



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:54 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 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>

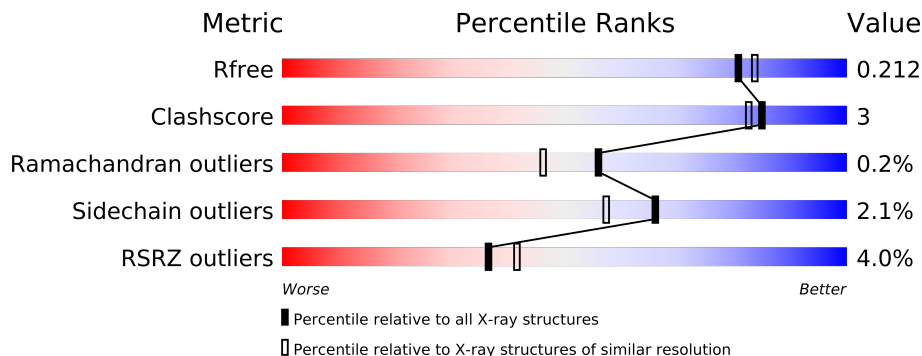
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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. 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	373	
1	B	373	
1	C	373	
1	D	373	
1	E	373	
1	F	373	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	NO3	A	513	X	-
6	NO3	A	514	X	-

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Mol	Type	Chain	Res	Geometry	Electron density
6	NO3	B	513	X	-
6	NO3	B	514	X	-
6	NO3	B	515	X	-
6	NO3	B	516	X	-
6	NO3	B	517	X	-
6	NO3	C	510	X	-
6	NO3	C	511	X	-
6	NO3	D	509	X	-
6	NO3	D	510	X	-
6	NO3	F	516	X	-
6	NO3	F	517	X	-
6	NO3	F	518	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 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 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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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

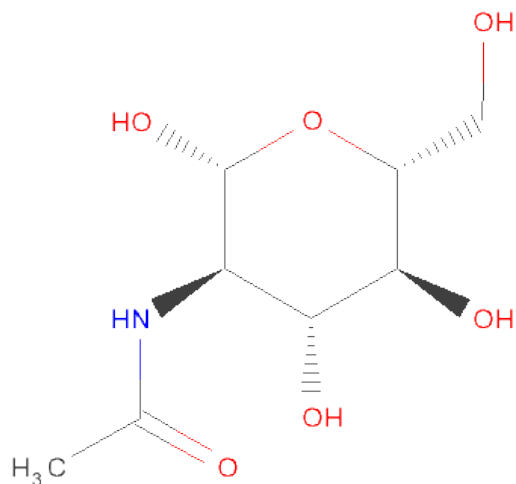
- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

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

There are 5 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

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

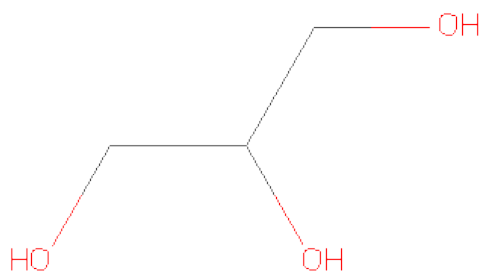


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	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 2 2	0	0
4	E	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	A	1	Total Ca 1 1	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



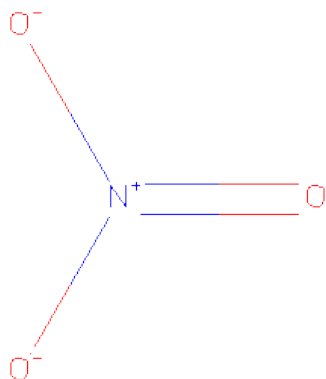
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	C	1	Total C H O 14 3 8 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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 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		

There are 5 discrepancies between the modelled and reference sequences:

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

- 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		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 12 is water.

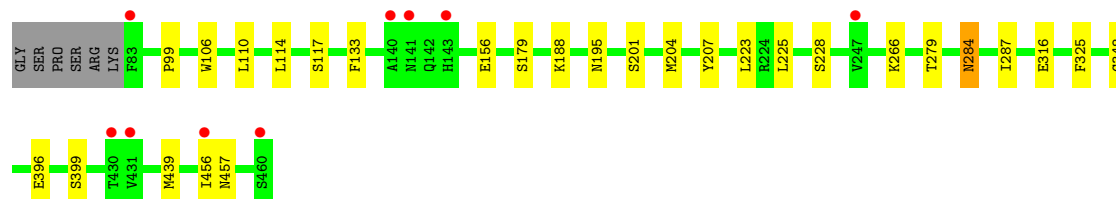
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	247	Total	O	0	0
			247	247		
12	B	246	Total	O	0	0
			246	246		
12	C	176	Total	O	0	0
			176	176		
12	D	213	Total	O	0	0
			213	213		
12	E	207	Total	O	0	0
			207	207		
12	F	319	Total	O	0	0
			319	319		

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.

