



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2016 – 09:36 PM EDT

PDB ID : 5T3X  
Title : 3.9 Angstrom Crystal Structure of a Fully and Natively Glycosylated BG505 SOSIP.664 HIV-1 Env Trimer in Complex with the Broadly Neutralizing Antibodies IOMA and 10-1074.  
Authors : Gristick, H.B.; Bjorkman, P.J.  
Deposited on : 2016-08-26  
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

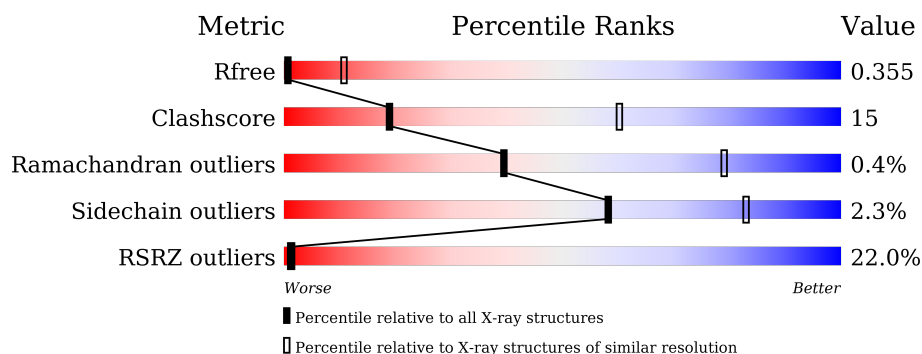
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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

Mol	Chain	Length	Quality of chain
1	B	153	<div> <div>10%</div> <div>49%</div> <div>32%</div> <div>•</div> <div>18%</div> </div>
2	G	481	<div> <div>7%</div> <div>58%</div> <div>34%</div> <div>•</div> <div>7%</div> </div>
3	H	238	<div> <div>29%</div> <div>67%</div> <div>29%</div> <div>••</div> </div>
4	L	214	<div> <div>20%</div> <div>67%</div> <div>29%</div> <div>••</div> </div>
5	D	232	<div> <div>29%</div> <div>59%</div> <div>37%</div> <div>••</div> </div>
6	E	214	<div> <div>42%</div> <div>67%</div> <div>29%</div> <div>••</div> </div>

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
10	MAN	G	3325	-	-	-	X
7	FUC	G	2760	-	-	-	X
8	NAG	G	3010	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	449	Total	C	N	O	S	0	0	0
			3532	2217	623	665	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called 10-1074 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			

- Molecule 4 is a protein called 10-1074 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			

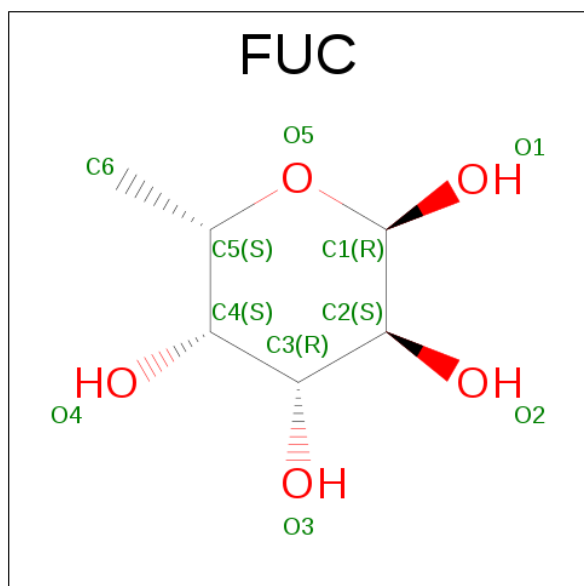
- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	229	Total	C	N	O	S	0	0	0
			1742	1100	298	332	12			

- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



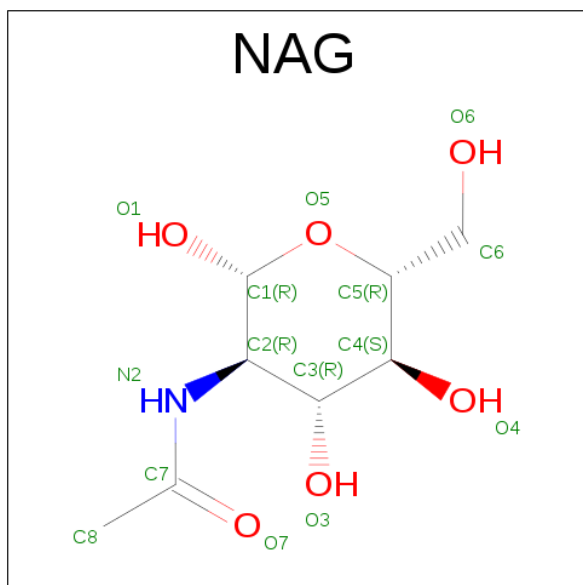
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

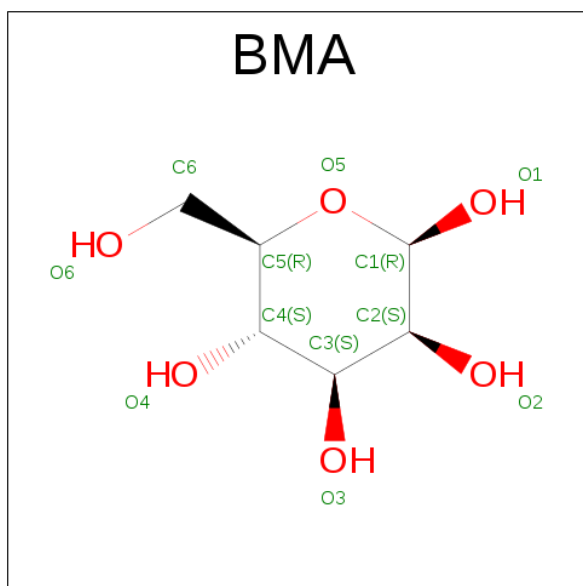
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



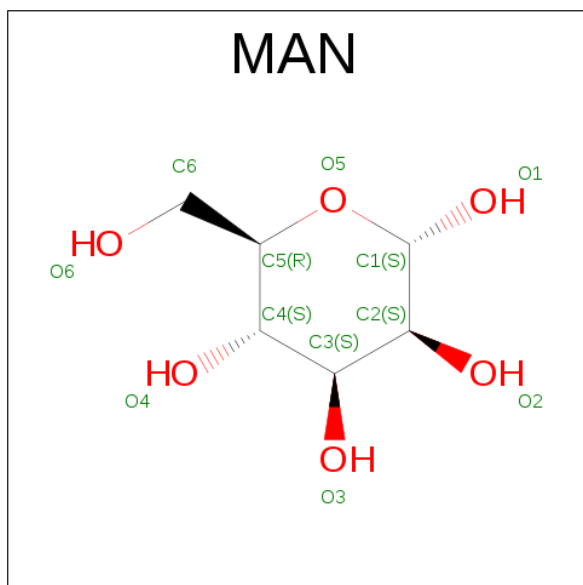
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 10 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

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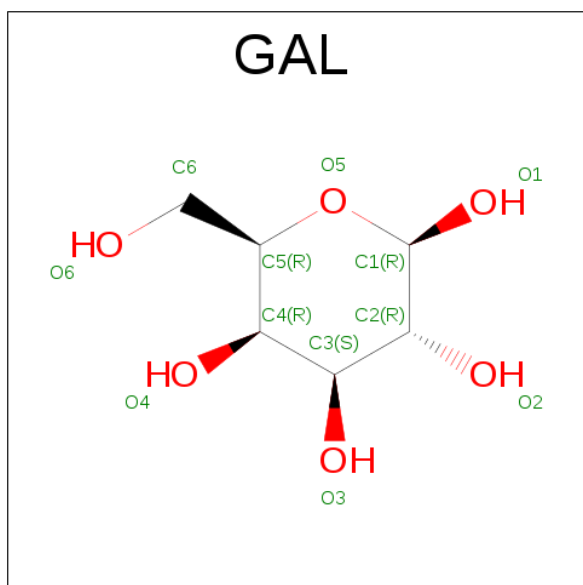
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11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

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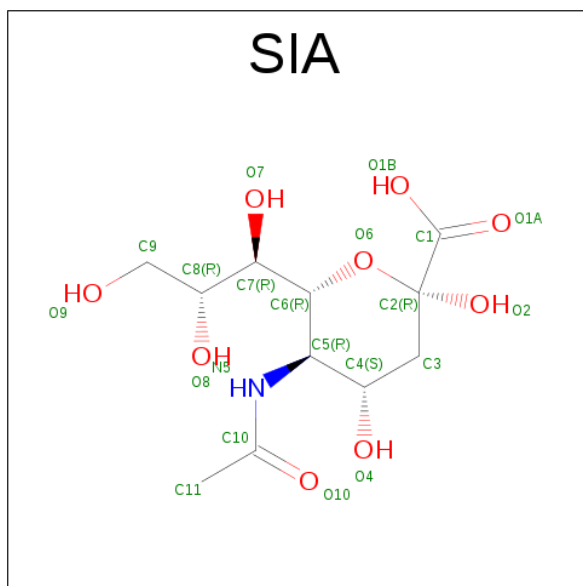
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 11 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 12 is O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).

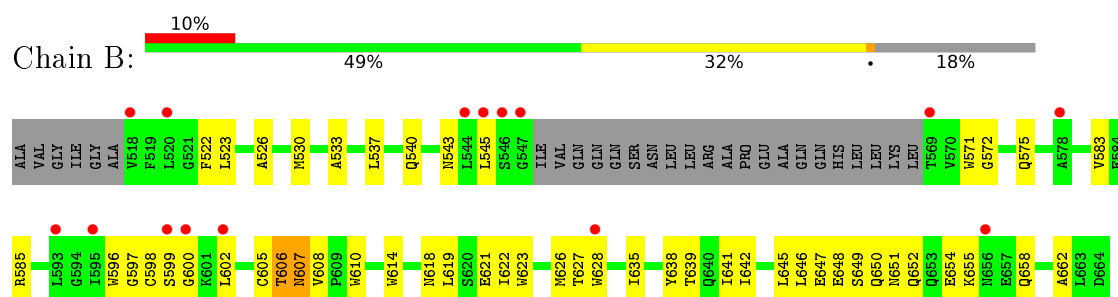


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			20	11	1	8		
12	G	1	Total	C	N	O	0	0
			20	11	1	8		
12	G	1	Total	C	N	O	0	0
			20	11	1	8		

