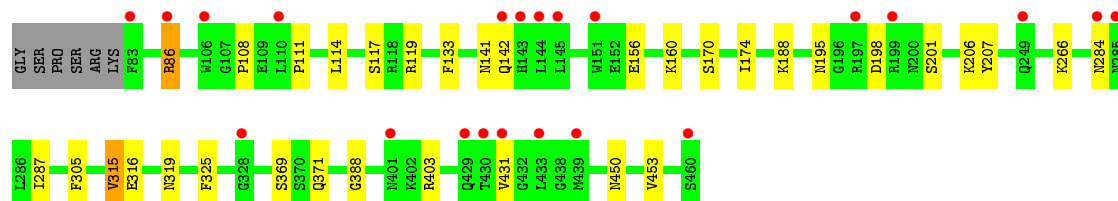
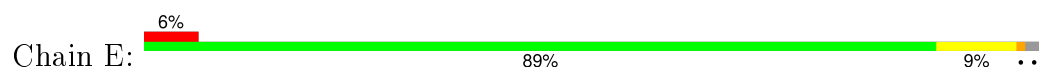


• Molecule 1: Neuraminidase

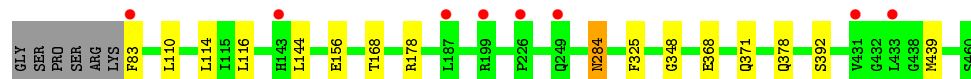
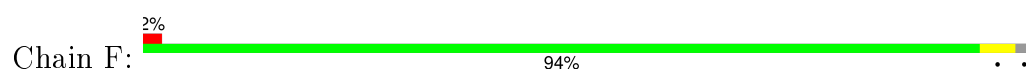




• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	176.32Å 176.32Å 193.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 1.95 40.11 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.11-1.95) 98.6 (40.11-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.2_869)	Depositor
R, R_{free}	0.180 , 0.223 0.181 , 0.223	Depositor DCC
R_{free} test set	10572 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.9	EDS
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 210682 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36150	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: GOL, BMA, NAG, CA, FUC, FUL, NO3, 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	0.39	0/2945	0.58	0/3990
1	B	0.40	0/2945	0.58	0/3990
1	C	0.35	0/2945	0.55	0/3990
1	D	0.37	0/2945	0.55	0/3990
1	E	0.37	0/2945	0.56	0/3990
1	F	0.42	0/2945	0.59	0/3990
All	All	0.39	0/17670	0.57	0/23940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2876	2778	2775	9	0
1	B	2876	2778	2776	12	0
1	C	2876	2778	2776	19	0
1	D	2876	2778	2776	15	0
1	E	2876	2778	2775	14	0
1	F	2876	2778	2775	8	0
2	A	59	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	39	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
3	E	28	0	26	1	0
3	F	28	0	26	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	18	24	24	2	0
5	B	12	16	16	0	0
5	C	6	8	8	0	0
5	D	6	8	8	1	0
5	E	18	24	24	1	0
5	F	24	32	32	0	0
6	A	8	0	0	1	0
6	B	20	0	0	1	0
6	C	8	0	0	1	0
6	D	8	0	0	0	0
6	F	12	0	0	0	0
7	B	70	0	61	1	0
8	C	48	0	43	0	0
8	E	48	0	43	0	0
8	F	48	0	43	0	0
9	D	38	0	34	0	0
10	E	24	0	22	0	0
11	F	38	0	34	0	0
12	A	247	0	0	0	0
12	B	246	0	0	1	0
12	C	176	0	0	0	0
12	D	213	0	0	1	0
12	E	207	0	0	1	0
12	F	319	0	0	1	0
All	All	19370	16780	17266	78	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 2.

All (78) 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:C:451:SER:HB2	1:C:452:PRO:CD	2.29	0.63
1:E:108:PRO:HB2	1:E:431:VAL:HG13	1.82	0.60
1:D:91:MET:HE1	1:D:356:GLU:HG3	1.84	0.59
1:B:396:GLU:OE2	1:B:399:SER:OG	2.19	0.58
1:D:103:GLY:O	5:D:508:GOL:O3	2.21	0.57
1:A:399:SER:OG	1:A:457:ASN:ND2	2.38	0.56
1:C:350:GLN:N	6:C:510:NO3:O1	2.33	0.56
1:D:287:ILE:HD13	1:D:305:PHE:CE2	2.41	0.56
1:F:325:PHE:CE1	1:F:371:GLN:HG3	2.43	0.54
1:D:91:MET:CE	1:D:356:GLU:HG3	2.38	0.54
1:C:399:SER:OG	1:C:457:ASN:ND2	2.41	0.53
1:A:456:ILE:HG12	1:B:200:ASN:HB3	1.90	0.52
1:D:427:GLU:OE1	1:D:441:GLN:HG3	2.10	0.52
1:E:119:ARG:NH2	1:E:156:GLU:OE2	2.43	0.52
1:E:117:SER:HB3	1:E:133:PHE:CD2	2.46	0.51
1:F:116:LEU:HD12	1:F:144:LEU:HD21	1.94	0.50
3:E:505:NAG:O7	5:E:511:GOL:O1	2.29	0.50
1:D:412:PRO:HG2	1:D:419:ARG:NH2	2.27	0.49
1:F:156:GLU:OE2	1:F:178:ARG:NH1	2.45	0.49
1:F:284:ASN:O	1:F:284:ASN:ND2	2.40	0.48
1:C:195:ASN:O	1:C:201:SER:HA	2.13	0.48
1:D:396:GLU:OE2	1:D:399:SER:OG	2.29	0.48
1:B:111:PRO:HG2	1:B:114:LEU:HD12	1.95	0.48