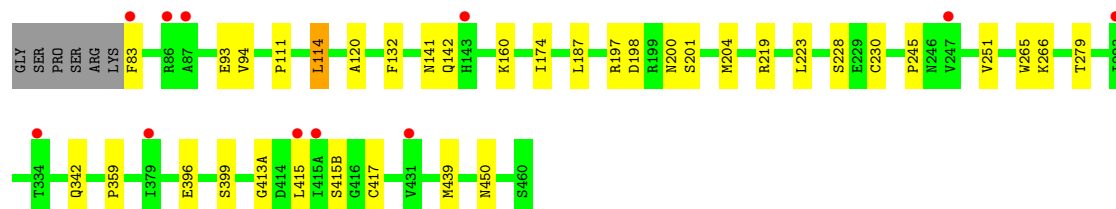
• Molecule 1: Neuraminidase

Chain A: 



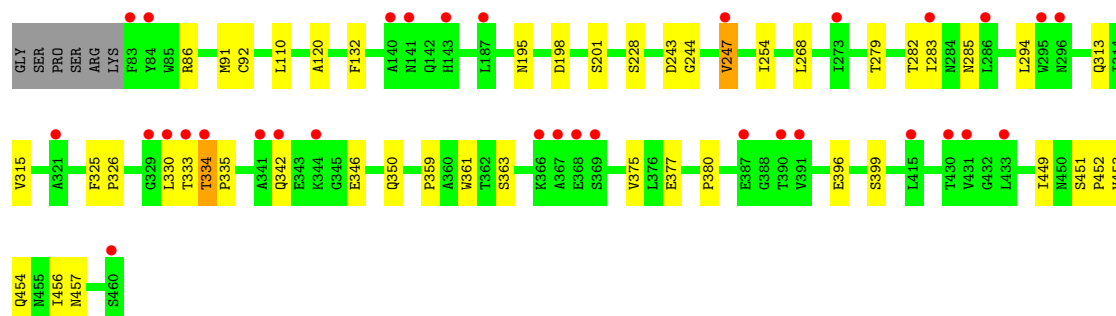
• Molecule 1: Neuraminidase

Chain B: 



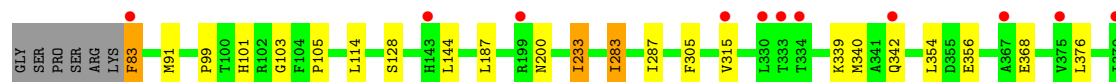
• Molecule 1: Neuraminidase

Chain C: 



• Molecule 1: Neuraminidase

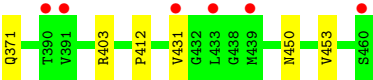
Chain D: 





● Molecule 1: Neuraminidase

Chain E:



● Molecule 1: Neuraminidase

Chain F:



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 0.170 , 0.212	Depositor DCC
R_{free} test set	10543 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.0	EDS
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 210682 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	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.