### 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: Envelope glycoprotein gp160

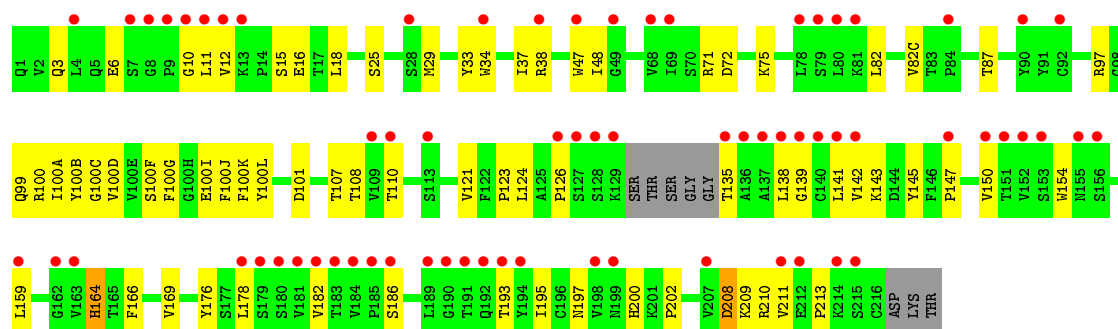


- Molecule 2: Envelope glycoprotein gp160

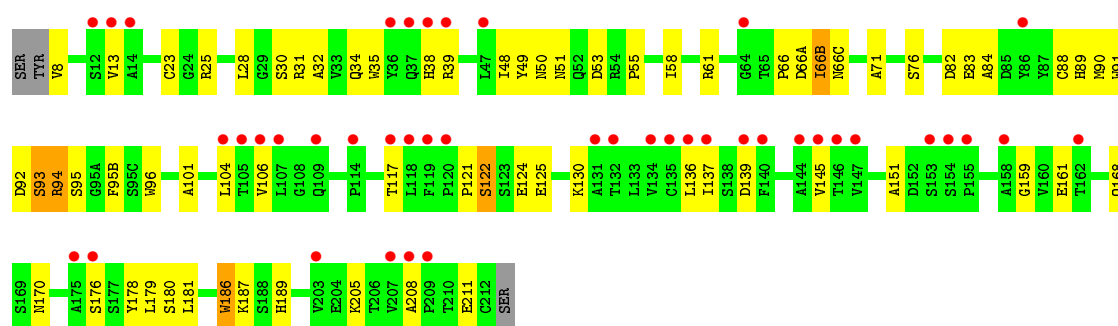


- Molecule 3: 10-1074 Heavy Chain

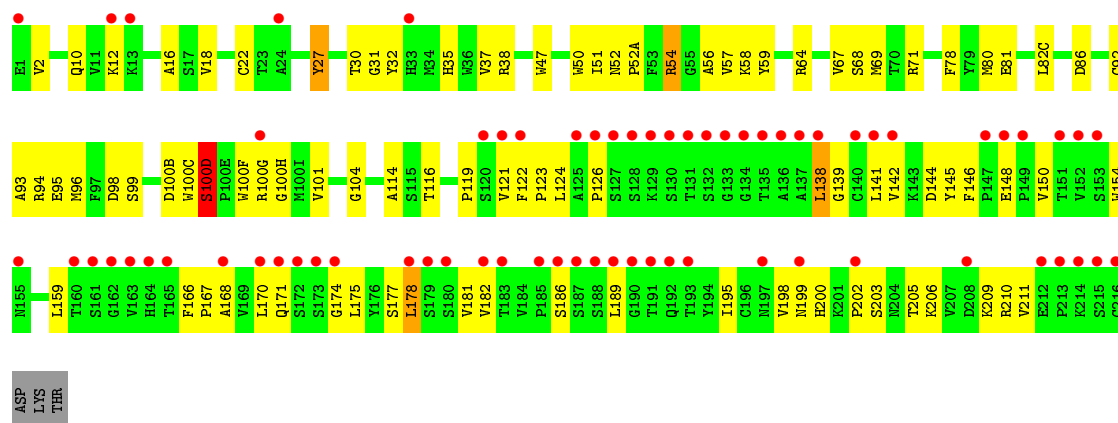




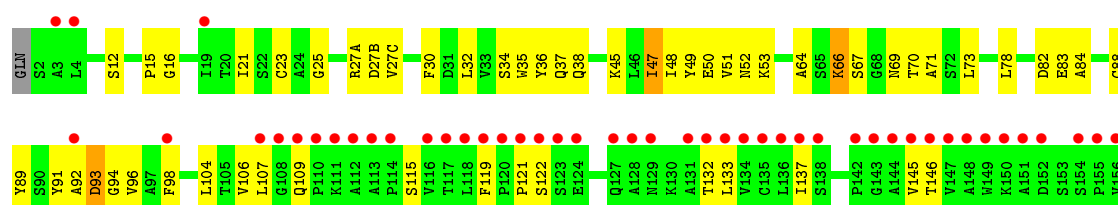
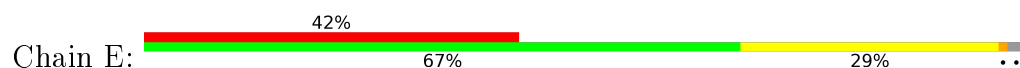
• Molecule 4: 10-1074 Light Chain