1:A:117:SER:HB3	1:A:133:PHE:CD2	2.49	0.48
1:F:325:PHE:O	1:F:348:GLY:HA2	2.15	0.47
1:E:325:PHE:CE1	1:E:371:GLN:HG3	2.50	0.47
1:C:333:THR:OG1	1:C:334:THR:N	2.42	0.47
1:B:83:PHE:HB3	1:B:187:LEU:HD11	1.97	0.47
1:C:282:THR:O	1:C:283:ILE:HG23	2.14	0.47
1:C:451:SER:HB2	1:C:452:PRO:HD2	1.96	0.46
1:A:188:LYS:HB2	1:A:207:TYR:CZ	2.50	0.46
1:B:219:ARG:HG3	1:B:251:VAL:HG21	1.97	0.46
5:A:511:GOL:H32	6:A:513:NO3:O2	2.14	0.46
1:C:325:PHE:HA	1:C:326:PRO:C	2.36	0.46
1:C:449:ILE:HD11	1:C:453:VAL:HB	1.97	0.46
1:A:325:PHE:O	1:A:348:GLY:HA2	2.16	0.45
1:E:111:PRO:HG2	1:E:114:LEU:HD13	1.98	0.45
1:E:195:ASN:O	1:E:201:SER:HA	2.16	0.45
1:D:233:ILE:HD11	1:D:287:ILE:HD11	1.98	0.45
1:B:160:LYS:HB2	1:B:174:ILE:HD11	1.99	0.45
1:E:86:ARG:NH1	12:E:688:HOH:O	2.50	0.45
1:C:247:VAL:HG21	1:C:294:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.44
1:D:101:HIS:HB3	1:D:445:THR:OG1	2.16	0.44
1:E:141:ASN:O	1:E:142:GLN:HB2	2.17	0.44
1:B:265:TRP:NE1	6:B:517:NO3:O2	2.49	0.44
1:A:316:GLU:HB2	5:A:512:GOL:H32	2.00	0.44
1:C:91:MET:HG2	1:C:92:CYS:O	2.18	0.44
1:C:313:GLN:HG2	1:C:315:VAL:HG23	2.00	0.43
1:C:359:PRO:HB3	1:C:380:PRO:HA	2.00	0.43
1:C:120:ALA:HA	1:C:132:PHE:O	2.19	0.43
1:C:456:ILE:CD1	1:D:200:ASN:HB3	2.48	0.43
1:E:160:LYS:HB2	1:E:174:ILE:HD11	2.01	0.42
1:D:283:ILE:HD11	1:D:356:GLU:OE2	2.18	0.42
7:B:503:BMA:H3	7:B:504:MAN:H2	1.41	0.42
1:A:106:TRP:NE1	1:A:114:LEU:HD21	2.34	0.42
1:E:188:LYS:HB2	1:E:207:TYR:CZ	2.55	0.42
1:A:195:ASN:O	1:A:201:SER:HA	2.20	0.42
1:D:83:PHE:HB3	1:D:187:LEU:HD11	2.01	0.42
1:B:197:ARG:HA	1:B:197:ARG:HD2	1.70	0.42
1:D:339:LYS:HE3	12:D:752:HOH:O	2.20	0.41
1:C:363:SER:HA	1:C:375:VAL:O	2.20	0.41
1:E:450:ASN:C	1:E:450:ASN:OD1	2.59	0.41
1:B:339:LYS:HD3	1:B:339:LYS:HA	1.86	0.41
1:B:413(A):GLY:O	1:B:415:LEU:N	2.53	0.41
1:B:245:PRO:HD2	12:B:721:HOH:O	2.19	0.41
1:C:243:ASP:OD1	1:C:244:GLY:N	2.51	0.41
1:E:315:VAL:CG1	1:E:316:GLU:N	2.84	0.41
1:F:114:LEU:HD23	1:F:168:THR:HG22	2.02	0.41
1:B:120:ALA:HA	1:B:132:PHE:O	2.21	0.41
1:F:378:GLN:OE1	1:F:392:SER:OG	2.32	0.41
1:E:287:ILE:HD12	1:E:305:PHE:CE2	2.55	0.40
1:D:114:LEU:HD22	1:D:168:THR:HG22	2.02	0.40
1:C:319:ASN:HB3	1:C:388:GLY:HA3	2.04	0.40
1:F:368:GLU:OE1	12:F:847:HOH:O	2.22	0.40
1:E:319:ASN:HB3	1:E:388:GLY:HA3	2.03	0.40
1:D:413(A):GLY:O	1:D:415:LEU:HG	2.22	0.40
1:C:254:ILE:HG13	1:C:268:LEU:HD21	2.03	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	365/373 (98%)	354 (97%)	10 (3%)	1 (0%)	46	35
1	B	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	C	365/373 (98%)	349 (96%)	13 (4%)	3 (1%)	24	11
1	D	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	E	365/373 (98%)	351 (96%)	13 (4%)	1 (0%)	46	35
1	F	365/373 (98%)	352 (96%)	13 (4%)	0	100	100
All	All	2190/2238 (98%)	2112 (96%)	73 (3%)	5 (0%)	52	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	C	198	ASP
1	C	285	ASN
1	E	198	ASP
1	C	335	PRO

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	320/325 (98%)	316 (99%)	4 (1%)	76	72
1	B	320/325 (98%)	314 (98%)	6 (2%)	65	58