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 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	2876	2778	0	17	0
1	B	2876	2778	0	20	0
1	C	2876	2778	0	22	0
1	D	2876	2778	0	18	0
1	E	2876	2778	0	13	0
1	F	2876	2778	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	59	0	0	0	0
3	A	42	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
3	E	28	0	0	1	0
3	F	28	0	0	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	0	2	0
5	B	12	16	0	4	0
5	C	6	8	0	0	0
5	D	6	8	0	2	0
5	E	18	24	0	2	0
5	F	24	32	0	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	0	0	0
8	C	48	0	0	0	0
8	E	48	0	0	0	0
8	F	48	0	0	0	0
9	D	38	0	0	0	0
10	E	24	0	0	0	0
11	F	38	0	0	0	0
12	A	247	0	0	1	0
12	B	246	0	0	2	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	0	97	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 (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:512:GOL:O3	12:B:727:HOH:O	2.12	0.67
1:F:228:SER:HG	1:F:279:THR:HG1	1.43	0.67
1:C:451:SER:HB2	1:C:452:PRO:CD	2.28	0.64
1:B:94:VAL:H	5:B:511:GOL:HO2	1.47	0.63
1:B:201:SER:HG	1:B:223:LEU:H	1.49	0.60
1:D:103:GLY:O	5:D:508:GOL:O3	2.21	0.59
1:B:396:GLU:OE2	1:B:399:SER:OG	2.19	0.59
1:E:108:PRO:HB2	1:E:431:VAL:HG13	1.84	0.59
1:B:228:SER:HG	1:B:279:THR:HG1	1.50	0.59
1:A:396:GLU:OE2	1:A:399:SER:OG	2.23	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:C:228:SER:HG	1:C:279:THR:HG1	1.53	0.56
1:A:316:GLU:HB2	5:A:512:GOL:H32	1.88	0.55
1:A:228:SER:HG	1:A:279:THR:HG1	1.54	0.55
5:A:511:GOL:H32	6:A:513:NO3:O2	2.06	0.55
1:D:287:ILE:HD13	1:D:305:PHE:CE2	2.42	0.55
1:D:415(B):SER:OG	1:D:417:CYS:O	2.26	0.54
1:F:325:PHE:CE1	1:F:371:GLN:HG3	2.44	0.53
1:C:399:SER:OG	1:C:457:ASN:ND2	2.41	0.53
1:D:91:MET:CE	1:D:356:GLU:HG3	2.39	0.53
1:E:119:ARG:NH2	1:E:156:GLU:OE2	2.43	0.52
1:D:91:MET:HE1	1:D:354:LEU:HD21	1.92	0.51
1:D:412:PRO:HG2	1:D:419:ARG:NH2	2.25	0.51
1:C:195:ASN:O	1:C:201:SER:HA	2.11	0.50
1:D:396:GLU:OE2	1:D:399:SER:OG	2.29	0.50
1:A:456:ILE:HG12	1:B:200:ASN:HB3	1.92	0.50
1:D:427:GLU:OE1	1:D:441:GLN:HG3	2.12	0.50
3:E:505:NAG:O7	5:E:511:GOL:O1	2.29	0.50
1:B:359:PRO:HD2	5:B:511:GOL:H31	1.94	0.49
1:E:117:SER:HB3	1:E:133:PHE:CD2	2.48	0.49
1:F:156:GLU:OE2	1:F:178:ARG:NH1	2.45	0.49
1:C:325:PHE:HA	1:C:326:PRO:C	2.32	0.49
1:F:284:ASN:O	1:F:284:ASN:ND2	2.40	0.48
1:B:111:PRO:HG2	1:B:114:LEU:HD12	1.94	0.48
1:A:201:SER:HG	1:A:223:LEU:H	1.61	0.48
1:F:325:PHE:O	1:F:348:GLY:HA2	2.14	0.48
1:B:415(B):SER:OG	1:B:417:CYS:O	2.32	0.48
1:E:325:PHE:CE1	1:E:371:GLN:HG3	2.49	0.47
1:F:116:LEU:HD12	1:F:144:LEU:HD21	1.97	0.47
1:A:204:MET:HE1	1:D:99:PRO:O	2.14	0.47
1:C:333:THR:OG1	1:C:334:THR:N	2.42	0.47
1:A:188:LYS:HB2	1:A:207:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:ARG:HG3	1:B:251:VAL:HG21	1.96	0.47
1:E:195:ASN:O	1:E:201:SER:HA	2.15	0.47
1:F:378:GLN:OE1	1:F:392:SER:OG	2.32	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	0.46
1:A:179:SER:HG	1:A:225:LEU:H	1.63	0.46
1:A:325:PHE:O	1:A:348:GLY:HA2	2.15	0.46
1:A:117:SER:HB3	1:A:133:PHE:CD2	2.51	0.46
1:E:412:PRO:HB3	5:E:512:GOL:H32	1.97	0.46
1:C:120:ALA:HA	1:C:132:PHE:O	2.17	0.45
1:E:141:ASN:O	1:E:142:GLN:HB2	2.16	0.45
1:C:449:ILE:HD11	1:C:453:VAL:HB	1.98	0.45
1:C:451:SER:HB2	1:C:452:PRO:HD2	1.97	0.45
1:E:86:ARG:NH1	12:E:688:HOH:O	2.50	0.45
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.44
1:C:359:PRO:HB3	1:C:380:PRO:HA	1.98	0.44
1:D:105:PRO:HA	5:D:508:GOL:H31	1.99	0.44
1:B:265:TRP:NE1	6:B:517:NO3:O2	2.49	0.44
1:B:197:ARG:HA	1:B:197:ARG:HD2	1.67	0.44
1:B:245:PRO:HD2	12:B:721:HOH:O	2.17	0.44
1:D:233:ILE:HD11	1:D:287:ILE:HD11	2.00	0.43
1:D:101:HIS:HB3	1:D:445:THR:OG1	2.17	0.43
1:A:195:ASN:O	1:A:201:SER:HA	2.18	0.43
1:C:91:MET:HG2	1:C:92:CYS:O	2.19	0.43
1:C:363:SER:HA	1:C:375:VAL:O	2.19	0.43
1:C:313:GLN:HG2	1:C:315:VAL:HG23	2.01	0.42
1:C:396:GLU:OE2	1:C:399:SER:OG	2.36	0.42
1:E:188:LYS:HB2	1:E:207:TYR:CZ	2.54	0.42
1:A:201:SER:HG	1:A:223:LEU:N	2.17	0.42
1:B:120:ALA:HA	1:B:132:PHE:O	2.19	0.42
1:E:111:PRO:HG2	1:E:114:LEU:HD13	2.00	0.42
1:B:160:LYS:HB2	1:B:174:ILE:HD11	2.01	0.42
1:D:339:LYS:HE3	12:D:752:HOH:O	2.19	0.42
1:C:247:VAL:HG21	1:C:294:LEU:HB2	2.01	0.42
1:C:361:TRP:HA	1:C:377:GLU:O	2.20	0.42
1:C:454:GLN:OE1	1:C:454:GLN:HA	2.20	0.42
1:E:201:SER:HG	1:E:223:LEU:H	1.67	0.41
1:E:450:ASN:C	1:E:450:ASN:OD1	2.59	0.41
1:B:413(A):GLY:O	1:B:415:LEU:N	2.53	0.41
1:D:83:PHE:HB3	1:D:187:LEU:HD11	2.02	0.41
1:C:243:ASP:OD1	1:C:244:GLY:N	2.51	0.41
1:A:106:TRP:NE1	1:A:114:LEU:HD21	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:ASN:O	1:B:142:GLN:HB2	2.19	0.41
1:E:315:VAL:CG1	1:E:316:GLU:N	2.84	0.41
1:B:94:VAL:HB	5:B:511:GOL:H2	2.02	0.41
1:D:283:ILE:HD11	1:D:356:GLU:OE2	2.20	0.41
1:A:99:PRO:O	1:B:204:MET:HE1	2.21	0.41
1:C:254:ILE:HG13	1:C:268:LEU:HD21	2.03	0.41
1:A:156:GLU:HG2	12:A:604:HOH:O	2.21	0.40
1:D:339:LYS:HG2	1:D:340:MET:O	2.22	0.40
1:D:402:LYS:HE3	1:D:459:ASP:O	2.22	0.40
1:F:368:GLU:OE1	12:F:847:HOH:O	2.22	0.40
1:C:456:ILE:CD1	1:D:200:ASN:HB3	2.51	0.40
1:B:93:GLU:O	1:B:450:ASN:HA	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	365/373 (98%)	354 (97%)	10 (3%)	1 (0%)	50	38
1	B	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	C	365/373 (98%)	349 (96%)	13 (4%)	3 (1%)	27	12
1	D	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	E	365/373 (98%)	351 (96%)	13 (4%)	1 (0%)	50	38
1	F	365/373 (98%)	352 (96%)	13 (4%)	0	100	100
All	All	2190/2238 (98%)	2112 (96%)	73 (3%)	5 (0%)	56	46