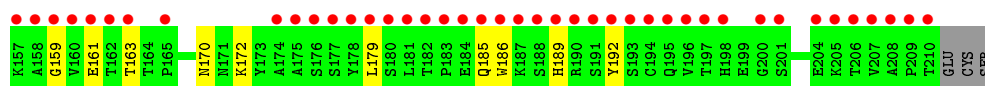


• Molecule 5: IOMA Heavy Chain



• Molecule 6: IOMA Light Chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.51Å 217.51Å 156.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.63 – 3.90 80.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.63-3.90) 95.7 (80.63-3.90)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.296 , 0.331 0.334 , 0.355	Depositor DCC
$R_{free}$ test set	1220 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	132.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 326.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.097 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.160 for k,h,-l	Depositor
Outliers	0 of 25072 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	302.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.25	0/1019	0.45	0/1382
2	G	0.28	0/3605	0.53	2/4895 (0.0%)
3	H	0.25	0/1796	0.48	0/2450
4	L	0.26	0/1649	0.47	0/2250
5	D	0.27	0/1790	0.55	2/2437 (0.1%)
6	E	0.26	0/1596	0.50	0/2175
All	All	0.26	0/11455	0.51	4/15589 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	100(D)	SER	C-N-CD	-8.05	102.89	120.60
2	G	458	GLY	O-C-N	-8.00	109.61	123.20
5	D	100(D)	SER	C-N-CA	6.31	148.50	122.00
2	G	458	GLY	CA-C-N	5.83	127.86	116.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	B	1001	0	976	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3532	0	3462	132	0
3	H	1753	0	1719	52	0
4	L	1607	0	1550	52	0
5	D	1742	0	1698	72	0
6	E	1558	0	1511	52	0
7	B	20	0	20	0	0
7	G	50	0	50	1	0
8	B	42	0	35	0	0
8	G	672	0	582	17	0
9	B	11	0	10	0	0
9	G	132	0	98	3	0
10	G	341	0	286	10	0
11	G	99	0	87	0	0
12	G	60	0	51	0	0
All	All	12620	0	12135	378	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 15.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.57	0.87
6:E:47:ILE:HG22	6:E:48:ILE:HG12	1.61	0.82
2:G:119:CYS:SG	2:G:205:CYS:N	2.50	0.81
5:D:199:ASN:OD1	5:D:206:LYS:NZ	2.13	0.80
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.63	0.78
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.66	0.77
2:G:51:THR:HA	2:G:103:GLN:HE22	1.52	0.75
2:G:175:LEU:O	2:G:320:THR:OG1	2.06	0.73
5:D:119:PRO:HD2	5:D:205:THR:HB	1.70	0.72
1:B:642:ILE:HG21	2:G:496:VAL:HG11	1.72	0.72
3:H:100:ARG:NH2	4:L:66(A):ASP:OD2	2.22	0.72
1:B:606:THR:HG21	1:B:646:LEU:HD22	1.71	0.72
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.54	0.71
5:D:35:HIS:HD2	5:D:50:TRP:HB3	1.55	0.69
4:L:13:VAL:HG23	4:L:104:LEU:HD11	1.75	0.69
2:G:65:LYS:HB2	2:G:68:VAL:HG23	1.75	0.69
5:D:51:ILE:HG23	5:D:57:VAL:HG12	1.74	0.69
5:D:150:VAL:HG11	5:D:198:VAL:HG13	1.75	0.68
9:G:2763:BMA:H2	10:G:2764:MAN:H5	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:279:ASN:HD22	2:G:282:LYS:HG2	1.58	0.68
8:G:1566:NAG:H81	8:G:1571:NAG:H82	1.76	0.67
1:B:606:THR:OG1	2:G:36:VAL:O	2.11	0.67
2:G:69:TRP:HE1	2:G:253:PRO:HG2	1.60	0.67
4:L:39:ARG:NH1	4:L:83:GLU:O	2.27	0.67
2:G:303:THR:HB	2:G:321:GLY:HA3	1.75	0.67
2:G:131:CYS:HB3	2:G:155:LYS:HB3	1.77	0.66
2:G:92:GLU:HA	2:G:238:PRO:HA	1.77	0.66
4:L:25:ARG:HH21	4:L:90:MET:H	1.42	0.66
3:H:38:ARG:HG3	3:H:48:ILE:HD11	1.79	0.65
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.61	0.65
2:G:258:GLN:NE2	2:G:371:VAL:O	2.29	0.65
2:G:424:ILE:HG22	2:G:426:MET:H	1.63	0.64
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.78	0.64
3:H:195:ILE:HG12	3:H:210:ARG:HG2	1.79	0.64
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.80	0.64
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.81	0.63
4:L:159:GLY:O	4:L:180:SER:N	2.27	0.63
3:H:100(B):TYR:CE2	4:L:93:SER:HB2	2.34	0.63
6:E:66:LYS:HA	6:E:71:ALA:HA	1.81	0.62
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.25	0.62
4:L:83:GLU:HG2	4:L:106:VAL:H	1.64	0.62
4:L:23:CYS:HB2	4:L:71:ALA:HB3	1.81	0.62
1:B:596:TRP:O	1:B:651:ASN:ND2	2.32	0.62
1:B:526:ALA:HA	2:G:43:PRO:HB2	1.82	0.62
4:L:61:ARG:NH1	4:L:76:SER:O	2.29	0.61
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.81	0.61
3:H:3:GLN:HG3	3:H:25:SER:HB2	1.82	0.61
2:G:439:ILE:HB	2:G:443:ILE:HD11	1.81	0.61
1:B:654:GLU:OE1	2:G:503:ARG:NH1	2.32	0.61
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.82	0.60
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.65	0.60
2:G:251:ILE:HG23	2:G:482:GLU:HG3	1.83	0.60
6:E:23:CYS:HB3	6:E:71:ALA:HB3	1.81	0.60
2:G:266:ALA:N	2:G:288:PHE:O	2.31	0.60
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.34	0.60
1:B:540:GLN:HE22	2:G:43:PRO:HG3	1.66	0.60
1:B:537:LEU:HD13	1:B:602:LEU:O	2.02	0.60
4:L:137:ILE:HD13	4:L:145:VAL:HG11	1.83	0.60
3:H:47:TRP:HE3	4:L:96:TRP:HA	1.67	0.60
4:L:25:ARG:NH2	4:L:90:MET:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:95:GLU:HA	5:D:100(H):GLY:O	2.03	0.59
4:L:28:LEU:HB3	4:L:94:ARG:HB2	1.84	0.59
2:G:274:SER:HB3	2:G:277:ILE:HG12	1.85	0.59
5:D:142:VAL:HG11	5:D:150:VAL:HG21	1.85	0.58
5:D:35:HIS:CD2	5:D:50:TRP:HB3	2.37	0.58
1:B:533:ALA:HB1	2:G:43:PRO:HG2	1.85	0.58
8:G:3860:NAG:O3	8:G:3861:NAG:N2	2.35	0.58
6:E:34:SER:N	6:E:89:TYR:O	2.31	0.58
2:G:195:ASN:ND2	2:G:199:SER:O	2.34	0.58
5:D:2:VAL:HG11	5:D:94:ARG:HH12	1.67	0.58
5:D:141:LEU:HD12	5:D:178:LEU:O	2.03	0.58
1:B:598:CYS:C	1:B:600:GLY:H	2.08	0.58
1:B:638:TYR:HA	1:B:641:ILE:HD12	1.86	0.58
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.86	0.57
5:D:150:VAL:HB	5:D:178:LEU:HD21	1.86	0.57
4:L:179:LEU:HG	4:L:181:LEU:HD13	1.86	0.57
5:D:116:THR:HG23	5:D:203:SER:HA	1.86	0.57
5:D:10:GLN:HB3	5:D:12:LYS:HE2	1.86	0.57
5:D:145:TYR:HE1	5:D:148:GLU:HA	1.70	0.57
6:E:92:ALA:C	6:E:94:GLY:H	2.07	0.57
1:B:650:GLN:O	1:B:654:GLU:N	2.32	0.57
5:D:47:TRP:HZ2	5:D:50:TRP:HD1	1.52	0.57
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.87	0.57
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.68	0.57
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.37	0.57
2:G:370:GLU:OE1	2:G:428:GLN:NE2	2.38	0.56
8:G:4480:NAG:O3	8:G:4481:NAG:N2	2.38	0.56
2:G:182:VAL:HG13	2:G:192:ARG:HD3	1.87	0.56
2:G:285:LEU:HD22	2:G:453:ILE:HG12	1.87	0.56
2:G:34:LEU:HB3	2:G:498:PRO:HB2	1.86	0.56
1:B:606:THR:OG1	2:G:36:VAL:HG23	2.06	0.56
3:H:147:PRO:O	3:H:200:HIS:NE2	2.38	0.56
5:D:68:SER:HB3	5:D:81:GLU:HB3	1.87	0.56
2:G:441:GLY:HA3	8:G:3010:NAG:H82	1.88	0.56
5:D:18:VAL:HG23	5:D:82(C):LEU:HD11	1.88	0.56
3:H:193:THR:HG21	3:H:210:ARG:CZ	2.36	0.56
5:D:52(A):PRO:HG3	5:D:78:PHE:CZ	2.39	0.56
2:G:155:LYS:O	2:G:175:LEU:HA	2.05	0.56
2:G:369:LEU:O	2:G:373:THR:OG1	2.23	0.55
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.88	0.55
4:L:32:ALA:N	4:L:91:TRP:O	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:385:CYS:HA	2:G:418:CYS:HA	1.87	0.55
6:E:21:ILE:HD12	6:E:73:LEU:HD23	1.88	0.55
2:G:380:GLY:HA3	2:G:439:ILE:HG13	1.89	0.54
4:L:117:THR:HA	4:L:205:LYS:HG3	1.89	0.54
5:D:142:VAL:O	5:D:177:SER:HA	2.06	0.54
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.88	0.54
4:L:186:TRP:CD1	4:L:187:LYS:HG3	2.42	0.54
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.47	0.54
2:G:325:ASP:OD1	4:L:30:SER:N	2.25	0.54
2:G:69:TRP:CG	2:G:70:ALA:N	2.75	0.54
8:G:1601:NAG:H62	8:G:1602:NAG:H82	1.89	0.54
5:D:52:ASN:HB3	5:D:56:ALA:HB3	1.90	0.54
1:B:628:TRP:CD1	2:G:43:PRO:HD2	2.42	0.54
1:B:530:MET:HG2	1:B:628:TRP:CG	2.43	0.54
5:D:69:MET:HG2	5:D:80:MET:HG2	1.90	0.54
2:G:100:MET:HB2	2:G:483:LEU:HD13	1.90	0.54
2:G:119:CYS:HB3	2:G:203:GLN:O	2.08	0.53
1:B:545:LEU:HD11	1:B:583:VAL:HG12	1.89	0.53
6:E:92:ALA:O	6:E:94:GLY:N	2.34	0.53
10:G:3328:MAN:O3	4:L:50:ASN:O	2.24	0.53
3:H:166:PHE:HB3	4:L:176:SER:HB3	1.90	0.53
2:G:98:ASN:ND2	2:G:486:TYR:O	2.42	0.53
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.29	0.53
2:G:320:THR:HG22	2:G:438:PRO:HG3	1.91	0.52
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.44	0.52
3:H:142:VAL:HB	3:H:178:LEU:HG	1.92	0.52
5:D:22:CYS:O	5:D:78:PHE:N	2.40	0.52
2:G:252:LYS:HE3	2:G:262:ASN:HB3	1.91	0.52
2:G:183:GLN:HA	2:G:191:TYR:HA	1.92	0.52
2:G:430:ILE:HG22	2:G:431:GLY:H	1.75	0.52
3:H:123:PRO:HD2	4:L:124:GLU:HB2	1.90	0.52
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.44	0.52
10:G:1564:MAN:O3	8:G:1565:NAG:O5	2.20	0.52
2:G:499:THR:HG23	2:G:501:CYS:H	1.75	0.52
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.90	0.52
1:B:610:TRP:NE1	1:B:614:TRP:O	2.42	0.52
2:G:358:ILE:HG12	2:G:396:ILE:HG23	1.91	0.52
2:G:473:GLY:O	5:D:54:ARG:NH1	2.40	0.51
5:D:52:ASN:N	5:D:56:ALA:O	2.38	0.51
6:E:145:VAL:HG12	6:E:146:THR:N	2.25	0.51
3:H:100(A):ILE:HG12	3:H:100(J):PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:HA	1:B:540:GLN:NE2	2.25	0.51
6:E:89:TYR:CE1	6:E:96:VAL:HG13	2.46	0.51
8:G:1330:NAG:O6	8:G:1331:NAG:N2	2.43	0.51
10:G:2769:MAN:O5	8:G:2775:NAG:H82	2.11	0.51
4:L:208:ALA:HB3	4:L:211:GLU:HG3	1.93	0.51
1:B:572:GLY:O	1:B:575:GLN:NE2	2.43	0.51
5:D:35:HIS:N	5:D:93:ALA:O	2.38	0.51
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.75	0.51
2:G:55:ALA:O	2:G:216:HIS:N	2.36	0.51
8:G:3321:NAG:H2	3:H:100(D):VAL:HA	1.92	0.51
4:L:34:GLN:HE21	4:L:91:TRP:HD1	1.59	0.51
6:E:12:SER:HB2	6:E:107:LEU:HD13	1.91	0.51
3:H:99:GLN:HG3	3:H:100(J):PHE:CD2	2.45	0.51
4:L:31:ARG:NH2	4:L:66:PRO:O	2.43	0.51
1:B:523:LEU:HA	1:B:540:GLN:HE21	1.74	0.51
5:D:126:PRO:HA	6:E:119:PHE:CE1	2.46	0.51
3:H:101:ASP:OD1	3:H:101:ASP:N	2.44	0.51
4:L:82:ASP:HB2	4:L:106:VAL:HG21	1.93	0.51
4:L:31:ARG:O	4:L:51:ASN:ND2	2.43	0.51
2:G:263:GLY:O	2:G:450:THR:HG21	2.12	0.50
2:G:55:ALA:N	2:G:216:HIS:O	2.44	0.50
4:L:28:LEU:O	4:L:92:ASP:HB2	2.11	0.50
2:G:274:SER:HB2	2:G:284:ILE:HG23	1.94	0.50
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.47	0.50
2:G:266:ALA:HB2	2:G:287:GLN:HB3	1.92	0.50
5:D:31:GLY:O	5:D:98:ASP:HB3	2.12	0.50
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.94	0.50
3:H:6:GLU:N	3:H:6:GLU:OE1	2.44	0.50
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.47	0.50
5:D:186:SER:HA	5:D:189:LEU:HG	1.92	0.50
2:G:335:LYS:H	2:G:413:SER:HA	1.76	0.50
5:D:100(G):ARG:HA	6:E:89:TYR:CE2	2.47	0.49
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.94	0.49
3:H:12:VAL:HG21	3:H:18:LEU:HD12	1.94	0.49
2:G:164:GLU:HA	2:G:312:GLY:O	2.12	0.49
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.94	0.49
2:G:55:ALA:HA	2:G:75:VAL:O	2.13	0.49
6:E:37:GLN:N	6:E:45:LYS:O	2.45	0.49
2:G:109:ILE:HG12	2:G:427:TRP:CD2	2.48	0.49
5:D:200:HIS:CE1	5:D:203:SER:HG	2.26	0.49
2:G:215:ILE:N	2:G:251:ILE:O	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:3922:NAG:H4	9:G:3923:BMA:O2	2.12	0.49
1:B:522:PHE:CD1	1:B:523:LEU:HG	2.47	0.48
5:D:100(G):ARG:HE	6:E:49:TYR:HD2	1.61	0.48
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.78	0.48
1:B:522:PHE:CE2	1:B:540:GLN:HA	2.47	0.48
5:D:100(C):TRP:O	5:D:100(D):SER:HB2	2.13	0.48
2:G:326:ILE:HG12	4:L:94:ARG:NE	2.28	0.48
5:D:166:PHE:HE2	5:D:181:VAL:HG13	1.78	0.48
2:G:393:SER:HB3	2:G:395:TRP:HE1	1.77	0.48
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.48	0.48
5:D:50:TRP:CE2	5:D:58:LYS:HB3	2.49	0.48
4:L:92:ASP:OD1	4:L:95:SER:OG	2.28	0.48
6:E:121:PRO:HD3	6:E:133:LEU:HD21	1.95	0.48
2:G:46:LYS:HG3	2:G:492:GLU:HG3	1.95	0.48
3:H:100(C):GLY:HA3	3:H:100(I):GLU:OE1	2.13	0.48
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.48	0.48
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.96	0.48
5:D:167:PRO:HD2	6:E:163:THR:HB	1.95	0.48
5:D:59:TYR:O	5:D:64:ARG:NH2	2.47	0.48
6:E:36:TYR:HE1	6:E:89:TYR:HB3	1.79	0.48
2:G:279:ASN:HB2	7:G:2760:FUC:H61	1.96	0.47
3:H:100(K):PHE:HE2	4:L:91:TRP:HB3	1.79	0.47
5:D:99:SER:OG	5:D:100(B):ASP:O	2.32	0.47
2:G:474:ASP:OD1	2:G:476:ARG:NH1	2.47	0.47
1:B:635:ILE:O	1:B:639:THR:HG23	2.14	0.47
3:H:121:VAL:HA	3:H:141:LEU:O	2.14	0.47
4:L:122:SER:OG	4:L:125:GLU:N	2.33	0.47
2:G:104:MET:HG2	2:G:217:TYR:CZ	2.50	0.47
8:G:3011:NAG:O3	9:G:3012:BMA:O2	2.19	0.47
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.97	0.47
1:B:605:CYS:HA	2:G:37:THR:HG22	1.95	0.47
1:B:607:ASN:N	1:B:607:ASN:OD1	2.47	0.47
2:G:107:ASP:OD2	2:G:217:TYR:OH	2.32	0.47
6:E:185:GLN:O	6:E:192:TYR:OH	2.33	0.47
6:E:27(B):ASP:O	6:E:30:PHE:HB2	2.14	0.47
1:B:522:PHE:CE2	1:B:543:ASN:HB2	2.50	0.47
5:D:67:VAL:HG11	5:D:69:MET:HE3	1.97	0.46
2:G:279:ASN:ND2	2:G:282:LYS:HG2	2.25	0.46
2:G:338:TRP:O	2:G:342:LEU:HG	2.15	0.46
2:G:298:ARG:HB2	2:G:383:PHE:HZ	1.79	0.46
1:B:571:TRP:CH2	2:G:74:CYS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:175:LEU:HD22	2:G:321(A):ASP:HA	1.97	0.46
3:H:124:LEU:HD23	4:L:122:SER:HB3	1.97	0.46
3:H:38:ARG:HH12	3:H:82:LEU:HD22	1.79	0.46
2:G:37:THR:OG1	2:G:497:ALA:O	2.33	0.46
2:G:206:PRO:HD3	2:G:318:TYR:CE2	2.51	0.46
1:B:645:LEU:HD12	1:B:649:SER:HB3	1.98	0.46
5:D:51:ILE:HD11	5:D:69:MET:HB3	1.98	0.46
6:E:27(B):ASP:OD1	6:E:27(C):VAL:N	2.43	0.46
10:G:1973:MAN:H4	8:G:1974:NAG:H83	1.97	0.46
4:L:151:ALA:HB1	4:L:189:HIS:CD2	2.51	0.46
5:D:168:ALA:HA	5:D:178:LEU:HB3	1.98	0.46
6:E:145:VAL:HG12	6:E:146:THR:H	1.80	0.46
2:G:192:ARG:NH2	2:G:193:LEU:O	2.44	0.46
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.98	0.45
1:B:651:ASN:O	1:B:655:LYS:HB2	2.15	0.45
6:E:48:ILE:HA	6:E:53:LYS:O	2.16	0.45
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.51	0.45
4:L:34:GLN:HB2	4:L:89:HIS:HB3	1.98	0.45
5:D:138:LEU:HB2	5:D:211:VAL:HG11	1.98	0.45
2:G:122:LEU:O	2:G:125:LEU:HB2	2.16	0.45
4:L:49:TYR:O	4:L:53:ASP:HB2	2.16	0.45
10:G:3327:MAN:O3	4:L:66(A):ASP:O	2.29	0.45
3:H:135:THR:N	3:H:186:SER:HG	2.14	0.45
5:D:38:ARG:HH22	5:D:86:ASP:HA	1.81	0.45
2:G:384:TYR:CE1	2:G:421:LYS:HB3	2.51	0.45
1:B:658:GLN:O	1:B:662:ALA:N	2.50	0.45
5:D:96:MET:HG2	5:D:101:VAL:HG23	1.97	0.45
2:G:44:VAL:HG12	2:G:492:GLU:HB2	1.98	0.45
1:B:623:TRP:HH2	2:G:39:TYR:CE1	2.35	0.45
5:D:121:VAL:HG21	5:D:198:VAL:HG11	1.99	0.45
6:E:35:TRP:CZ3	6:E:88:CYS:HB3	2.52	0.44
2:G:80:ASN:O	2:G:82:GLN:N	2.49	0.44
3:H:142:VAL:HG11	3:H:150:VAL:HG11	1.99	0.44
1:B:571:TRP:HZ3	2:G:72:HIS:H	1.65	0.44
2:G:339:ASN:OD1	8:G:3390:NAG:N2	2.51	0.44
2:G:434:MET:HG2	2:G:435:TYR:N	2.33	0.44
2:G:35:TRP:O	2:G:498:PRO:HA	2.18	0.44
2:G:384:TYR:O	2:G:419:ARG:N	2.46	0.44
10:G:2764:MAN:H2	8:G:2775:NAG:H61	1.99	0.44
5:D:170:LEU:HD11	5:D:174:GLY:HA2	1.98	0.44
5:D:171:GLN:HG2	6:E:161:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:185:GLN:O	6:E:189:HIS:ND1	2.48	0.44
1:B:618:ASN:HB2	1:B:621:GLU:HG3	1.98	0.44
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.83	0.44
5:D:122:PHE:CE2	5:D:141:LEU:HD23	2.53	0.44
2:G:120:VAL:HG11	2:G:316:ALA:O	2.17	0.44
3:H:10:GLY:HA3	3:H:202:PRO:HG3	2.00	0.44
4:L:66(B):ILE:O	4:L:66(C):ASN:HB2	2.18	0.44
2:G:198:THR:OG1	2:G:199:SER:N	2.51	0.43
10:G:3324:MAN:H2	10:G:3325:MAN:H2	1.78	0.43
6:E:16:GLY:H	6:E:78:LEU:HB2	1.82	0.43
2:G:298:ARG:HB2	2:G:383:PHE:CZ	2.53	0.43
2:G:350:ARG:NH2	2:G:396:ILE:O	2.48	0.43
2:G:312:GLY:HA2	2:G:315:GLN:HB2	1.98	0.43
2:G:393:SER:HB3	2:G:395:TRP:NE1	2.32	0.43
3:H:139:GLY:HA2	3:H:154:TRP:CZ2	2.53	0.43
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.52	0.43
5:D:124:LEU:HB3	6:E:119:PHE:CD2	2.53	0.43
5:D:16:ALA:O	5:D:82(C):LEU:HG	2.18	0.43
5:D:92:CYS:O	5:D:104:GLY:N	2.48	0.43
3:H:164:HIS:NE2	4:L:168:GLN:OE1	2.51	0.43
5:D:122:PHE:HE2	5:D:141:LEU:HD23	1.83	0.43
6:E:170:ASN:OD1	6:E:170:ASN:N	2.39	0.43
2:G:69:TRP:CH2	2:G:108:ILE:HG23	2.54	0.43
5:D:100(G):ARG:HA	6:E:89:TYR:HE2	1.83	0.43
2:G:112:TRP:O	2:G:115:SER:OG	2.31	0.43
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.48	0.43
2:G:321(A):ASP:OD1	2:G:322:ILE:N	2.51	0.43
3:H:107:THR:OG1	3:H:108:THR:N	2.50	0.43
3:H:87:THR:HG23	3:H:110:THR:HA	2.00	0.43
6:E:30:PHE:HB3	6:E:32:LEU:HG	2.00	0.43
6:E:50:GLU:HB2	6:E:53:LYS:HG2	1.99	0.43
3:H:209:LYS:HE2	3:H:209:LYS:HB2	1.78	0.43
6:E:83:GLU:HG3	6:E:104:LEU:O	2.19	0.43
8:G:3011:NAG:H61	10:G:3015:MAN:H3	2.01	0.43
2:G:462:ASN:OD1	6:E:27(A):ARG:NH1	2.52	0.43
6:E:89:TYR:HB2	6:E:98:PHE:CD1	2.53	0.43
2:G:157:CYS:O	2:G:173:TYR:HA	2.18	0.43
2:G:231:LYS:HD2	2:G:267:GLU:HG3	2.01	0.43
2:G:380:GLY:HA3	2:G:439:ILE:CG1	2.48	0.43
2:G:96:TRP:CG	2:G:275:GLU:HB2	2.54	0.43
5:D:141:LEU:HD11	5:D:177:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:252:LYS:O	2:G:254:VAL:N	2.52	0.42
2:G:300:ASN:HB3	2:G:322:ILE:HD13	2.01	0.42
2:G:93:PHE:HZ	2:G:226:LEU:HB2	1.84	0.42
5:D:145:TYR:HD1	5:D:200:HIS:NE2	2.17	0.42
5:D:200:HIS:CD2	5:D:202:PRO:HD2	2.54	0.42
3:H:100(G):PHE:HB2	3:H:100(I):GLU:HG3	2.01	0.42
6:E:25:GLY:O	6:E:69:ASN:HB3	2.19	0.42
1:B:610:TRP:CH2	2:G:498:PRO:HD3	2.53	0.42
1:B:622:ILE:O	1:B:626:MET:HB2	2.20	0.42
1:B:614:TRP:CD1	1:B:638:TYR:CG	3.08	0.42
6:E:32:LEU:HD12	6:E:91:TYR:HB3	2.02	0.42
1:B:607:ASN:HA	2:G:502:LYS:HG3	2.02	0.42
5:D:145:TYR:CE1	5:D:150:VAL:HG23	2.55	0.42
6:E:115:SER:O	6:E:137:ILE:HA	2.20	0.42
1:B:608:VAL:HB	2:G:36:VAL:CG2	2.50	0.42
2:G:226:LEU:O	2:G:486:TYR:HA	2.20	0.42
1:B:597:GLY:HA3	2:G:503:ARG:CZ	2.50	0.42
1:B:614:TRP:CZ3	1:B:642:ILE:HG12	2.55	0.42
2:G:427:TRP:O	2:G:429:ARG:N	2.53	0.42
4:L:32:ALA:HA	4:L:51:ASN:ND2	2.35	0.42
5:D:100(G):ARG:HG3	5:D:100(H):GLY:N	2.35	0.42
5:D:139:GLY:HA2	5:D:154:TRP:CH2	2.55	0.42
2:G:376:PHE:O	2:G:382:PHE:HA	2.19	0.42
3:H:138:LEU:HD13	3:H:211:VAL:HG11	2.02	0.42
4:L:161:GLU:HB2	4:L:178:TYR:HB2	2.01	0.42
4:L:38:HIS:O	4:L:84:ALA:HB1	2.19	0.42
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.54	0.41
2:G:116:LEU:HD22	2:G:434:MET:HG3	2.02	0.41
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.53	0.41
5:D:145:TYR:CE1	5:D:148:GLU:HA	2.52	0.41
6:E:35:TRP:CD1	6:E:48:ILE:HB	2.56	0.41
2:G:134:VAL:HB	2:G:154:LEU:O	2.20	0.41
3:H:15:SER:N	3:H:82(C):VAL:O	2.37	0.41
3:H:143:LYS:HZ3	4:L:130:LYS:HB3	1.85	0.41
1:B:523:LEU:HD11	2:G:491:ILE:HD11	2.02	0.41
1:B:540:GLN:HE22	2:G:43:PRO:CG	2.33	0.41
3:H:126:PRO:HB3	3:H:138:LEU:HB3	2.01	0.41
2:G:59:LYS:HD2	2:G:59:LYS:HA	1.84	0.41
3:H:150:VAL:HB	3:H:178:LEU:HD21	2.02	0.41
3:H:72:ASP:HB3	3:H:75:LYS:HB2	2.02	0.41
4:L:121:PRO:HD2	4:L:186:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:GLU:HG3	2:G:308:ARG:HB3	2.02	0.41
3:H:200:HIS:CD2	3:H:202:PRO:HD2	2.56	0.41
2:G:461:THR:HB	2:G:464:THR:HG21	2.02	0.41
3:H:100(D):VAL:HG13	3:H:100(G):PHE:HB2	2.01	0.41
3:H:33:TYR:HE2	3:H:97:ARG:HD3	1.86	0.41
1:B:646:LEU:O	1:B:650:GLN:HB2	2.19	0.41
6:E:23:CYS:O	6:E:71:ALA:N	2.32	0.41
2:G:346:VAL:O	2:G:350:ARG:HG3	2.20	0.41
5:D:12:LYS:HG3	5:D:18:VAL:CG2	2.51	0.41
6:E:159:GLY:O	6:E:179:LEU:HA	2.21	0.41
2:G:282:LYS:HA	2:G:282:LYS:HD3	1.84	0.41
2:G:295:ASN:O	2:G:331:CYS:HA	2.21	0.41
1:B:585:ARG:NE	2:G:491:ILE:O	2.41	0.41
3:H:145:TYR:CZ	3:H:176:TYR:HB2	2.55	0.41
1:B:648:GLU:O	1:B:652:GLN:HB3	2.20	0.41
5:D:122:PHE:HB2	6:E:122:SER:OG	2.21	0.41
8:G:2775:NAG:HO3	8:G:2775:NAG:C7	2.33	0.41
2:G:446:VAL:O	8:G:2620:NAG:H5	2.21	0.41
1:B:642:ILE:HD13	2:G:496:VAL:HG11	2.03	0.41
6:E:67:SER:N	6:E:70:THR:O	2.44	0.40
3:H:29:MET:O	3:H:71:ARG:NH1	2.54	0.40
6:E:23:CYS:HB2	6:E:35:TRP:CH2	2.57	0.40
6:E:38:GLN:O	6:E:84:ALA:HB1	2.20	0.40
4:L:31:ARG:HA	4:L:92:ASP:HA	2.03	0.40
6:E:82:ASP:O	6:E:104:LEU:HD23	2.22	0.40
10:G:2625:MAN:H2	10:G:2626:MAN:H2	1.65	0.40
2:G:96:TRP:HH2	2:G:285:LEU:HG	1.86	0.40
5:D:114:ALA:HB3	5:D:146:PHE:CD1	2.57	0.40
2:G:213:ILE:O	2:G:215:ILE:HG13	2.22	0.40
6:E:132:THR:HA	6:E:179:LEU:O	2.22	0.40
2:G:152:GLY:C	2:G:154:LEU:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	122/153 (80%)	106 (87%)	15 (12%)	1 (1%)	24	68
2	G	441/481 (92%)	407 (92%)	32 (7%)	2 (0%)	34	76
3	H	226/238 (95%)	216 (96%)	10 (4%)	0	100	100
4	L	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
5	D	227/232 (98%)	216 (95%)	10 (4%)	1 (0%)	39	79
6	E	208/214 (97%)	193 (93%)	13 (6%)	2 (1%)	19	64
All	All	1433/1532 (94%)	1337 (93%)	90 (6%)	6 (0%)	39	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	599	SER
2	G	138	ILE
5	D	100(D)	SER
6	E	93	ASP
2	G	457	ASP
6	E	51	VAL