1	C	320/325 (98%)	313 (98%)	7 (2%)	60	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	320/325 (98%)	310 (97%)	10 (3%)	47	34
1	E	320/325 (98%)	311 (97%)	9 (3%)	51	39
1	F	320/325 (98%)	316 (99%)	4 (1%)	76	72
All	All	1920/1950 (98%)	1880 (98%)	40 (2%)	61	53

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	266	LYS
1	A	284	ASN
1	A	439	MET
1	B	114	LEU
1	B	198	ASP
1	B	230	CYS
1	B	266	LYS
1	B	342	GLN
1	B	439	MET
1	C	86	ARG
1	C	110	LEU
1	C	247	VAL
1	C	330	LEU
1	C	334	THR
1	C	342	GLN
1	C	346	GLU
1	D	83	PHE
1	D	114	LEU
1	D	128	SER
1	D	144	LEU
1	D	233	ILE
1	D	283	ILE
1	D	315	VAL
1	D	342	GLN
1	D	368	GLU
1	D	376	LEU
1	E	86	ARG
1	E	170	SER
1	E	206	LYS
1	E	266	LYS
1	E	284	ASN
1	E	315	VAL

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Mol	Chain	Res	Type
1	E	369	SER
1	E	403	ARG
1	E	453	VAL
1	F	83	PHE
1	F	110	LEU
1	F	284	ASN
1	F	439	MET

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

Mol	Chain	Res	Type
1	C	143	HIS

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 ⓘ

31 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	501	1,2	14,14,15	0.53	0	15,19,21	1.23	2 (13%)
2	NAG	A	502	2	14,14,15	0.43	0	15,19,21	0.69	0
2	BMA	A	503	2	11,11,12	0.59	0	14,15,17	0.69	0
2	FUC	A	504	2	10,10,11	0.63	0	14,14,16	1.01	1 (7%)
2	FUL	A	505	2	10,10,11	0.69	0	14,14,16	2.25	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	501	1,7	14,14,15	0.60	0	15,19,21	1.43	2 (13%)
7	NAG	B	502	7	14,14,15	0.44	0	15,19,21	0.59	0
7	BMA	B	503	7	11,11,12	0.62	0	14,15,17	0.60	0
7	MAN	B	504	7	11,11,12	0.53	0	14,15,17	1.04	2 (14%)
7	FUC	B	505	7	10,10,11	0.66	0	14,14,16	1.21	2 (14%)
7	FUL	B	506	7	10,10,11	0.78	0	14,14,16	2.80	5 (35%)
8	NAG	C	501	1,8	14,14,15	0.63	0	15,19,21	1.25	2 (13%)
8	NAG	C	502	8	14,14,15	0.42	0	15,19,21	0.95	0
8	FUC	C	503	8	10,10,11	0.57	0	14,14,16	1.05	1 (7%)
8	FUL	C	504	8	10,10,11	0.59	0	14,14,16	0.77	0
9	NAG	D	501	9,1	14,14,15	0.58	0	15,19,21	1.12	1 (6%)
9	NAG	D	502	9	14,14,15	0.42	0	15,19,21	0.78	0
9	FUC	D	503	9	10,10,11	0.55	0	14,14,16	0.85	0
8	NAG	E	501	1,8	14,14,15	0.53	0	15,19,21	1.14	2 (13%)
8	NAG	E	502	8	14,14,15	0.47	0	15,19,21	0.62	0
8	FUC	E	503	8	10,10,11	0.62	0	14,14,16	1.02	2 (14%)
8	FUL	E	504	8	10,10,11	0.68	0	14,14,16	2.41	4 (28%)
10	NAG	E	506	1,10	14,14,15	0.51	0	15,19,21	1.14	2 (13%)
10	FUC	E	507	10	10,10,11	0.71	0	14,14,16	1.20	1 (7%)
8	NAG	F	501	1,8	14,14,15	0.48	0	15,19,21	1.24	1 (6%)
8	NAG	F	502	8	14,14,15	0.49	0	15,19,21	0.86	0
8	FUC	F	503	8	10,10,11	0.68	0	14,14,16	1.23	1 (7%)
8	FUL	F	504	8	10,10,11	0.64	0	14,14,16	2.19	4 (28%)
11	NAG	F	507	11,1	14,14,15	0.57	0	15,19,21	1.18	2 (13%)
11	NAG	F	508	11	14,14,15	0.47	0	15,19,21	0.81	0
11	FUL	F	509	11	10,10,11	0.60	0	14,14,16	0.74	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
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	2	-	0/2/19/22	0/1/1/1
2	FUC	A	504	2	-	0/0/17/20	0/1/1/1
2	FUL	A	505	2	-	0/0/17/20	0/1/1/1
7	NAG	B	501	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	502	7	-	0/6/23/26	0/1/1/1
7	BMA	B	503	7	-	0/2/19/22	1/1/1/1
7	MAN	B	504	7	-	0/2/19/22	1/1/1/1