All (5) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	80	76
1	B	320/325 (98%)	314 (98%)	6 (2%)	69	62
1	C	320/325 (98%)	313 (98%)	7 (2%)	64	55
1	D	320/325 (98%)	310 (97%)	10 (3%)	52	38
1	E	320/325 (98%)	311 (97%)	9 (3%)	56	43
1	F	320/325 (98%)	316 (99%)	4 (1%)	80	76
All	All	1920/1950 (98%)	1880 (98%)	40 (2%)	66	57

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

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Mol	Chain	Res	Type
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
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	263	GLN
1	A	371	GLN
1	B	195	ASN
1	B	263	GLN
1	B	313	GLN
1	B	342	GLN
1	B	371	GLN
1	B	429	GLN
1	C	143	HIS
1	C	195	ASN
1	D	195	ASN
1	D	263	GLN
1	D	313	GLN
1	E	195	ASN

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Mol	Chain	Res	Type
1	E	258	GLN
1	E	284	ASN
1	E	311	ASN
1	E	342	GLN
1	F	195	ASN
1	F	263	GLN
1	F	284	ASN
1	F	311	ASN
1	F	313	GLN
1	F	342	GLN

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 ⓘ

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	12,14,15	0.70	0	15,19,21	1.29	3 (20%)
2	NAG	A	502	2	12,14,15	0.60	0	15,19,21	0.92	1 (6%)
2	BMA	A	503	2	10,11,12	0.80	0	11,15,17	0.71	0
2	FUC	A	504	2	9,10,11	0.85	0	10,14,16	0.93	1 (10%)
2	FUL	A	505	2	9,10,11	0.83	0	10,14,16	1.21	1 (10%)
7	NAG	B	501	1,7	12,14,15	0.73	1 (8%)	15,19,21	1.46	3 (20%)
7	NAG	B	502	7	12,14,15	0.65	1 (8%)	15,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	B	503	7	10,11,12	0.82	1 (10%)	11,15,17	0.97	1 (9%)
7	MAN	B	504	7	10,11,12	0.75	0	11,15,17	1.21	2 (18%)
7	FUC	B	505	7	9,10,11	0.81	0	10,14,16	1.26	1 (10%)
7	FUL	B	506	7	9,10,11	0.88	0	10,14,16	1.59	2 (20%)
8	NAG	C	501	1,8	12,14,15	0.73	1 (8%)	15,19,21	1.22	2 (13%)
8	NAG	C	502	8	12,14,15	0.59	0	15,19,21	0.99	1 (6%)
8	FUC	C	503	8	9,10,11	0.75	0	10,14,16	0.84	0
8	FUL	C	504	8	9,10,11	0.89	1 (11%)	10,14,16	0.64	0
9	NAG	D	501	9,1	12,14,15	0.74	1 (8%)	15,19,21	0.97	0
9	NAG	D	502	9	12,14,15	0.63	0	15,19,21	0.94	1 (6%)
9	FUC	D	503	9	9,10,11	0.80	0	10,14,16	0.77	0
8	NAG	E	501	1,8	12,14,15	0.70	0	15,19,21	1.04	0
8	NAG	E	502	8	12,14,15	0.66	0	15,19,21	1.00	1 (6%)
8	FUC	E	503	8	9,10,11	0.72	0	10,14,16	1.01	1 (10%)
8	FUL	E	504	8	9,10,11	0.85	0	10,14,16	1.22	1 (10%)
10	NAG	E	506	1,10	12,14,15	0.61	0	15,19,21	1.14	2 (13%)
10	FUC	E	507	10	9,10,11	0.87	0	10,14,16	0.79	0
8	NAG	F	501	1,8	12,14,15	0.65	0	15,19,21	1.31	2 (13%)
8	NAG	F	502	8	12,14,15	0.65	0	15,19,21	1.00	1 (6%)
8	FUC	F	503	8	9,10,11	0.80	0	10,14,16	1.14	0
8	FUL	F	504	8	9,10,11	0.86	0	10,14,16	0.76	0
11	NAG	F	507	11,1	12,14,15	0.66	0	15,19,21	1.25	1 (6%)
11	NAG	F	508	11	12,14,15	0.64	0	15,19,21	1.05	1 (6%)
11	FUL	F	509	11	9,10,11	0.92	1 (11%)	10,14,16	0.71	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
7	NAG	B	502	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	B	503	7	-	0/2/19/22	0/1/1/1
7	MAN	B	504	7	-	0/2/19/22	0/1/1/1