### 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	B	108/129 (84%)	104 (96%)	4 (4%)	41	75
2	G	401/428 (94%)	395 (98%)	6 (2%)	72	89
3	H	202/208 (97%)	197 (98%)	5 (2%)	55	82
4	L	175/178 (98%)	169 (97%)	6 (3%)	44	77
5	D	194/197 (98%)	189 (97%)	5 (3%)	54	81
6	E	173/177 (98%)	170 (98%)	3 (2%)	68	88
All	All	1253/1317 (95%)	1224 (98%)	29 (2%)	58	83

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	606	THR
1	B	607	ASN
1	B	619	LEU
1	B	627	THR
2	G	57	ASP
2	G	192	ARG
2	G	195	ASN
2	G	205	CYS
2	G	322	ILE
2	G	396	ILE
3	H	37	ILE
3	H	100(F)	SER
3	H	100(L)	TYR
3	H	164	HIS
3	H	208	ASP
4	L	66(B)	ILE
4	L	93	SER
4	L	94	ARG
4	L	95(B)	PHE
4	L	122	SER
4	L	186	TRP
5	D	27	TYR
5	D	54	ARG
5	D	71	ARG
5	D	138	LEU
5	D	178	LEU
6	E	47	ILE
6	E	52	ASN
6	E	66	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	540	GLN
2	G	428	GLN
3	H	60	ASN
3	H	171	GLN
4	L	52	GLN
5	D	35	HIS
5	D	155	ASN
6	E	109	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