7	FUC	B	505	7	-	0/0/17/20	0/1/1/1
7	FUL	B	506	7	-	0/0/17/20	0/1/1/1
8	NAG	C	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	502	8	-	0/6/23/26	0/1/1/1
8	FUC	C	503	8	-	0/0/17/20	0/1/1/1
8	FUL	C	504	8	-	0/0/17/20	0/1/1/1
9	NAG	D	501	9,1	-	0/6/23/26	0/1/1/1
9	NAG	D	502	9	-	0/6/23/26	0/1/1/1
9	FUC	D	503	9	-	0/0/17/20	0/1/1/1
8	NAG	E	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	502	8	-	0/6/23/26	0/1/1/1
8	FUC	E	503	8	-	0/0/17/20	0/1/1/1
8	FUL	E	504	8	-	0/0/17/20	0/1/1/1
10	NAG	E	506	1,10	-	0/6/23/26	0/1/1/1
10	FUC	E	507	10	-	0/0/17/20	0/1/1/1
8	NAG	F	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	F	502	8	-	0/6/23/26	0/1/1/1
8	FUC	F	503	8	-	0/0/17/20	0/1/1/1
8	FUL	F	504	8	-	0/0/17/20	0/1/1/1
11	NAG	F	507	11,1	-	0/6/23/26	0/1/1/1
11	NAG	F	508	11	-	0/6/23/26	0/1/1/1
11	FUL	F	509	11	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	506	FUL	C1-C2-C3	-7.39	100.80	109.54
8	E	504	FUL	C1-C2-C3	-6.30	102.09	109.54
2	A	505	FUL	C1-C2-C3	-5.63	102.88	109.54
8	F	504	FUL	C1-O5-C5	-5.08	104.53	112.38
8	F	504	FUL	C1-C2-C3	-4.65	104.03	109.54
7	B	506	FUL	C1-O5-C5	-3.99	106.22	112.38
8	E	504	FUL	O5-C1-C2	-3.63	104.96	110.86
2	A	501	NAG	C2-N2-C7	-3.48	118.57	123.04
7	B	501	NAG	O3-C3-C2	-3.29	102.60	109.11
2	A	505	FUL	C1-O5-C5	-3.24	107.37	112.38
2	A	505	FUL	O5-C1-C2	-3.22	105.63	110.86
7	B	506	FUL	O5-C1-C2	-3.19	105.69	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	507	FUC	O5-C1-C2	-3.09	105.85	110.86
8	F	501	NAG	O3-C3-C2	-3.08	103.01	109.11
8	E	504	FUL	C1-O5-C5	-3.01	107.72	112.38
7	B	501	NAG	C2-N2-C7	-2.97	119.22	123.04
8	F	504	FUL	O5-C1-C2	-2.85	106.23	110.86
10	E	506	NAG	C2-N2-C7	-2.58	119.73	123.04
8	E	501	NAG	C2-N2-C7	-2.52	119.80	123.04
7	B	505	FUC	C6-C5-C4	-2.50	108.15	113.08
2	A	501	NAG	O3-C3-C2	-2.41	104.33	109.11
8	C	501	NAG	O3-C3-C4	-2.41	104.90	110.34
8	E	504	FUL	C2-C3-C4	-2.12	107.44	111.04
7	B	504	MAN	C2-C3-C4	-2.09	107.49	111.04
8	E	503	FUC	C6-C5-C4	-2.08	108.98	113.08
2	A	504	FUC	C2-C3-C4	-2.07	107.53	111.04
9	D	501	NAG	C3-C4-C5	2.01	113.71	110.20
11	F	507	NAG	C4-C3-C2	2.08	114.47	111.23
8	E	501	NAG	C1-O5-C5	2.14	114.97	112.25
8	C	501	NAG	C3-C4-C5	2.22	114.07	110.20
11	F	507	NAG	C1-O5-C5	2.27	115.13	112.25
8	E	503	FUC	O5-C5-C6	2.29	109.91	106.13
10	E	506	NAG	C1-O5-C5	2.43	115.33	112.25
7	B	506	FUL	O5-C5-C4	2.53	113.91	109.53
7	B	505	FUC	O5-C5-C6	2.54	110.33	106.13
2	A	505	FUL	C3-C4-C5	2.60	114.09	109.72
8	F	504	FUL	O5-C5-C6	2.64	110.50	106.13
7	B	504	MAN	C1-O5-C5	2.73	115.71	112.25
8	C	503	FUC	O5-C5-C6	2.77	110.70	106.13
8	F	503	FUC	O5-C5-C6	2.97	111.03	106.13
7	B	506	FUL	C3-C4-C5	3.49	115.59	109.72

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	503	BMA	C1-C2-C3-C4-C5-O5
7	B	504	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	BMA	1	0
7	B	504	MAN	1	0

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 11 are monoatomic - leaving 41 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	506	1	14,14,15	0.49	0	15,19,21	0.87	0
3	NAG	A	507	1	14,14,15	0.40	0	15,19,21	1.32	2 (13%)