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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	NAG	O5-C5	-2.30	1.41	1.45
11	F	509	FUL	O5-C5	-2.19	1.41	1.45
8	C	501	NAG	O5-C5	-2.18	1.41	1.45
8	C	504	FUL	O5-C5	-2.15	1.41	1.45
7	B	501	NAG	O5-C5	-2.08	1.41	1.45
7	B	503	BMA	O5-C5	-2.05	1.41	1.45
7	B	502	NAG	O5-C5	-2.03	1.41	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	507	NAG	O5-C5-C6	3.59	110.74	106.98
7	B	506	FUL	C3-C4-C5	3.46	115.59	109.84
7	B	504	MAN	O5-C5-C6	3.11	110.24	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	NAG	O3-C3-C2	-3.09	102.60	109.09
11	F	508	NAG	O5-C5-C6	3.07	110.20	106.98
8	E	502	NAG	O5-C5-C6	3.05	110.18	106.98
7	B	505	FUC	C6-C5-C4	-3.02	108.15	113.06
8	F	501	NAG	O3-C3-C2	-2.89	103.01	109.09
10	E	506	NAG	O5-C5-C6	2.80	109.92	106.98
9	D	502	NAG	O5-C5-C6	2.79	109.91	106.98
2	A	501	NAG	C2-N2-C7	-2.69	118.57	123.09
7	B	503	BMA	O5-C5-C6	2.68	109.79	106.98
2	A	501	NAG	O5-C5-C6	2.61	109.72	106.98
2	A	502	NAG	O5-C5-C6	2.61	109.72	106.98
8	C	502	NAG	O5-C5-C6	2.59	109.70	106.98
2	A	505	FUL	C3-C4-C5	2.55	114.09	109.84
8	E	503	FUC	C6-C5-C4	-2.51	108.98	113.06
7	B	506	FUL	O5-C5-C4	2.44	113.91	110.22
8	C	501	NAG	O3-C3-C4	-2.43	104.90	110.35
7	B	501	NAG	C2-N2-C7	-2.31	119.22	123.09
8	F	502	NAG	O5-C5-C6	2.29	109.39	106.98
8	E	504	FUL	C4-C3-C2	-2.28	107.44	110.50
2	A	501	NAG	O3-C3-C2	-2.27	104.33	109.09
7	B	504	MAN	C4-C3-C2	-2.25	107.49	110.50
2	A	504	FUC	C4-C3-C2	-2.22	107.53	110.50
8	C	501	NAG	C3-C4-C5	2.17	114.07	110.20
7	B	501	NAG	O5-C5-C6	2.12	109.20	106.98
8	F	501	NAG	C3-C2-N2	-2.04	108.65	111.76
10	E	506	NAG	C2-N2-C7	-2.00	119.73	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	12,14,15	0.61	0	15,19,21	0.94	1 (6%)
3	NAG	A	507	1	12,14,15	0.56	0	15,19,21	1.32	1 (6%)
3	NAG	A	508	1	12,14,15	0.70	0	15,19,21	1.35	1 (6%)
5	GOL	A	510	-	5,5,5	0.28	0	5,5,5	0.52	0
5	GOL	A	511	-	5,5,5	0.42	0	5,5,5	0.23	0
5	GOL	A	512	-	5,5,5	0.39	0	5,5,5	0.24	0
6	NO3	A	513	-	3,3,3	3.14	3 (100%)	3,3,3	0.11	0
6	NO3	A	514	-	3,3,3	3.26	3 (100%)	3,3,3	0.13	0
3	NAG	B	507	1	12,14,15	0.72	1 (8%)	15,19,21	0.87	0
3	NAG	B	508	1	12,14,15	0.63	0	15,19,21	1.00	1 (6%)
5	GOL	B	511	-	5,5,5	0.27	0	5,5,5	0.43	0
5	GOL	B	512	-	5,5,5	0.28	0	5,5,5	0.29	0
6	NO3	B	513	-	3,3,3	3.25	3 (100%)	3,3,3	0.07	0
6	NO3	B	514	-	3,3,3	3.11	3 (100%)	3,3,3	0.14	0
6	NO3	B	515	-	3,3,3	3.22	3 (100%)	3,3,3	0.16	0
6	NO3	B	516	-	3,3,3	3.02	3 (100%)	3,3,3	0.13	0
6	NO3	B	517	-	3,3,3	3.19	3 (100%)	3,3,3	0.16	0
3	NAG	C	505	1	12,14,15	0.69	1 (8%)	15,19,21	0.85	0
3	NAG	C	506	1	12,14,15	0.76	1 (8%)	15,19,21	1.06	0
5	GOL	C	509	-	5,5,5	0.29	0	5,5,5	0.53	0
6	NO3	C	510	-	3,3,3	3.15	3 (100%)	3,3,3	0.20	0
6	NO3	C	511	-	3,3,3	3.12	3 (100%)	3,3,3	0.19	0
3	NAG	D	504	1	12,14,15	0.71	1 (8%)	15,19,21	1.07	1 (6%)
3	NAG	D	505	1	12,14,15	0.73	1 (8%)	15,19,21	1.27	1 (6%)
5	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.36	0
6	NO3	D	509	-	3,3,3	3.19	3 (100%)	3,3,3	0.18	0
6	NO3	D	510	-	3,3,3	3.18	3 (100%)	3,3,3	0.06	0