114 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$
7	FUC	B	6110	8	10,10,11	0.72	0	13,14,16	0.81	0
8	NAG	B	6111	1,7	14,14,15	0.26	0	15,19,21	0.71	0
7	FUC	B	6370	8	10,10,11	0.65	0	13,14,16	0.76	0
8	NAG	B	6371	1,8,7	14,14,15	0.33	0	15,19,21	1.43	2 (13%)
8	NAG	B	6372	9,8	14,14,15	0.30	0	15,19,21	0.93	1 (6%)
9	BMA	B	6373	8	11,11,12	0.25	0	15,15,17	0.71	0
8	NAG	G	1330	8,2	14,14,15	0.42	0	15,19,21	1.32	3 (20%)
8	NAG	G	1331	9,8	14,14,15	0.31	0	15,19,21	0.87	0
9	BMA	G	1332	8	11,11,12	0.24	0	15,15,17	0.79	0
7	FUC	G	1560	8	10,10,11	0.66	0	13,14,16	0.76	0
8	NAG	G	1561	8,2,7	14,14,15	0.37	0	15,19,21	0.70	0
8	NAG	G	1562	9,8	14,14,15	0.35	0	15,19,21	0.94	0
9	BMA	G	1563	8,10	11,11,12	0.46	0	15,15,17	1.41	2 (13%)
10	MAN	G	1564	9,8	11,11,12	0.38	0	15,15,17	1.92	3 (20%)
8	NAG	G	1565	10	14,14,15	0.30	0	15,19,21	1.00	1 (6%)
8	NAG	G	1566	11,10	14,14,15	0.45	0	15,19,21	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	GAL	G	1567	8	11,11,12	0.24	0	15,15,17	0.73	0
10	MAN	G	1568	9,8	11,11,12	0.50	0	15,15,17	1.90	2 (13%)
8	NAG	G	1569	11,10	14,14,15	0.31	0	15,19,21	0.72	0
11	GAL	G	1570	8	11,11,12	0.25	0	15,15,17	0.74	0
8	NAG	G	1571	11,10	14,14,15	0.33	0	15,19,21	1.10	2 (13%)
11	GAL	G	1572	8	11,11,12	0.24	0	15,15,17	0.74	0
7	FUC	G	1600	8	10,10,11	0.67	0	13,14,16	0.83	0
8	NAG	G	1601	8,2,7	14,14,15	0.46	0	15,19,21	1.10	1 (6%)
8	NAG	G	1602	9,8	14,14,15	0.56	0	15,19,21	2.19	2 (13%)
9	BMA	G	1603	8,10	11,11,12	0.36	0	15,15,17	1.56	3 (20%)
10	MAN	G	1604	9,8	11,11,12	0.38	0	15,15,17	0.96	1 (6%)
8	NAG	G	1605	11,10	14,14,15	0.33	0	15,19,21	0.85	0
11	GAL	G	1606	8	11,11,12	0.27	0	15,15,17	0.75	0
10	MAN	G	1607	9,8	11,11,12	0.25	0	15,15,17	1.03	1 (6%)
8	NAG	G	1608	11,10	14,14,15	0.24	0	15,19,21	0.51	0
11	GAL	G	1609	8	11,11,12	0.24	0	15,15,17	0.73	0
8	NAG	G	1970	8,2	14,14,15	0.58	0	15,19,21	2.48	6 (40%)
8	NAG	G	1971	9,8	14,14,15	0.68	0	15,19,21	1.77	3 (20%)
9	BMA	G	1972	8,10	11,11,12	0.52	0	15,15,17	1.49	3 (20%)
10	MAN	G	1973	9,8	11,11,12	0.39	0	15,15,17	1.48	3 (20%)
8	NAG	G	1974	11,10	14,14,15	0.32	0	15,19,21	0.65	0
11	GAL	G	1975	8,12	11,11,12	0.25	0	15,15,17	0.85	0
12	SIA	G	1976	11	17,20,21	0.84	0	18,28,31	1.19	2 (11%)
10	MAN	G	1977	9,8	11,11,12	0.25	0	15,15,17	1.06	1 (6%)
8	NAG	G	1978	10	14,14,15	0.24	0	15,19,21	0.60	0
8	NAG	G	2340	8,2	14,14,15	0.31	0	15,19,21	1.45	2 (13%)
8	NAG	G	2341	8	14,14,15	0.24	0	15,19,21	0.73	0
8	NAG	G	2620	8,2	14,14,15	0.36	0	15,19,21	0.78	0
8	NAG	G	2621	9,8	14,14,15	0.29	0	15,19,21	1.02	2 (13%)
9	BMA	G	2622	8,10	11,11,12	0.31	0	15,15,17	0.90	0
10	MAN	G	2623	9,10	11,11,12	0.27	0	15,15,17	0.87	1 (6%)
10	MAN	G	2624	10	11,11,12	0.33	0	15,15,17	0.83	1 (6%)
10	MAN	G	2625	9,10	11,11,12	0.24	0	15,15,17	0.86	0
10	MAN	G	2626	10	11,11,12	0.28	0	15,15,17	0.80	0
7	FUC	G	2760	8	10,10,11	0.56	0	13,14,16	0.81	0
8	NAG	G	2761	8,2,7	14,14,15	0.46	0	15,19,21	1.16	2 (13%)
8	NAG	G	2762	9,8	14,14,15	0.29	0	15,19,21	0.98	2 (13%)
9	BMA	G	2763	8,10	11,11,12	0.42	0	15,15,17	1.82	6 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	G	2764	9,8	11,11,12	0.36	0	15,15,17	1.65	4 (26%)
8	NAG	G	2765	11,10	14,14,15	0.26	0	15,19,21	0.53	0
11	GAL	G	2766	8,12	11,11,12	0.25	0	15,15,17	0.74	0
12	SIA	G	2767	11	17,20,21	0.85	0	18,28,31	1.15	2 (11%)
8	NAG	G	2768	10	14,14,15	0.26	0	15,19,21	0.60	0
10	MAN	G	2769	9,8	11,11,12	0.91	0	15,15,17	2.89	9 (60%)
8	NAG	G	2770	11,10	14,14,15	0.38	0	15,19,21	1.40	3 (20%)
11	GAL	G	2771	8,12	11,11,12	0.28	0	15,15,17	1.08	2 (13%)
12	SIA	G	2772	11	17,20,21	0.84	0	18,28,31	1.27	2 (11%)
8	NAG	G	2773	11,10	14,14,15	0.44	0	15,19,21	1.06	1 (6%)
11	GAL	G	2774	8	11,11,12	0.24	0	15,15,17	0.88	1 (6%)
8	NAG	G	2775	9	14,14,15	0.52	0	15,19,21	1.01	0
8	NAG	G	2950	8,2	14,14,15	0.34	0	15,19,21	0.69	0
8	NAG	G	2951	8	14,14,15	0.28	0	15,19,21	0.61	0
8	NAG	G	3010	8,2	14,14,15	0.46	0	15,19,21	1.48	2 (13%)
8	NAG	G	3011	9,8	14,14,15	0.35	0	15,19,21	0.69	1 (6%)
9	BMA	G	3012	8,10	11,11,12	0.28	0	15,15,17	0.96	1 (6%)
10	MAN	G	3013	9,8	11,11,12	0.27	0	15,15,17	1.12	1 (6%)
8	NAG	G	3014	10	14,14,15	0.29	0	15,19,21	0.41	0
10	MAN	G	3015	9,8	11,11,12	0.25	0	15,15,17	0.82	0
8	NAG	G	3016	10	14,14,15	0.26	0	15,19,21	0.62	0
8	NAG	G	3320	8,2	14,14,15	0.29	0	15,19,21	0.70	0
8	NAG	G	3321	9,8	14,14,15	0.23	0	15,19,21	1.11	0
9	BMA	G	3322	8,10	11,11,12	0.32	0	15,15,17	1.02	1 (6%)
10	MAN	G	3323	9,10	11,11,12	0.24	0	15,15,17	1.23	2 (13%)
10	MAN	G	3324	10	11,11,12	0.45	0	15,15,17	1.25	1 (6%)
10	MAN	G	3325	10	11,11,12	0.22	0	15,15,17	0.84	1 (6%)
10	MAN	G	3326	10	11,11,12	0.26	0	15,15,17	0.78	0
10	MAN	G	3327	9,10	11,11,12	0.34	0	15,15,17	1.48	2 (13%)
10	MAN	G	3328	10	11,11,12	0.32	0	15,15,17	1.35	2 (13%)
10	MAN	G	3329	10	11,11,12	0.22	0	15,15,17	1.00	1 (6%)
8	NAG	G	3390	2	14,14,15	0.31	0	15,19,21	0.55	0
8	NAG	G	3550	8,2	14,14,15	0.33	0	15,19,21	0.55	0
8	NAG	G	3551	8	14,14,15	0.30	0	15,19,21	0.55	0
8	NAG	G	3630	8,2	14,14,15	0.52	0	15,19,21	2.12	4 (26%)
8	NAG	G	3631	9,8	14,14,15	0.44	0	15,19,21	1.87	3 (20%)
9	BMA	G	3632	8,10	11,11,12	0.41	0	15,15,17	1.26	2 (13%)
10	MAN	G	3633	9,10	11,11,12	0.39	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	G	3634	10	11,11,12	0.28	0	15,15,17	0.79	0
10	MAN	G	3635	10	11,11,12	0.26	0	15,15,17	0.81	0
10	MAN	G	3636	9	11,11,12	0.31	0	15,15,17	0.83	1 (6%)
8	NAG	G	3860	8,2	14,14,15	0.31	0	15,19,21	1.19	1 (6%)
8	NAG	G	3861	9,8	14,14,15	0.60	0	15,19,21	1.46	3 (20%)
9	BMA	G	3862	8,10	11,11,12	0.34	0	15,15,17	1.17	2 (13%)
10	MAN	G	3863	9	11,11,12	0.27	0	15,15,17	0.74	0
10	MAN	G	3864	9	11,11,12	0.27	0	15,15,17	0.78	1 (6%)
7	FUC	G	3920	8	10,10,11	0.86	0	13,14,16	1.06	1 (7%)
8	NAG	G	3921	8,2,7	14,14,15	0.35	0	15,19,21	0.93	0
8	NAG	G	3922	9,8	14,14,15	0.27	0	15,19,21	0.85	0
9	BMA	G	3923	8,10	11,11,12	0.43	0	15,15,17	1.57	2 (13%)
10	MAN	G	3924	9	11,11,12	0.26	0	15,15,17	0.76	1 (6%)
10	MAN	G	3925	9	11,11,12	0.26	0	15,15,17	0.80	0
8	NAG	G	4480	8,2	14,14,15	0.27	0	15,19,21	1.15	1 (6%)
8	NAG	G	4481	9,8	14,14,15	0.57	0	15,19,21	1.85	2 (13%)
9	BMA	G	4482	8,10	11,11,12	0.31	0	15,15,17	1.10	2 (13%)
10	MAN	G	4483	9,10	11,11,12	0.24	0	15,15,17	0.67	0
10	MAN	G	4484	10	11,11,12	0.24	0	15,15,17	0.72	0
7	FUC	G	880	8	10,10,11	0.68	0	13,14,16	0.84	0
8	NAG	G	881	8,2,7	14,14,15	0.30	0	15,19,21	0.78	0
8	NAG	G	882	8	14,14,15	0.26	0	15,19,21	0.62	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
7	FUC	B	6110	8	-	0/0/17/20	0/1/1/1
8	NAG	B	6111	1,7	-	0/6/23/26	0/1/1/1
7	FUC	B	6370	8	-	0/0/17/20	0/1/1/1
8	NAG	B	6371	1,8,7	-	0/6/23/26	0/1/1/1
8	NAG	B	6372	9,8	-	0/6/23/26	0/1/1/1
9	BMA	B	6373	8	-	0/2/19/22	0/1/1/1
8	NAG	G	1330	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	1331	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1332	8	-	0/2/19/22	0/1/1/1
7	FUC	G	1560	8	-	0/0/17/20	0/1/1/1
8	NAG	G	1561	8,2,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	G	1562	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1563	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1564	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1565	10	-	0/6/23/26	0/1/1/1
8	NAG	G	1566	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1567	8	-	0/2/19/22	0/1/1/1
10	MAN	G	1568	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1569	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1570	8	-	0/2/19/22	0/1/1/1
8	NAG	G	1571	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1572	8	-	0/2/19/22	0/1/1/1
7	FUC	G	1600	8	-	0/0/17/20	0/1/1/1
8	NAG	G	1601	8,2,7	-	0/6/23/26	0/1/1/1
8	NAG	G	1602	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1603	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1604	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1605	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1606	8	-	0/2/19/22	0/1/1/1
10	MAN	G	1607	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1608	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1609	8	-	0/2/19/22	0/1/1/1
8	NAG	G	1970	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	1971	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1972	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1973	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1974	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	1975	8,12	-	0/2/19/22	0/1/1/1
12	SIA	G	1976	11	-	0/14/34/38	0/1/1/1
10	MAN	G	1977	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1978	10	-	0/6/23/26	0/1/1/1
8	NAG	G	2340	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	2341	8	-	0/6/23/26	0/1/1/1
8	NAG	G	2620	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	2621	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	2622	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	2623	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	2624	10	-	0/2/19/22	0/1/1/1
10	MAN	G	2625	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	2626	10	-	0/2/19/22	0/1/1/1
7	FUC	G	2760	8	-	0/0/17/20	0/1/1/1
8	NAG	G	2761	8,2,7	-	0/6/23/26	0/1/1/1
8	NAG	G	2762	9,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	G	2763	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	2764	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	2765	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	2766	8,12	-	0/2/19/22	0/1/1/1
12	SIA	G	2767	11	-	0/14/34/38	0/1/1/1
8	NAG	G	2768	10	-	0/6/23/26	0/1/1/1
10	MAN	G	2769	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	2770	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	2771	8,12	-	0/2/19/22	0/1/1/1
12	SIA	G	2772	11	-	0/14/34/38	0/1/1/1
8	NAG	G	2773	11,10	-	0/6/23/26	0/1/1/1
11	GAL	G	2774	8	-	0/2/19/22	0/1/1/1
8	NAG	G	2775	9	-	0/6/23/26	0/1/1/1
8	NAG	G	2950	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	2951	8	-	0/6/23/26	0/1/1/1
8	NAG	G	3010	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	3011	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	3012	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3013	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	3014	10	-	0/6/23/26	0/1/1/1
10	MAN	G	3015	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	3016	10	-	0/6/23/26	0/1/1/1
8	NAG	G	3320	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	3321	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	3322	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3323	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3324	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3325	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3326	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3327	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3328	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3329	10	-	0/2/19/22	0/1/1/1
8	NAG	G	3390	2	-	0/6/23/26	0/1/1/1
8	NAG	G	3550	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	3551	8	-	0/6/23/26	0/1/1/1
8	NAG	G	3630	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	3631	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	3632	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3633	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3634	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3635	10	-	0/2/19/22	0/1/1/1
10	MAN	G	3636	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	G	3860	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	3861	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	3862	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3863	9	-	0/2/19/22	0/1/1/1
10	MAN	G	3864	9	-	0/2/19/22	0/1/1/1
7	FUC	G	3920	8	-	0/0/17/20	0/1/1/1
8	NAG	G	3921	8,2,7	-	0/6/23/26	0/1/1/1
8	NAG	G	3922	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	3923	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	3924	9	-	0/2/19/22	0/1/1/1
10	MAN	G	3925	9	-	0/2/19/22	0/1/1/1
8	NAG	G	4480	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	4481	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	4482	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	4483	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	4484	10	-	0/2/19/22	0/1/1/1
7	FUC	G	880	8	-	0/0/17/20	0/1/1/1
8	NAG	G	881	8,2,7	-	0/6/23/26	0/1/1/1
8	NAG	G	882	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	4481	NAG	O4-C4-C3	-5.79	97.31	110.36
8	G	1970	NAG	O3-C3-C2	-5.74	97.10	109.37
10	G	1564	MAN	C1-C2-C3	-5.19	103.26	109.55
8	G	1970	NAG	O4-C4-C3	-4.24	100.79	110.36
10	G	2764	MAN	O5-C1-C2	-4.20	104.18	110.89
8	G	1971	NAG	O4-C4-C3	-4.11	101.09	110.36
8	G	1970	NAG	O4-C4-C5	-3.84	99.11	109.23
8	G	3010	NAG	O4-C4-C3	-3.72	101.98	110.36
10	G	3324	MAN	C1-O5-C5	-3.57	106.89	112.14
10	G	2769	MAN	O5-C1-C2	-3.40	105.46	110.89
8	G	3861	NAG	O4-C4-C3	-3.39	102.72	110.36
9	G	3923	BMA	O5-C1-C2	-3.30	105.62	110.89
10	G	2769	MAN	O5-C5-C6	-3.23	100.42	107.34
9	G	3923	BMA	O2-C2-C3	-3.20	103.74	110.19
10	G	3328	MAN	O5-C1-C2	-3.19	105.79	110.89
10	G	1973	MAN	C1-C2-C3	-3.17	105.71	109.55
9	G	1972	BMA	O5-C1-C2	-3.08	105.97	110.89
8	G	1330	NAG	C2-N2-C7	-3.08	119.10	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	2761	NAG	O4-C4-C5	-3.04	101.21	109.23
8	G	4480	NAG	O4-C4-C3	-3.01	103.56	110.36
8	G	1971	NAG	O4-C4-C5	-2.93	101.50	109.23
8	G	3010	NAG	O5-C5-C6	-2.91	101.10	107.34
8	G	2340	NAG	C4-C3-C2	-2.84	106.93	111.34
8	G	3630	NAG	C4-C3-C2	-2.81	106.98	111.34
8	G	1571	NAG	C2-N2-C7	-2.76	119.52	123.11
9	G	2763	BMA	O3-C3-C2	-2.75	104.97	110.01
8	G	1970	NAG	C1-O5-C5	-2.74	108.11	112.14
8	G	3860	NAG	C3-C4-C5	-2.73	105.36	110.23
8	G	3861	NAG	O4-C4-C5	-2.73	102.03	109.23
10	G	1607	MAN	O5-C1-C2	-2.71	106.56	110.89
8	G	1566	NAG	C8-C7-N2	-2.70	110.91	116.10
10	G	3329	MAN	O5-C1-C2	-2.62	106.71	110.89
10	G	3013	MAN	O5-C1-C2	-2.61	106.72	110.89
8	G	2762	NAG	O4-C4-C5	-2.61	102.36	109.23
10	G	2769	MAN	O4-C4-C3	-2.60	104.49	110.36
12	G	2772	SIA	C7-C6-C5	-2.59	110.50	114.06
9	G	4482	BMA	O5-C1-C2	-2.58	106.77	110.89
10	G	1604	MAN	C1-O5-C5	-2.58	108.35	112.14
9	G	3632	BMA	O5-C1-C2	-2.56	106.80	110.89
9	G	3322	BMA	O3-C3-C2	-2.54	105.34	110.01
12	G	2767	SIA	C7-C6-C5	-2.53	110.57	114.06
9	G	1972	BMA	C1-O5-C5	-2.52	108.43	112.14
10	G	1973	MAN	O5-C1-C2	-2.50	106.90	110.89
10	G	3323	MAN	C1-C2-C3	-2.49	106.53	109.55
9	G	2763	BMA	C2-C3-C4	-2.49	106.70	111.05
9	G	1563	BMA	O3-C3-C2	-2.45	105.52	110.01
10	G	3633	MAN	O5-C1-C2	-2.44	106.99	110.89
10	G	2769	MAN	C3-C4-C5	-2.42	105.92	110.23
10	G	1564	MAN	O5-C1-C2	-2.41	107.04	110.89
9	G	1972	BMA	O3-C3-C4	-2.40	104.94	110.36
10	G	1977	MAN	O5-C1-C2	-2.40	107.06	110.89
10	G	1973	MAN	O2-C2-C3	-2.39	105.37	110.19
9	G	1603	BMA	O3-C3-C4	-2.37	105.01	110.36
10	G	3636	MAN	O5-C1-C2	-2.34	107.15	110.89
9	G	4482	BMA	C1-O5-C5	-2.33	108.71	112.14
8	G	1330	NAG	O4-C4-C5	-2.32	103.10	109.23
9	G	2763	BMA	C3-C4-C5	-2.32	106.10	110.23
12	G	1976	SIA	C7-C6-C5	-2.21	111.01	114.06
10	G	2624	MAN	C1-O5-C5	-2.21	108.89	112.14
10	G	2764	MAN	O2-C2-C1	-2.21	104.81	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	3325	MAN	O5-C1-C2	-2.18	107.40	110.89
11	G	2771	GAL	O5-C1-C2	-2.18	107.41	110.89
9	G	3862	BMA	O3-C3-C2	-2.17	106.04	110.01
10	G	2623	MAN	O5-C1-C2	-2.16	107.44	110.89
11	G	2774	GAL	O5-C1-C2	-2.14	107.47	110.89
10	G	3328	MAN	O2-C2-C1	-2.13	104.97	109.23
8	G	1970	NAG	O3-C3-C4	-2.13	105.56	110.36
8	G	1330	NAG	O4-C4-C3	-2.11	105.59	110.36
8	G	3011	NAG	O4-C4-C3	-2.11	105.60	110.36
8	G	2762	NAG	O4-C4-C3	-2.10	105.62	110.36
8	G	2621	NAG	O4-C4-C5	-2.09	103.72	109.23
8	G	2761	NAG	O3-C3-C2	-2.06	104.97	109.37
8	G	2770	NAG	C6-C5-C4	-2.05	107.84	112.99
9	G	3012	BMA	O5-C1-C2	-2.04	107.63	110.89
8	B	6371	NAG	O4-C4-C5	-2.04	103.85	109.23
10	G	3924	MAN	O5-C1-C2	-2.02	107.67	110.89
8	G	3630	NAG	C2-N2-C7	-2.02	120.48	123.11
10	G	2764	MAN	C3-C4-C5	-2.01	106.64	110.23
10	G	3864	MAN	O5-C1-C2	-2.01	107.68	110.89
8	B	6372	NAG	C2-N2-C7	2.00	125.71	123.11
8	G	2621	NAG	C2-N2-C7	2.03	125.75	123.11
8	G	3861	NAG	C2-N2-C7	2.04	125.75	123.11
11	G	2771	GAL	C1-C2-C3	2.06	112.05	109.55
10	G	3323	MAN	O3-C3-C4	2.11	115.11	110.36
10	G	2769	MAN	C1-O5-C5	2.12	115.26	112.14
8	G	1970	NAG	C4-C3-C2	2.21	114.77	111.34
9	G	1603	BMA	O5-C5-C6	2.24	112.13	107.34
10	G	2764	MAN	C1-O5-C5	2.33	115.57	112.14
9	G	2763	BMA	O3-C3-C4	2.34	115.63	110.36
8	G	4481	NAG	C2-N2-C7	2.39	126.21	123.11
7	G	3920	FUC	O2-C2-C1	2.47	114.18	109.23
8	G	2770	NAG	O4-C4-C5	2.47	115.75	109.23
9	G	2763	BMA	O4-C4-C3	2.49	115.96	110.36
8	G	1571	NAG	C1-O5-C5	2.69	116.10	112.14
9	G	1563	BMA	C1-C2-C3	2.70	112.82	109.55
12	G	2767	SIA	O6-C6-C5	2.73	112.95	108.48
8	G	1565	NAG	C1-O5-C5	2.75	116.18	112.14
8	B	6371	NAG	O5-C5-C6	2.77	113.27	107.34
8	G	1602	NAG	C8-C7-N2	2.80	121.46	116.10
8	G	2773	NAG	C1-O5-C5	2.92	116.44	112.14
12	G	1976	SIA	O6-C6-C5	3.00	113.39	108.48
9	G	3632	BMA	C1-C2-C3	3.00	113.19	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	2772	SIA	O6-C6-C5	3.01	113.41	108.48
8	G	2770	NAG	C1-O5-C5	3.02	116.58	112.14
9	G	3862	BMA	C1-C2-C3	3.05	113.24	109.55
10	G	3327	MAN	O2-C2-C3	3.13	116.48	110.19
9	G	1603	BMA	C1-C2-C3	3.14	113.35	109.55
9	G	2763	BMA	C1-C2-C3	3.28	113.53	109.55
10	G	1564	MAN	O4-C4-C5	3.33	118.00	109.23
10	G	2769	MAN	C1-C2-C3	3.33	113.58	109.55
8	G	3630	NAG	C1-O5-C5	3.43	117.18	112.14
8	G	3631	NAG	C1-O5-C5	3.43	117.19	112.14
8	G	1601	NAG	C1-O5-C5	3.47	117.25	112.14
10	G	1568	MAN	O3-C3-C2	3.56	116.53	110.01
8	G	1971	NAG	C4-C3-C2	3.56	116.87	111.34
8	G	2340	NAG	O4-C4-C3	3.74	118.79	110.36
8	G	3631	NAG	O4-C4-C3	3.76	118.84	110.36
10	G	3327	MAN	C1-C2-C3	3.78	114.14	109.55
10	G	2769	MAN	O2-C2-C1	3.85	116.95	109.23
8	G	3631	NAG	O4-C4-C5	4.00	119.77	109.23
10	G	2769	MAN	O4-C4-C5	4.95	122.26	109.23
10	G	2769	MAN	O2-C2-C3	5.02	120.30	110.19
10	G	1568	MAN	O2-C2-C3	5.45	121.17	110.19
8	G	3630	NAG	O4-C4-C5	5.87	124.69	109.23
8	G	1602	NAG	C2-N2-C7	7.23	132.51	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	1330	NAG	1	0
8	G	1331	NAG	1	0
10	G	1564	MAN	1	0
8	G	1565	NAG	1	0
8	G	1566	NAG	1	0
8	G	1571	NAG	1	0
8	G	1601	NAG	1	0
8	G	1602	NAG	1	0
10	G	1973	MAN	1	0
8	G	1974	NAG	1	0
8	G	2620	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	2625	MAN	1	0
10	G	2626	MAN	1	0
7	G	2760	FUC	1	0
9	G	2763	BMA	1	0
10	G	2764	MAN	2	0
10	G	2769	MAN	1	0
8	G	2775	NAG	3	0
8	G	3010	NAG	1	0
8	G	3011	NAG	2	0
9	G	3012	BMA	1	0
10	G	3015	MAN	1	0
8	G	3321	NAG	1	0
10	G	3324	MAN	1	0
10	G	3325	MAN	1	0
10	G	3327	MAN	1	0
10	G	3328	MAN	1	0
8	G	3390	NAG	1	0
8	G	3860	NAG	1	0
8	G	3861	NAG	1	0
8	G	3922	NAG	1	0
9	G	3923	BMA	1	0
8	G	4480	NAG	1	0
8	G	4481	NAG	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	126/153 (82%)	0.66	15 (11%) 6 5	163, 268, 331, 391	0
2	G	449/481 (93%)	0.59	36 (8%) 15 10	45, 199, 352, 455	0
3	H	230/238 (96%)	1.69	69 (30%) 1 1	154, 314, 444, 501	0
4	L	211/214 (98%)	0.98	43 (20%) 1 1	147, 347, 430, 482	0
5	D	229/232 (98%)	1.91	68 (29%) 1 1	109, 244, 640, 874	0
6	E	210/214 (98%)	3.39	89 (42%) 0 1	23, 310, 886, 970	0
All	All	1455/1532 (94%)	1.44	320 (21%) 1 1	23, 266, 631, 970	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	133	GLY	23.9
6	E	206	THR	21.3
6	E	155	PRO	21.2
6	E	148	ALA	20.8
5	D	216	CYS	20.2
6	E	146	THR	19.6
5	D	126	PRO	19.4
6	E	143	GLY	16.8
6	E	149	TRP	15.6
5	D	127	SER	15.5
6	E	190	ARG	15.4
6	E	188	SER	15.0
6	E	144	ALA	14.9
6	E	108	GLY	14.6
5	D	134	GLY	14.4
5	D	128	SER	14.4
5	D	135	THR	14.3
6	E	145	VAL	13.4
6	E	147	VAL	13.4