3	NAG	A	508	1	14,14,15	0.55	0	15,19,21	0.95	0
5	GOL	A	510	-	5,5,5	0.29	0	5,5,5	0.45	0
5	GOL	A	511	-	5,5,5	0.43	0	5,5,5	0.21	0
5	GOL	A	512	-	5,5,5	0.41	0	5,5,5	0.21	0
6	NO3	A	513	-	3,3,3	3.21	3 (100%)	3,3,3	0.08	0
6	NO3	A	514	-	3,3,3	3.34	3 (100%)	3,3,3	0.17	0
3	NAG	B	507	1	14,14,15	0.60	0	15,19,21	0.92	0
3	NAG	B	508	1	14,14,15	0.52	0	15,19,21	0.82	0
5	GOL	B	511	-	5,5,5	0.28	0	5,5,5	0.40	0
5	GOL	B	512	-	5,5,5	0.29	0	5,5,5	0.27	0
6	NO3	B	513	-	3,3,3	3.33	3 (100%)	3,3,3	0.11	0
6	NO3	B	514	-	3,3,3	3.19	3 (100%)	3,3,3	0.17	0
6	NO3	B	515	-	3,3,3	3.30	3 (100%)	3,3,3	0.12	0
6	NO3	B	516	-	3,3,3	3.10	3 (100%)	3,3,3	0.16	0
6	NO3	B	517	-	3,3,3	3.27	3 (100%)	3,3,3	0.18	0
3	NAG	C	505	1	14,14,15	0.54	0	15,19,21	0.75	0
3	NAG	C	506	1	14,14,15	0.63	0	15,19,21	1.11	2 (13%)
5	GOL	C	509	-	5,5,5	0.30	0	5,5,5	0.49	0
6	NO3	C	510	-	3,3,3	3.23	3 (100%)	3,3,3	0.24	0
6	NO3	C	511	-	3,3,3	3.20	3 (100%)	3,3,3	0.22	0
3	NAG	D	504	1	14,14,15	0.52	0	15,19,21	1.47	1 (6%)
3	NAG	D	505	1	14,14,15	0.56	0	15,19,21	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.36	0
6	NO3	D	509	-	3,3,3	3.27	3 (100%)	3,3,3	0.22	0
6	NO3	D	510	-	3,3,3	3.26	3 (100%)	3,3,3	0.11	0
3	NAG	E	505	1	14,14,15	0.60	0	15,19,21	0.88	0
3	NAG	E	508	1	14,14,15	0.65	0	15,19,21	1.28	2 (13%)
5	GOL	E	511	-	5,5,5	0.29	0	5,5,5	0.42	0
5	GOL	E	512	-	5,5,5	0.45	0	5,5,5	0.28	0
5	GOL	E	513	-	5,5,5	0.32	0	5,5,5	0.27	0
3	NAG	F	505	1	14,14,15	0.56	0	15,19,21	0.75	0
3	NAG	F	506	1	14,14,15	0.49	0	15,19,21	0.96	1 (6%)
5	GOL	F	512	-	5,5,5	0.51	0	5,5,5	0.63	0
5	GOL	F	513	-	5,5,5	0.30	0	5,5,5	0.46	0
5	GOL	F	514	-	5,5,5	0.31	0	5,5,5	0.32	0
5	GOL	F	515	-	5,5,5	0.34	0	5,5,5	0.48	0
6	NO3	F	516	-	3,3,3	3.27	3 (100%)	3,3,3	0.16	0
6	NO3	F	517	-	3,3,3	3.40	3 (100%)	3,3,3	0.05	0
6	NO3	F	518	-	3,3,3	3.18	3 (100%)	3,3,3	0.13	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
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	NAG	A	508	1	-	0/6/23/26	0/1/1/1
5	GOL	A	510	-	-	0/4/4/4	0/0/0/0
5	GOL	A	511	-	-	0/4/4/4	0/0/0/0
5	GOL	A	512	-	-	0/4/4/4	0/0/0/0
6	NO3	A	513	-	-	0/0/0/0	0/0/0/0
6	NO3	A	514	-	-	0/0/0/0	0/0/0/0
3	NAG	B	507	1	-	0/6/23/26	0/1/1/1
3	NAG	B	508	1	-	0/6/23/26	0/1/1/1
5	GOL	B	511	-	-	0/4/4/4	0/0/0/0
5	GOL	B	512	-	-	0/4/4/4	0/0/0/0
6	NO3	B	513	-	-	0/0/0/0	0/0/0/0
6	NO3	B	514	-	-	0/0/0/0	0/0/0/0
6	NO3	B	515	-	-	0/0/0/0	0/0/0/0
6	NO3	B	516	-	-	0/0/0/0	0/0/0/0
6	NO3	B	517	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	505	1	-	0/6/23/26	0/1/1/1
3	NAG	C	506	1	-	0/6/23/26	0/1/1/1
5	GOL	C	509	-	-	0/4/4/4	0/0/0/0
6	NO3	C	510	-	-	0/0/0/0	0/0/0/0
6	NO3	C	511	-	-	0/0/0/0	0/0/0/0
3	NAG	D	504	1	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1	-	0/6/23/26	0/1/1/1
5	GOL	D	508	-	-	0/4/4/4	0/0/0/0
6	NO3	D	509	-	-	0/0/0/0	0/0/0/0
6	NO3	D	510	-	-	0/0/0/0	0/0/0/0
3	NAG	E	505	1	-	0/6/23/26	0/1/1/1
3	NAG	E	508	1	-	0/6/23/26	0/1/1/1
5	GOL	E	511	-	-	0/4/4/4	0/0/0/0
5	GOL	E	512	-	-	0/4/4/4	0/0/0/0
5	GOL	E	513	-	-	0/4/4/4	0/0/0/0
3	NAG	F	505	1	-	0/6/23/26	0/1/1/1
3	NAG	F	506	1	-	0/6/23/26	0/1/1/1