3	NAG	E	505	1	12,14,15	0.77	1 (8%)	15,19,21	0.88	0
3	NAG	E	508	1	12,14,15	0.80	1 (8%)	15,19,21	1.18	3 (20%)
5	GOL	E	511	-	5,5,5	0.28	0	5,5,5	0.45	0
5	GOL	E	512	-	5,5,5	0.43	0	5,5,5	0.29	0
5	GOL	E	513	-	5,5,5	0.31	0	5,5,5	0.32	0
3	NAG	F	505	1	12,14,15	0.67	1 (8%)	15,19,21	1.14	1 (6%)
3	NAG	F	506	1	12,14,15	0.67	0	15,19,21	1.07	1 (6%)
5	GOL	F	512	-	5,5,5	0.49	0	5,5,5	0.69	0
5	GOL	F	513	-	5,5,5	0.29	0	5,5,5	0.50	0
5	GOL	F	514	-	5,5,5	0.31	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	F	515	-	5,5,5	0.33	0	5,5,5	0.49	0
6	NO3	F	516	-	3,3,3	3.19	3 (100%)	3,3,3	0.12	0
6	NO3	F	517	-	3,3,3	3.31	3 (100%)	3,3,3	0.05	0
6	NO3	F	518	-	3,3,3	3.11	3 (100%)	3,3,3	0.10	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	517	NO3	O1-N	4.02	1.41	1.24
6	B	515	NO3	O1-N	3.98	1.41	1.24
6	B	513	NO3	O1-N	3.93	1.40	1.24
6	A	514	NO3	O1-N	3.88	1.40	1.24
6	D	510	NO3	O1-N	3.81	1.40	1.24
6	F	516	NO3	O1-N	3.80	1.40	1.24
6	B	517	NO3	O1-N	3.80	1.40	1.24
6	A	513	NO3	O1-N	3.76	1.40	1.24
6	C	511	NO3	O1-N	3.72	1.40	1.24
6	F	518	NO3	O1-N	3.71	1.40	1.24
6	B	514	NO3	O1-N	3.70	1.39	1.24
6	D	509	NO3	O1-N	3.66	1.39	1.24
6	C	510	NO3	O1-N	3.59	1.39	1.24
6	B	516	NO3	O1-N	3.53	1.39	1.24
6	D	509	NO3	O3-N	3.02	1.41	1.25
6	C	510	NO3	O3-N	2.99	1.41	1.25
6	A	514	NO3	O2-N	2.97	1.41	1.25
6	A	513	NO3	O2-N	2.93	1.40	1.25
6	F	517	NO3	O2-N	2.91	1.40	1.25
6	B	517	NO3	O3-N	2.91	1.40	1.25
6	B	513	NO3	O2-N	2.88	1.40	1.25
6	F	516	NO3	O2-N	2.88	1.40	1.25
6	F	517	NO3	O3-N	2.87	1.40	1.25
6	C	511	NO3	O3-N	2.84	1.40	1.25
6	D	510	NO3	O3-N	2.83	1.40	1.25
6	A	514	NO3	O3-N	2.83	1.40	1.25
6	D	509	NO3	O2-N	2.83	1.40	1.25
6	C	510	NO3	O2-N	2.83	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	516	NO3	O3-N	2.81	1.40	1.25
6	B	513	NO3	O3-N	2.81	1.40	1.25
6	D	510	NO3	O2-N	2.80	1.40	1.25
6	B	514	NO3	O3-N	2.78	1.40	1.25
6	B	515	NO3	O3-N	2.78	1.40	1.25
6	B	516	NO3	O3-N	2.76	1.40	1.25
6	F	518	NO3	O2-N	2.76	1.39	1.25
6	B	514	NO3	O2-N	2.75	1.39	1.25
6	B	517	NO3	O2-N	2.75	1.39	1.25
6	F	518	NO3	O3-N	2.75	1.39	1.25
6	B	515	NO3	O2-N	2.75	1.39	1.25
6	B	516	NO3	O2-N	2.70	1.39	1.25
6	C	511	NO3	O2-N	2.70	1.39	1.25
6	A	513	NO3	O3-N	2.61	1.39	1.25
3	E	508	NAG	O5-C5	-2.44	1.40	1.45
3	E	505	NAG	O5-C5	-2.42	1.40	1.45
3	B	507	NAG	O5-C5	-2.25	1.41	1.45
3	C	506	NAG	O5-C5	-2.25	1.41	1.45
3	C	505	NAG	O5-C5	-2.16	1.41	1.45
3	D	505	NAG	O5-C5	-2.10	1.41	1.45
3	D	504	NAG	O5-C5	-2.03	1.41	1.45
3	F	505	NAG	O5-C5	-2.03	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NAG	O5-C5-C6	4.14	111.33	106.98
3	A	507	NAG	O5-C5-C6	3.93	111.11	106.98
3	D	505	NAG	O5-C5-C6	3.54	110.69	106.98
3	F	505	NAG	O5-C5-C6	3.46	110.61	106.98
3	B	508	NAG	O5-C5-C6	3.13	110.27	106.98
3	E	508	NAG	C2-N2-C7	-2.68	118.59	123.09
3	F	506	NAG	O5-C5-C6	2.66	109.77	106.98
3	D	504	NAG	C3-C2-N2	-2.41	108.09	111.76
3	E	508	NAG	O5-C5-C4	-2.32	107.71	110.65
3	A	506	NAG	O5-C5-C6	2.31	109.41	106.98
3	E	508	NAG	O5-C5-C6	2.13	109.22	106.98