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Mol	Chain	Res	Type	RSRZ
6	E	210	THR	13.3
6	E	151	ALA	13.2
6	E	191	SER	12.9
6	E	175	ALA	12.8
5	D	161	SER	12.7
4	L	145	VAL	12.7
6	E	156	VAL	12.4
3	H	181	VAL	12.1
6	E	189	HIS	12.0
3	H	180	SER	11.8
3	H	152	VAL	11.8
6	E	205	LYS	11.6
3	H	135	THR	11.6
6	E	135	CYS	11.4
5	D	173	SER	11.2
5	D	160	THR	11.0
6	E	133	LEU	11.0
3	H	138	LEU	11.0
3	H	179	SER	10.9
6	E	117	THR	10.3
5	D	132	SER	10.3
5	D	162	GLY	10.2
6	E	193	SER	10.2
6	E	136	LEU	10.2
6	E	128	ALA	10.1
6	E	194	CYS	9.9
6	E	207	VAL	9.5
6	E	158	ALA	9.3
2	G	187	SER	9.3
6	E	157	LYS	9.1
6	E	118	LEU	9.0
3	H	10	GLY	8.8
3	H	212	GLU	8.8
6	E	107	LEU	8.7
3	H	184	VAL	8.5
6	E	195	GLN	8.5
5	D	192	GLN	8.3
6	E	111	LYS	8.2
3	H	11	LEU	8.1
4	L	144	ALA	8.1
3	H	151	THR	7.9
3	H	215	SER	7.9