5	GOL	F	512	-	-	0/4/4/4	0/0/0/0
5	GOL	F	513	-	-	0/4/4/4	0/0/0/0
5	GOL	F	514	-	-	0/4/4/4	0/0/0/0
5	GOL	F	515	-	-	0/4/4/4	0/0/0/0
6	NO3	F	516	-	-	0/0/0/0	0/0/0/0
6	NO3	F	517	-	-	0/0/0/0	0/0/0/0
6	NO3	F	518	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	513	NO3	O3-N	2.67	1.39	1.25
6	C	511	NO3	O2-N	2.76	1.39	1.25
6	B	516	NO3	O2-N	2.77	1.39	1.25
6	B	515	NO3	O2-N	2.81	1.39	1.25
6	B	517	NO3	O2-N	2.82	1.39	1.25
6	F	518	NO3	O3-N	2.82	1.39	1.25
6	B	514	NO3	O2-N	2.82	1.39	1.25
6	F	518	NO3	O2-N	2.83	1.39	1.25
6	B	516	NO3	O3-N	2.83	1.40	1.25
6	B	515	NO3	O3-N	2.85	1.40	1.25
6	B	514	NO3	O3-N	2.85	1.40	1.25
6	D	510	NO3	O2-N	2.87	1.40	1.25
6	B	513	NO3	O3-N	2.88	1.40	1.25
6	F	516	NO3	O3-N	2.88	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	510	NO3	O2-N	2.90	1.40	1.25
6	D	509	NO3	O2-N	2.90	1.40	1.25
6	A	514	NO3	O3-N	2.91	1.40	1.25
6	D	510	NO3	O3-N	2.91	1.40	1.25
6	C	511	NO3	O3-N	2.91	1.40	1.25
6	F	517	NO3	O3-N	2.95	1.40	1.25
6	F	516	NO3	O2-N	2.95	1.40	1.25
6	B	513	NO3	O2-N	2.95	1.40	1.25
6	B	517	NO3	O3-N	2.98	1.40	1.25
6	F	517	NO3	O2-N	2.99	1.40	1.25
6	A	513	NO3	O2-N	3.01	1.40	1.25
6	A	514	NO3	O2-N	3.04	1.41	1.25
6	C	510	NO3	O3-N	3.06	1.41	1.25
6	D	509	NO3	O3-N	3.10	1.41	1.25
6	B	516	NO3	O1-N	3.62	1.39	1.24
6	C	510	NO3	O1-N	3.68	1.39	1.24
6	D	509	NO3	O1-N	3.75	1.39	1.24
6	B	514	NO3	O1-N	3.79	1.39	1.24
6	F	518	NO3	O1-N	3.80	1.40	1.24
6	C	511	NO3	O1-N	3.81	1.40	1.24
6	A	513	NO3	O1-N	3.85	1.40	1.24
6	B	517	NO3	O1-N	3.89	1.40	1.24
6	F	516	NO3	O1-N	3.89	1.40	1.24
6	D	510	NO3	O1-N	3.91	1.40	1.24
6	A	514	NO3	O1-N	3.98	1.40	1.24
6	B	513	NO3	O1-N	4.02	1.40	1.24
6	B	515	NO3	O1-N	4.08	1.41	1.24
6	F	517	NO3	O1-N	4.12	1.41	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	508	NAG	C2-N2-C7	-3.46	118.59	123.04
3	A	507	NAG	C4-C3-C2	-3.02	106.53	111.23
3	E	508	NAG	C1-O5-C5	-2.74	108.77	112.25
3	F	506	NAG	C2-N2-C7	-2.47	119.86	123.04
3	C	506	NAG	C2-N2-C7	-2.22	120.19	123.04
3	A	507	NAG	C1-O5-C5	2.44	115.35	112.25
3	C	506	NAG	C4-C3-C2	2.61	115.28	111.23
3	D	505	NAG	C4-C3-C2	2.78	115.55	111.23
3	D	504	NAG	C1-O5-C5	4.73	118.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	511	GOL	1	0
5	A	512	GOL	1	0
6	A	513	NO3	1	0
6	B	517	NO3	1	0
6	C	510	NO3	1	0
5	D	508	GOL	1	0
3	E	505	NAG	1	0
5	E	511	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	367/373 (98%)	0.36	12 (3%)	50	61	19, 30, 52, 77	0
1	B	367/373 (98%)	0.45	27 (7%)	17	27	20, 32, 61, 93	0
1	C	367/373 (98%)	0.62	37 (10%)	9	14	23, 39, 66, 85	0
1	D	367/373 (98%)	0.51	27 (7%)	17	27	23, 36, 62, 88	0
1	E	367/373 (98%)	0.48	22 (5%)	25	35	22, 36, 60, 92	0
1	F	367/373 (98%)	0.23	8 (2%)	65	74	18, 28, 49, 76	0
All	All	2202/2238 (98%)	0.44	133 (6%)	25	35	18, 33, 60, 93	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	7.6
1	C	83	PHE	7.0
1	E	83	PHE	6.5
1	F	83	PHE	6.4
1	B	83	PHE	6.3
1	A	83	PHE	6.3
1	E	431	VAL	5.5
1	B	415(A)	ILE	5.3
1	D	143	HIS	4.7
1	D	330	LEU	4.7
1	E	143	HIS	4.5
1	C	329	GLY	4.4
1	C	330	LEU	4.3
1	E	460	SER	4.3
1	D	415	LEU	4.2
1	C	431	VAL	4.2
1	D	415(A)	ILE	4.1
1	D	431	VAL	4.0