There are no chirality outliers.

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	367/373 (98%)	0.18	9 (2%) 54 62	19, 31, 52, 77	0
1	B	367/373 (98%)	0.29	11 (2%) 48 55	20, 32, 61, 93	0
1	C	367/373 (98%)	0.45	32 (8%) 10 13	23, 40, 66, 88	0
1	D	367/373 (98%)	0.34	19 (5%) 26 32	23, 37, 63, 88	0
1	E	367/373 (98%)	0.33	14 (3%) 38 45	22, 36, 61, 92	0
1	F	367/373 (98%)	0.05	6 (1%) 68 77	18, 28, 50, 76	0
All	All	2202/2238 (98%)	0.27	91 (4%) 36 40	18, 34, 61, 93	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	431	VAL	7.2
1	D	83	PHE	6.5
1	E	431	VAL	6.4
1	D	431	VAL	6.3
1	C	83	PHE	6.3
1	E	83	PHE	6.1
1	A	431	VAL	5.9
1	B	83	PHE	5.9
1	A	83	PHE	5.3
1	F	431	VAL	5.3
1	F	83	PHE	5.1
1	B	431	VAL	4.8
1	B	415(A)	ILE	4.8
1	C	330	LEU	4.2
1	C	321	ALA	3.8
1	D	330	LEU	3.8
1	D	415(A)	ILE	3.5
1	E	460	SER	3.4
1	D	199	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	143	HIS	3.4
1	C	333	THR	3.4
1	B	247	VAL	3.3
1	D	415	LEU	3.3
1	C	247	VAL	3.3
1	D	390	THR	3.3
1	E	315	VAL	3.1
1	C	390	THR	3.1
1	A	460	SER	3.1
1	C	329	GLY	3.1
1	C	344	LYS	3.0
1	C	342	GLN	3.0
1	C	460	SER	2.9
1	E	390	THR	2.9
1	D	143	HIS	2.9
1	C	433	LEU	2.9
1	C	430	THR	2.9
1	B	86	ARG	2.9
1	C	334	THR	2.8
1	E	151	TRP	2.8
1	B	415	LEU	2.8
1	C	415	LEU	2.8
1	E	328	GLY	2.7
1	C	295	TRP	2.7
1	D	433	LEU	2.7
1	D	367	ALA	2.7
1	D	334	THR	2.7
1	C	341	ALA	2.6
1	D	430	THR	2.6
1	F	247	VAL	2.6
1	C	283	ILE	2.6
1	E	433	LEU	2.6
1	D	333	THR	2.5
1	A	141	ASN	2.5
1	C	296	ASN	2.5
1	C	143	HIS	2.5
1	F	283	ILE	2.5
1	F	249	GLN	2.5
1	C	273	ILE	2.5
1	C	84	TYR	2.5
1	C	391	VAL	2.5
1	C	366	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	391	VAL	2.4
1	C	187	LEU	2.4
1	B	283	ILE	2.4
1	A	143	HIS	2.4
1	E	391	VAL	2.3
1	A	430	THR	2.3
1	E	110	LEU	2.2
1	D	342	GLN	2.2
1	A	247	VAL	2.2
1	C	140	ALA	2.2
1	D	375	VAL	2.2
1	E	284	ASN	2.2
1	C	141	ASN	2.2
1	B	334	THR	2.2
1	C	387	GLU	2.1
1	B	87	ALA	2.1
1	E	439	MET	2.1
1	A	456	ILE	2.1
1	D	379	ILE	2.1
1	D	440	ILE	2.1
1	C	369	SER	2.1
1	B	143	HIS	2.1
1	A	140	ALA	2.1
1	B	379	ILE	2.1
1	C	368	GLU	2.1
1	F	271	THR	2.0
1	C	286	LEU	2.0
1	C	367	ALA	2.0
1	E	285	ASN	2.0
1	D	315	VAL	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
2	NAG	A	501	14/15	0.11	-	38,47,53,63	0
8	NAG	E	502	14/15	0.23	-	53,64,80,89	0
8	FUL	C	504	10/11	0.31	-	100,113,123,132	0
8	FUC	C	503	10/11	0.16	-	47,64,80,86	0
8	NAG	C	501	14/15	0.17	-	64,72,87,101	0
2	FUL	A	505	10/11	0.21	-	59,70,83,96	0
2	NAG	A	502	14/15	0.13	-	48,62,76,87	0
8	FUC	F	503	10/11	0.09	-	27,35,40,47	0
8	FUL	F	504	10/11	0.17	-	66,72,76,90	0
7	FUC	B	505	10/11	0.09	-	30,45,49,51	0
7	FUL	B	506	10/11	0.29	-	63,76,83,83	0
8	FUL	E	504	10/11	0.26	-	73,80,87,88	0
9	FUC	D	503	10/11	0.19	-	49,55,64,70	0
7	MAN	B	504	11/12	0.43	-	106,118,121,124	0
7	BMA	B	503	11/12	0.35	-	98,112,119,120	0