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Mol	Chain	Res	Type	RSRZ
6	E	152	ASP	7.7
6	E	208	ALA	7.7
1	B	547	GLY	7.7
4	L	154	SER	7.6
6	E	176	SER	7.6
6	E	129	ASN	7.4
5	D	125	ALA	7.4
3	H	194	TYR	7.4
5	D	129	LYS	7.4
6	E	181	LEU	7.0
6	E	137	ILE	6.9
3	H	192	GLN	6.9
4	L	118	LEU	6.8
3	H	127	SER	6.8
3	H	186	SER	6.5
3	H	150	VAL	6.5
6	E	196	VAL	6.4
6	E	150	LYS	6.3
6	E	187	LYS	6.3
5	D	172	SER	6.3
3	H	136	ALA	6.1
6	E	209	PRO	6.1
2	G	188	ASN	6.1
6	E	204	GLU	6.1
5	D	208	ASP	6.1
5	D	151	THR	6.0
6	E	127	GLN	5.9
6	E	183	PRO	5.9
3	H	141	LEU	5.9
5	D	185	PRO	5.8
1	B	602	LEU	5.8
6	E	180	SER	5.8
5	D	165	THR	5.8
3	H	198	VAL	5.8
3	H	182	VAL	5.7
6	E	179	LEU	5.7
6	E	142	PRO	5.6
1	B	545	LEU	5.5
6	E	162	THR	5.5
3	H	9	PRO	5.4
6	E	124	GLU	5.4
6	E	120	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
3	H	183	THR	5.3
6	E	134	VAL	5.3
2	G	465	THR	5.3
6	E	116	VAL	5.2
4	L	117	THR	5.2
6	E	192	TYR	5.1
1	B	520	LEU	5.1
5	D	152	VAL	5.1
5	D	140	CYS	5.1
6	E	3	ALA	5.1
3	H	190	GLY	5.0
5	D	174	GLY	5.0
4	L	104	LEU	4.9
6	E	182	THR	4.8
5	D	214	LYS	4.8
3	H	90	TYR	4.8
5	D	189	LEU	4.7
4	L	86	TYR	4.7
5	D	191	THR	4.7
6	E	201	SER	4.7
5	D	137	ALA	4.6
4	L	209	PRO	4.6
5	D	186	SER	4.6
2	G	236	THR	4.6
3	H	153	SER	4.5
6	E	112	ALA	4.5
5	D	136	ALA	4.5
5	D	180	SER	4.5
6	E	197	THR	4.5
3	H	81	LYS	4.5
4	L	114	PRO	4.4
4	L	132	THR	4.4
6	E	109	GLN	4.4
5	D	141	LEU	4.4
5	D	12	LYS	4.4
6	E	174	ALA	4.3
3	H	155	ASN	4.3
3	H	207	VAL	4.3
4	L	37	GLN	4.2
1	B	599	SER	4.2
3	H	178	LEU	4.2
6	E	122	SER	4.2