1	A	431	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	321	ALA	3.9
1	C	295	TRP	3.9
1	E	151	TRP	3.9
1	C	341	ALA	3.9
1	E	433	LEU	3.7
1	A	460	SER	3.6
1	C	140	ALA	3.4
1	D	367	ALA	3.4
1	C	415	LEU	3.3
1	C	84	TYR	3.3
1	D	199	ARG	3.3
1	C	369	SER	3.3
1	C	460	SER	3.3
1	C	433	LEU	3.3
1	C	334	THR	3.2
1	C	296	ASN	3.2
1	B	415	LEU	3.2
1	C	143	HIS	3.2
1	F	431	VAL	3.1
1	B	86	ARG	3.1
1	E	110	LEU	3.0
1	A	433	LEU	3.0
1	D	433	LEU	3.0
1	C	342	GLN	3.0
1	C	344	LYS	3.0
1	D	390	THR	3.0
1	C	387	GLU	2.9
1	C	187	LEU	2.9
1	B	415(B)	SER	2.9
1	C	388	GLY	2.9
1	A	141	ASN	2.8
1	C	333	THR	2.8
1	C	141	ASN	2.8
1	C	390	THR	2.8
1	C	328	GLY	2.8
1	B	158	LEU	2.7
1	C	368	GLU	2.7
1	A	140	ALA	2.7
1	F	143	HIS	2.7
1	C	367	ALA	2.7
1	B	88	LYS	2.7
1	B	121	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	328	GLY	2.7
1	C	249	GLN	2.7
1	D	342	GLN	2.7
1	E	106	TRP	2.7
1	B	143	HIS	2.6
1	F	249	GLN	2.6
1	D	141	ASN	2.6
1	A	86	ARG	2.6
1	C	247	VAL	2.6
1	B	141	ASN	2.5
1	C	430	THR	2.5
1	D	249	GLN	2.5
1	E	142	GLN	2.5
1	C	366	LYS	2.4
1	E	249	GLN	2.4
1	C	86	ARG	2.4
1	E	285	ASN	2.4
1	F	199	ARG	2.4
1	B	295	TRP	2.4
1	D	321	ALA	2.4
1	A	249	GLN	2.4
1	D	86	ARG	2.4
1	D	144	LEU	2.4
1	F	433	LEU	2.4
1	D	142	GLN	2.4
1	A	145	LEU	2.4
1	B	120	ALA	2.4
1	E	429	GLN	2.3
1	B	460	SER	2.3
1	B	132	PHE	2.3
1	C	347	GLY	2.3
1	E	86	ARG	2.3
1	E	197	ARG	2.3
1	B	87	ALA	2.3
1	E	199	ARG	2.3
1	B	432	GLY	2.3
1	A	143	HIS	2.3
1	B	429	GLN	2.3
1	D	329	GLY	2.3
1	C	401	ASN	2.3
1	A	432	GLY	2.3
1	B	443	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	246	ASN	2.2
1	B	285	ASN	2.2
1	E	284	ASN	2.2
1	D	337	CYS	2.2
1	D	140	ALA	2.2
1	B	393	LEU	2.2
1	D	430	THR	2.2
1	D	387	GLU	2.2
1	C	142	GLN	2.2
1	D	334	THR	2.2
1	E	430	THR	2.1
1	E	144	LEU	2.1
1	C	246	ASN	2.1
1	E	439	MET	2.1
1	D	339	LYS	2.1
1	B	89	SER	2.1
1	D	110	LEU	2.1
1	B	392	SER	2.1
1	C	346	GLU	2.1
1	B	126	LEU	2.1
1	E	401	ASN	2.1
1	D	432	GLY	2.1
1	A	121	TYR	2.1
1	B	433	LEU	2.1
1	F	187	LEU	2.1
1	B	84	TYR	2.0
1	D	369	SER	2.0
1	E	145	LEU	2.0
1	B	151	TRP	2.0
1	F	226	PRO	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	FUC	D	503	10/11	0.92	0.21	3.43	49,55,64,70	0
2	FUC	A	504	10/11	0.90	0.15	1.45	23,39,45,49	0
8	FUC	E	503	10/11	0.93	0.16	0.81	35,41,50,56	0
8	FUC	C	503	10/11	0.87	0.16	0.09	47,64,80,86	0
7	FUC	B	505	10/11	0.94	0.10	-0.02	30,45,49,51	0
7	NAG	B	501	14/15	0.92	0.13	-0.22	40,43,55,59	0
8	FUC	F	503	10/11	0.96	0.10	-0.59	27,35,40,47	0
8	NAG	E	502	14/15	0.92	0.23	-	53,64,80,89	0
8	FUL	F	504	10/11	0.82	0.19	-	66,72,76,90	0
8	FUL	C	504	10/11	0.75	0.30	-	100,113,123,132	0
7	FUL	B	506	10/11	0.78	0.30	-	63,76,83,83	0
8	FUL	E	504	10/11	0.75	0.30	-	73,80,87,88	0
2	NAG	A	501	14/15	0.93	0.16	-	38,47,53,63	0
7	MAN	B	504	11/12	0.54	0.46	-	106,118,121,124	0
7	BMA	B	503	11/12	0.77	0.38	-	98,112,119,120	0
8	NAG	C	501	14/15	0.83	0.19	-	64,72,87,101	0
8	NAG	C	502	14/15	0.78	0.28	-	72,83,94,98	0
2	FUL	A	505	10/11	0.79	0.23	-	59,70,83,96	0
8	NAG	F	501	14/15	0.93	0.10	-	28,35,51,57	0
2	BMA	A	503	11/12	0.66	0.28	-	102,115,122,126	0
7	NAG	B	502	14/15	0.89	0.17	-	46,54,72,83	0