8	FUC	E	503	10/11	0.15	-	35,41,50,56	0
8	NAG	C	502	14/15	0.27	-	72,83,94,98	0
2	FUC	A	504	10/11	0.11	-	23,39,45,49	0
8	NAG	F	501	14/15	0.07	-	28,35,51,57	0
2	BMA	A	503	11/12	0.28	-	102,115,122,126	0
7	NAG	B	502	14/15	0.18	-	46,54,72,83	0
8	NAG	F	502	14/15	0.14	-	41,58,67,89	0
7	NAG	B	501	14/15	0.11	-	40,43,55,59	0
9	NAG	D	502	14/15	0.31	-	71,78,90,96	0
11	NAG	F	507	14/15	0.22	-	53,72,95,97	0
11	FUL	F	509	10/11	0.41	-	103,113,123,131	0
11	NAG	F	508	14/15	0.41	-	90,105,113,114	0
10	FUC	E	507	10/11	0.21	-	87,96,100,100	0
8	NAG	E	501	14/15	0.14	-	39,45,68,70	0
10	NAG	E	506	14/15	0.17	-	48,55,72,75	0
9	NAG	D	501	14/15	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NO3	C	510	4/4	0.20	-	37,54,59,70	0
6	NO3	B	517	4/4	0.18	-	53,57,58,72	0
6	NO3	F	518	4/4	0.17	-	36,48,50,62	0
6	NO3	D	510	4/4	0.17	-	50,57,61,64	0
3	NAG	D	504	14/15	0.18	-	37,54,69,73	0
4	CA	D	507	1/1	0.06	-	55,55,55,55	0
4	CA	A	509	1/1	0.10	-	25,25,25,25	0
5	GOL	A	512	6/6	0.25	-	42,58,69,69	0
3	NAG	B	508	14/15	0.31	-	68,73,90,92	0
3	NAG	A	508	14/15	0.27	-	65,82,93,98	0
4	CA	F	510	1/1	0.06	-	22,22,22,22	0
5	GOL	B	512	6/6	0.17	-	43,60,74,75	0
6	NO3	B	513	4/4	0.13	-	27,50,51,69	0
4	CA	C	508	1/1	0.05	-	75,75,75,75	0
6	NO3	D	509	4/4	0.17	-	46,48,54,61	0
5	GOL	A	510	6/6	0.11	-	26,39,55,66	0
3	NAG	A	507	14/15	0.24	-	67,79,88,89	0
3	NAG	A	506	14/15	0.27	-	47,82,97,105	0
5	GOL	C	509	6/6	0.12	-	36,49,58,66	0
6	NO3	A	514	4/4	0.21	-	26,46,53,69	0
4	CA	B	510	1/1	0.07	-	59,59,59,59	0
6	NO3	B	516	4/4	0.13	-	32,35,37,42	0
3	NAG	F	506	14/15	0.34	-	66,80,88,95	0
5	GOL	F	512	6/6	0.22	-	33,58,76,92	0
3	NAG	F	505	14/15	0.19	-	50,67,74,92	0
5	GOL	D	508	6/6	0.19	-	54,73,85,87	0
6	NO3	C	511	4/4	0.13	-	42,45,49,52	0
3	NAG	B	507	14/15	0.22	-	65,86,92,100	0
6	NO3	B	514	4/4	0.14	-	36,41,47,50	0
4	CA	E	509	1/1	0.06	-	32,32,32,32	0
5	GOL	F	513	6/6	0.11	-	31,52,68,70	0
5	GOL	E	511	6/6	0.23	-	62,74,80,87	0
4	CA	C	507	1/1	0.07	-	48,48,48,48	0
4	CA	E	510	1/1	0.07	-	69,69,69,69	0
3	NAG	C	505	14/15	0.25	-	62,73,80,87	0
6	NO3	F	517	4/4	0.13	-	62,66,73,74	0
5	GOL	B	511	6/6	0.20	-	37,64,76,77	0
5	GOL	E	513	6/6	0.15	-	73,88,97,97	0
6	NO3	F	516	4/4	0.14	-	55,66,66,76	0
4	CA	D	506	1/1	0.06	-	33,33,33,33	0
4	CA	F	511	1/1	0.05	-	45,45,45,45	0
5	GOL	F	515	6/6	0.15	-	47,56,58,58	0
5	GOL	F	514	6/6	0.10	-	28,40,70,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NO3	B	515	4/4	0.17	-	37,38,43,61	0
5	GOL	A	511	6/6	0.13	-	32,61,82,89	0
3	NAG	C	506	14/15	0.31	-	65,74,98,101	0
3	NAG	E	505	14/15	0.21	-	35,55,63,68	0
4	CA	B	509	1/1	0.07	-	25,25,25,25	0
3	NAG	D	505	14/15	0.33	-	56,75,86,92	0
5	GOL	E	512	6/6	0.12	-	33,43,74,88	0
6	NO3	A	513	4/4	0.15	-	37,46,49,50	0
3	NAG	E	508	14/15	0.30	-	68,87,102,114	0

6.5 Other polymers ⓘ

There are no such residues in this entry.