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Mol	Chain	Res	Type	RSRZ
3	H	142	VAL	4.2
4	L	119	PHE	4.2
2	G	496	VAL	4.1
6	E	132	THR	4.1
6	E	154	SER	4.1
3	H	140	CYS	4.0
5	D	149	PRO	4.0
5	D	138	LEU	4.0
3	H	185	PRO	4.0
2	G	33	ASN	4.0
3	H	38	ARG	3.9
5	D	179	SER	3.9
5	D	130	SER	3.9
6	E	4	LEU	3.9
3	H	193	THR	3.8
3	H	191	THR	3.8
5	D	199	ASN	3.8
3	H	137	ALA	3.8
3	H	189	LEU	3.8
4	L	39	ARG	3.8
3	H	4	LEU	3.7
3	H	163	VAL	3.7
6	E	131	ALA	3.7
3	H	80	LEU	3.6
5	D	193	THR	3.6
6	E	113	ALA	3.5
6	E	159	GLY	3.5
4	L	139	ASP	3.5
4	L	176	SER	3.5
5	D	122	PHE	3.5
1	B	544	LEU	3.4
5	D	188	SER	3.5
3	H	69	ILE	3.4
4	L	38	HIS	3.4
4	L	203	VAL	3.4
4	L	208	ALA	3.4
3	H	214	LYS	3.3
2	G	505	VAL	3.3
5	D	120	SER	3.3
3	H	7	SER	3.3
5	D	131	THR	3.3
3	H	47	TRP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	L	109	GLN	3.2
2	G	500	ARG	3.2
2	G	411	ASN	3.2
4	L	162	THR	3.2
1	B	578	ALA	3.2
6	E	184	GLU	3.2
2	G	93	PHE	3.2
3	H	12	VAL	3.2
4	L	135	CYS	3.2
3	H	113	SER	3.2
2	G	504	ARG	3.2
4	L	136	LEU	3.1
1	B	656	ASN	3.1
2	G	499	THR	3.1
2	G	494	LEU	3.1
4	L	155	PRO	3.1
3	H	49	GLY	3.1
5	D	202	PRO	3.1
6	E	185	GLN	3.0
6	E	200	GLY	3.0
1	B	546	SER	3.0
4	L	207	VAL	3.0
2	G	466	GLU	3.0
1	B	518	VAL	3.0
6	E	161	GLU	3.0
6	E	114	PRO	3.0
6	E	92	ALA	3.0
2	G	95	MET	3.0
2	G	498	PRO	3.0
4	L	140	PHE	3.0
5	D	100(G)	ARG	3.0
2	G	468	PHE	2.9
3	H	110	THR	2.9
3	H	129	LYS	2.9
5	D	215	SER	2.9
4	L	175	ALA	2.9
2	G	40	TYR	2.9
6	E	198	HIS	2.9
5	D	187	SER	2.9
1	B	569	THR	2.9
5	D	170	LEU	2.9
5	D	197	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
4	L	153	SER	2.9
5	D	148	GLU	2.8
6	E	123	SER	2.8
5	D	13	LYS	2.8
4	L	131	ALA	2.8
1	B	593	LEU	2.8
4	L	147	VAL	2.8
4	L	47	LEU	2.8
5	D	155	ASN	2.8
3	H	68	VAL	2.7
5	D	24	ALA	2.7
2	G	358	ILE	2.7
2	G	237	GLY	2.7
1	B	600	GLY	2.7
2	G	38	VAL	2.7
1	B	595	ILE	2.7
3	H	139	GLY	2.7
3	H	199	ASN	2.7
6	E	121	PRO	2.6
5	D	142	VAL	2.6
2	G	141	ASP	2.6
2	G	293	GLN	2.6
6	E	98	PHE	2.6
2	G	356	ASN	2.6
4	L	105	THR	2.6
2	G	467	THR	2.6
4	L	13	VAL	2.6
3	H	92	CYS	2.6
4	L	107	LEU	2.6
5	D	212	GLU	2.6
5	D	171	GLN	2.5
5	D	1	GLU	2.5
5	D	213	PRO	2.5
5	D	147	PRO	2.5
2	G	235	GLY	2.5
5	D	190	GLY	2.5
3	H	109	VAL	2.5
3	H	126	PRO	2.5
6	E	186	TRP	2.5
3	H	159	LEU	2.4
2	G	73	ALA	2.4
2	G	86	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	13	LYS	2.4
6	E	165	PRO	2.4
3	H	156	SER	2.4
5	D	153	SER	2.4
4	L	120	PRO	2.4
6	E	177	SER	2.3
3	H	8	GLY	2.3
5	D	183	THR	2.3
4	L	36	TYR	2.3
4	L	134	VAL	2.3
3	H	147	PRO	2.3
3	H	128	SER	2.3
3	H	211	VAL	2.3
2	G	72	HIS	2.3
6	E	160	VAL	2.3
3	H	84	PRO	2.3
4	L	158	ALA	2.2
3	H	162	GLY	2.2
3	H	34	TRP	2.2
4	L	106	VAL	2.2
5	D	163	VAL	2.2
5	D	33	HIS	2.2
3	H	28	SER	2.2
4	L	146	THR	2.2
6	E	163	THR	2.2
6	E	119	PHE	2.1
5	D	164	HIS	2.1
3	H	79	SER	2.1
5	D	182	VAL	2.1
4	L	137	ILE	2.1
6	E	178	TYR	2.1
2	G	463	SER	2.1
2	G	360	ARG	2.1
4	L	64	GLY	2.1
5	D	168	ALA	2.1
3	H	78	LEU	2.1
6	E	138	SER	2.1
2	G	85	HIS	2.1
4	L	12	SER	2.1
5	D	121	VAL	2.1
4	L	14	ALA	2.1
2	G	139	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	217	TYR	2.0
1	B	628	TRP	2.0
2	G	455	THR	2.0
6	E	19	ILE	2.0
2	G	69	TRP	2.0
6	E	110	PRO	2.0
5	D	178	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	MAN	G	3325	11/12	0.58	0.46	2.49	280,280,280,280	0
7	FUC	G	2760	10/11	0.47	0.59	1.99	309,309,309,309	0
8	NAG	G	1970	14/15	0.86	0.39	1.52	198,208,226,229	0
8	NAG	G	3010	14/15	0.77	0.45	1.13	258,258,258,258	0
10	MAN	G	2625	11/12	0.74	0.35	0.59	281,286,304,324	0
8	NAG	G	1330	14/15	0.84	0.37	0.34	251,251,251,251	0
8	NAG	G	2621	14/15	0.88	0.33	0.21	203,219,240,245	0
8	NAG	G	2620	14/15	0.93	0.32	0.11	169,179,197,202	0
10	MAN	G	3329	11/12	0.83	0.33	0.05	203,208,213,213	0
8	NAG	G	3320	14/15	0.89	0.31	0.04	200,211,228,234	0
8	NAG	G	1601	14/15	0.87	0.34	-0.22	236,260,269,281	0
8	NAG	G	2950	14/15	0.83	0.31	-0.69	204,220,246,255	0
8	NAG	G	3321	14/15	0.94	0.27	-0.73	162,179,199,205	0
10	MAN	G	3328	11/12	0.86	0.16	-0.98	180,183,196,204	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	G	2340	14/15	0.87	0.29	-1.03	232,246,263,271	0
8	NAG	G	1561	14/15	0.93	0.24	-1.22	211,224,277,278	0
10	MAN	G	3327	11/12	0.88	0.19	-1.57	195,200,218,238	0
8	NAG	G	2761	14/15	0.67	0.32	-	289,299,317,320	0
10	MAN	G	3633	11/12	0.82	0.21	-	350,368,374,383	0
10	MAN	G	1977	11/12	0.77	0.26	-	283,291,296,297	0
8	NAG	G	2951	14/15	0.85	0.35	-	283,298,308,317	0
8	NAG	G	881	14/15	0.73	0.27	-	331,341,358,361	0
11	GAL	G	1572	11/12	0.80	0.22	-	336,336,336,336	0
7	FUC	G	3920	10/11	0.79	0.39	-	308,313,323,331	0
8	NAG	G	3550	14/15	0.72	0.18	-	385,385,385,385	0
8	NAG	B	6111	14/15	0.76	0.22	-	285,298,351,352	0
8	NAG	G	2775	14/15	0.67	0.47	-	376,376,376,376	0
8	NAG	G	4480	14/15	0.77	0.42	-	215,226,243,248	0
8	NAG	G	1602	14/15	0.69	0.23	-	277,290,302,308	0
8	NAG	G	1971	14/15	0.79	0.34	-	221,241,244,244	0
11	GAL	G	2774	11/12	0.65	0.50	-	367,367,367,367	0
10	MAN	G	2764	11/12	0.83	0.44	-	393,393,393,393	0
8	NAG	G	2762	14/15	0.46	0.29	-	297,317,320,320	0
8	NAG	G	3861	14/15	0.87	0.34	-	326,343,363,369	0
9	BMA	G	4482	11/12	0.83	0.33	-	307,324,340,341	0
12	SIA	G	1976	20/21	0.72	0.42	-	371,371,371,371	0
8	NAG	G	2341	14/15	0.78	0.37	-	270,272,275,276	0
9	BMA	G	1563	11/12	0.78	0.15	-	313,313,313,313	0
10	MAN	G	2769	11/12	0.42	0.34	-	390,390,390,390	0
10	MAN	G	2624	11/12	0.59	0.51	-	399,413,420,421	0
9	BMA	G	2763	11/12	0.72	0.24	-	355,362,366,371	0
10	MAN	G	3323	11/12	0.81	0.27	-	208,225,231,240	0
10	MAN	G	1564	11/12	0.62	0.18	-	340,340,340,340	0
11	GAL	G	2771	11/12	0.56	0.20	-	435,435,435,435	0
8	NAG	G	2770	14/15	0.44	0.39	-	404,417,422,424	0
8	NAG	G	3011	14/15	0.66	0.43	-	338,352,362,366	0
9	BMA	G	3632	11/12	0.49	0.36	-	397,414,429,431	0
12	SIA	G	2772	20/21	0.66	0.48	-	456,456,456,456	0
8	NAG	G	2768	14/15	0.69	0.24	-	371,371,371,371	0
8	NAG	G	1605	14/15	0.49	0.25	-	363,363,363,363	0
11	GAL	G	1609	11/12	0.80	0.19	-	350,355,364,366	0
8	NAG	G	3860	14/15	0.85	0.37	-	245,256,273,279	0
7	FUC	B	6370	10/11	0.80	0.26	-	351,351,351,351	0
10	MAN	G	3324	11/12	0.81	0.26	-	261,274,297,307	0
10	MAN	G	3925	11/12	0.67	0.58	-	400,400,400,400	0
10	MAN	G	3635	11/12	0.61	0.32	-	342,342,342,342	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	G	3922	14/15	0.72	0.22	-	300,321,323,323	0
10	MAN	G	3634	11/12	0.74	0.36	-	355,370,377,378	0
8	NAG	G	3390	14/15	0.61	0.36	-	288,306,313,318	0
8	NAG	G	1562	14/15	0.82	0.27	-	254,274,287,287	0
8	NAG	G	3016	14/15	0.71	0.35	-	332,345,349,351	0
8	NAG	G	3631	14/15	0.71	0.74	-	431,431,431,431	0
12	SIA	G	2767	20/21	0.78	0.21	-	397,397,397,397	0
9	BMA	G	1332	11/12	0.83	0.23	-	274,274,274,274	0
10	MAN	G	2623	11/12	0.49	0.50	-	318,335,341,351	0
10	MAN	G	4484	11/12	0.62	0.71	-	408,410,419,425	0
8	NAG	G	882	14/15	0.70	0.33	-	336,357,359,360	0
10	MAN	G	3013	11/12	0.74	0.28	-	317,323,334,335	0
9	BMA	G	3862	11/12	0.71	0.24	-	318,336,351,352	0
8	NAG	G	1569	14/15	0.69	0.35	-	383,383,383,383	0
10	MAN	G	3864	11/12	0.58	0.42	-	313,318,336,356	0
11	GAL	G	1567	11/12	0.74	0.27	-	350,350,350,350	0
7	FUC	G	880	10/11	0.67	0.50	-	318,324,334,342	0
7	FUC	G	1600	10/11	0.86	0.57	-	329,329,329,329	0
8	NAG	G	2765	14/15	0.77	0.15	-	352,366,370,372	0
10	MAN	G	3924	11/12	0.66	0.38	-	294,294,294,294	0
8	NAG	G	3551	14/15	0.74	0.22	-	369,369,369,369	0
11	GAL	G	1975	11/12	0.71	0.22	-	358,363,372,375	0
7	FUC	G	1560	10/11	0.79	0.35	-	294,294,294,294	0
10	MAN	G	3863	11/12	0.71	0.38	-	314,331,337,347	0
8	NAG	G	1331	14/15	0.77	0.22	-	271,271,271,271	0
10	MAN	G	1973	11/12	0.84	0.22	-	337,337,337,337	0
9	BMA	G	3322	11/12	0.92	0.22	-	136,153,169,170	0
8	NAG	G	3014	14/15	0.74	0.52	-	347,356,371,376	0
9	BMA	G	3012	11/12	0.48	0.20	-	350,357,361,366	0
8	NAG	G	1565	14/15	0.72	0.27	-	340,340,340,340	0
10	MAN	G	3636	11/12	0.72	0.38	-	370,375,393,413	0
9	BMA	G	1972	11/12	0.89	0.23	-	254,261,265,270	0
8	NAG	B	6371	14/15	0.89	0.16	-	333,351,364,365	0
8	NAG	G	3630	14/15	0.78	0.43	-	290,299,323,342	0
8	NAG	G	1978	14/15	0.71	0.45	-	307,320,324,326	0
11	GAL	G	1570	11/12	0.81	0.39	-	401,401,401,401	0
7	FUC	B	6110	10/11	0.58	0.55	-	312,312,312,312	0
8	NAG	G	1566	14/15	0.76	0.18	-	346,346,346,346	0
10	MAN	G	2626	11/12	0.65	0.43	-	311,311,311,311	0
11	GAL	G	1606	11/12	0.68	0.42	-	411,411,411,411	0
8	NAG	G	1974	14/15	0.60	0.35	-	355,368,372,374	0
9	BMA	G	1603	11/12	0.75	0.11	-	330,330,330,330	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	BMA	B	6373	11/12	0.82	0.38	-	311,311,311,311	0
8	NAG	G	3921	14/15	0.85	0.25	-	296,306,324,327	0
8	NAG	G	4481	14/15	0.86	0.42	-	241,258,278,284	0
8	NAG	B	6372	14/15	0.95	0.18	-	318,318,318,318	0
8	NAG	G	1608	14/15	0.80	0.19	-	339,352,356,358	0
8	NAG	G	2773	14/15	0.43	0.44	-	394,394,394,394	0
8	NAG	G	1571	14/15	0.65	0.20	-	315,315,315,315	0
10	MAN	G	1607	11/12	0.69	0.23	-	350,350,350,350	0
10	MAN	G	3015	11/12	0.89	0.20	-	360,369,374,374	0
9	BMA	G	3923	11/12	0.78	0.19	-	314,321,325,329	0
11	GAL	G	2766	11/12	0.86	0.12	-	351,351,351,351	0
10	MAN	G	1568	11/12	0.57	0.19	-	330,330,330,330	0
10	MAN	G	4483	11/12	0.71	0.42	-	380,397,403,413	0
9	BMA	G	2622	11/12	0.59	0.38	-	287,304,319,321	0
10	MAN	G	3326	11/12	0.88	0.35	-	250,252,261,267	0
10	MAN	G	1604	11/12	0.66	0.25	-	338,338,338,338	0

## 6.5 Other polymers

There are no such residues in this entry.