8	NAG	F	502	14/15	0.91	0.18	-	41,58,67,89	0
2	NAG	A	502	14/15	0.93	0.14	-	48,62,76,87	0
9	NAG	D	502	14/15	0.83	0.37	-	71,78,90,96	0
11	NAG	F	507	14/15	0.79	0.25	-	53,72,95,97	0
11	FUL	F	509	10/11	0.68	0.45	-	103,113,123,131	0
11	NAG	F	508	14/15	0.69	0.43	-	90,105,113,114	0
10	FUC	E	507	10/11	0.87	0.24	-	87,96,100,100	0
8	NAG	E	501	14/15	0.89	0.16	-	39,45,68,70	0
10	NAG	E	506	14/15	0.87	0.19	-	48,55,72,75	0
9	NAG	D	501	14/15	0.79	0.23	-	50,64,73,92	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
5	GOL	E	511	6/6	0.67	0.26	13.53	62,74,80,87	0
6	NO3	B	517	4/4	0.92	0.22	9.42	53,57,58,72	0
5	GOL	F	512	6/6	0.88	0.25	7.64	33,58,76,92	0
5	GOL	B	511	6/6	0.53	0.22	5.04	37,64,76,77	0
6	NO3	A	514	4/4	0.90	0.25	4.72	26,46,53,69	0
6	NO3	C	511	4/4	0.97	0.15	3.98	42,45,49,52	0
5	GOL	D	508	6/6	0.77	0.20	3.82	54,73,85,87	0
6	NO3	F	518	4/4	0.97	0.20	3.67	36,48,50,62	0
6	NO3	B	516	4/4	0.98	0.15	3.59	32,35,37,42	0
6	NO3	D	510	4/4	0.97	0.19	3.11	50,57,61,64	0
5	GOL	A	512	6/6	0.93	0.23	2.97	42,58,69,69	0
6	NO3	C	510	4/4	0.92	0.21	2.93	37,54,59,70	0
5	GOL	F	515	6/6	0.89	0.16	2.62	47,56,58,58	0
3	NAG	F	505	14/15	0.85	0.22	2.46	50,67,74,92	0
6	NO3	A	513	4/4	0.93	0.18	2.35	37,46,49,50	0
5	GOL	E	512	6/6	0.92	0.15	2.11	33,43,74,88	0
6	NO3	F	517	4/4	0.81	0.16	1.95	62,66,73,74	0
5	GOL	B	512	6/6	0.86	0.17	1.83	43,60,74,75	0
3	NAG	E	505	14/15	0.85	0.20	1.81	35,55,63,68	0
6	NO3	D	509	4/4	0.92	0.19	1.76	46,48,54,61	0
3	NAG	A	506	14/15	0.73	0.29	1.71	47,82,97,105	0
6	NO3	F	516	4/4	0.94	0.12	1.62	55,66,66,76	0
6	NO3	B	514	4/4	0.98	0.16	1.34	36,41,47,50	0
5	GOL	A	511	6/6	0.96	0.16	1.06	32,61,82,89	0
5	GOL	E	513	6/6	0.81	0.16	1.05	73,88,97,97	0
3	NAG	C	505	14/15	0.73	0.29	0.99	62,73,80,87	0
5	GOL	F	513	6/6	0.91	0.12	0.97	31,52,68,70	0
3	NAG	D	504	14/15	0.86	0.18	0.95	37,54,69,73	0
5	GOL	C	509	6/6	0.95	0.13	0.58	36,49,58,66	0
5	GOL	F	514	6/6	0.93	0.11	0.58	28,40,70,84	0
5	GOL	A	510	6/6	0.96	0.12	0.54	26,39,55,66	0
6	NO3	B	515	4/4	0.97	0.19	0.33	37,38,43,61	0
4	CA	E	510	1/1	0.91	0.10	0.09	69,69,69,69	0
4	CA	A	509	1/1	1.00	0.11	-0.07	25,25,25,25	0
6	NO3	B	513	4/4	0.97	0.15	-0.25	27,50,51,69	0
4	CA	F	510	1/1	0.99	0.09	-0.72	22,22,22,22	0
4	CA	B	509	1/1	0.99	0.08	-0.96	25,25,25,25	0
4	CA	E	509	1/1	0.97	0.07	-1.18	32,32,32,32	0
4	CA	C	507	1/1	0.94	0.07	-1.20	48,48,48,48	0
4	CA	D	506	1/1	0.98	0.06	-1.45	33,33,33,33	0
4	CA	D	507	1/1	0.89	0.05	-2.93	55,55,55,55	0
4	CA	F	511	1/1	0.97	0.05	-3.90	45,45,45,45	0
4	CA	C	508	1/1	0.76	0.06	-4.69	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	B	510	1/1	0.95	0.04	-9.41	59,59,59,59	0
3	NAG	B	508	14/15	0.77	0.32	-	68,73,90,92	0
3	NAG	C	506	14/15	0.74	0.31	-	65,74,98,101	0
3	NAG	A	508	14/15	0.73	0.27	-	65,82,93,98	0
3	NAG	F	506	14/15	0.74	0.36	-	66,80,88,95	0
3	NAG	D	505	14/15	0.68	0.33	-	56,75,86,92	0
3	NAG	B	507	14/15	0.84	0.22	-	65,86,92,100	0
3	NAG	A	507	14/15	0.81	0.26	-	67,79,88,89	0
3	NAG	E	508	14/15	0.68	0.29	-	68,87,102,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.