



wwPDB X-ray Structure Validation Summary 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 An-
tibodies IOMA and 10-1074.
Authors : Gristick, H.B.; Bjorkman, P.J.
Deposited on : 2016-08-26
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (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

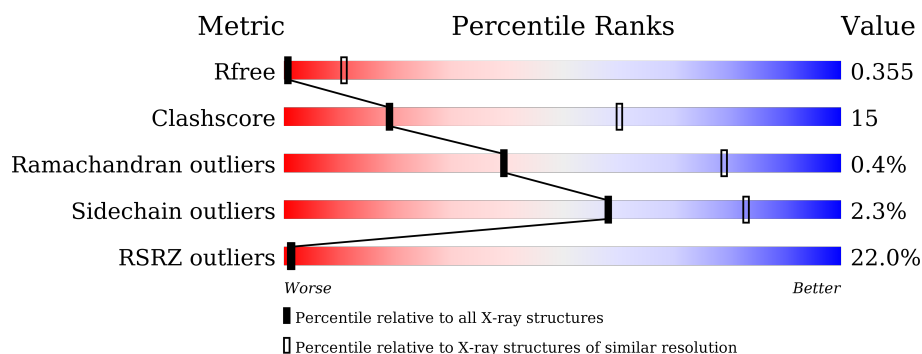
1 Overall quality at a glance ⓘ

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 ≥ 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> <div>49%</div> <div>32%</div> <div>•</div> <div>18%</div> </div> </div>
2	G	481	<div> <div>7%</div> <div> <div>58%</div> <div>34%</div> <div>•</div> <div>7%</div> </div> </div>
3	H	238	<div> <div>29%</div> <div> <div>67%</div> <div>29%</div> <div>••</div> </div> </div>
4	L	214	<div> <div>20%</div> <div> <div>67%</div> <div>29%</div> <div>••</div> </div> </div>
5	D	232	<div> <div>29%</div> <div> <div>59%</div> <div>37%</div> <div>••</div> </div> </div>
6	E	214	<div> <div>42%</div> <div> <div>67%</div> <div>29%</div> <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			

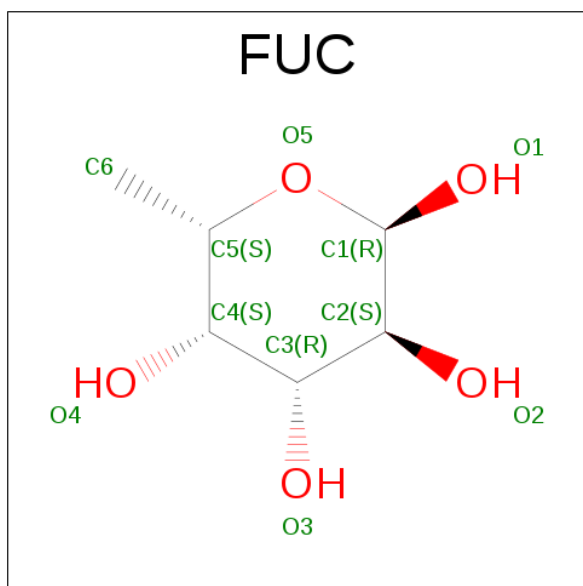
- Molecule 5 is a protein called IOMA Heavy Chain.

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: $C_6H_{12}O_5$).



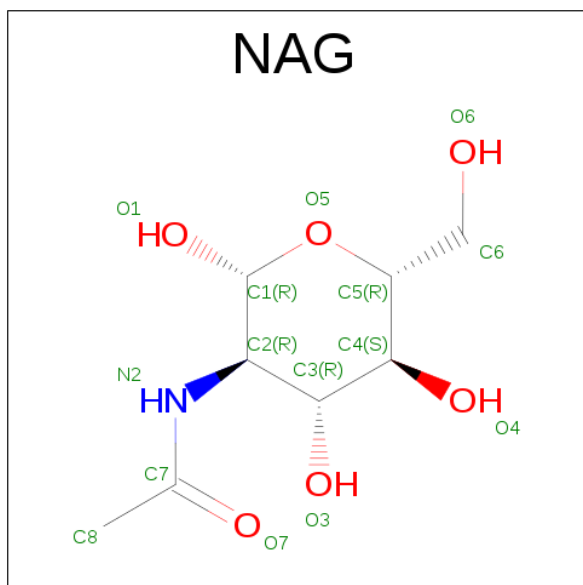
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		

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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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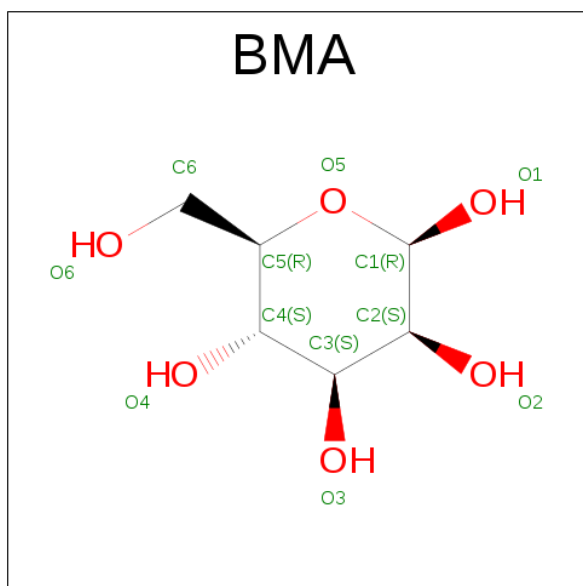
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	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: $C_6H_{12}O_6$).



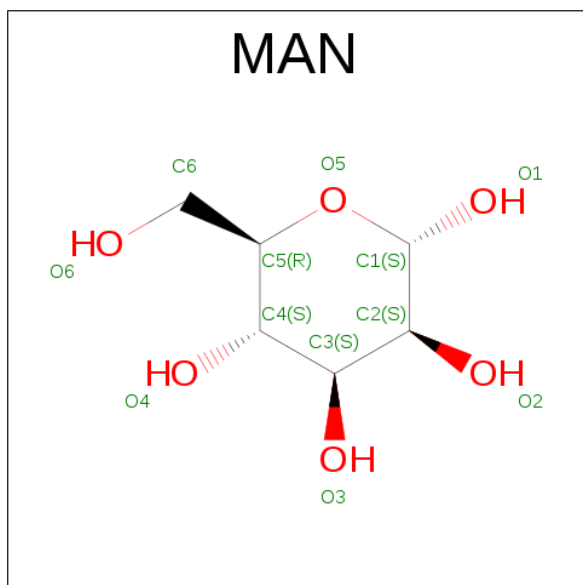
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		

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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: $C_6H_{12}O_6$).



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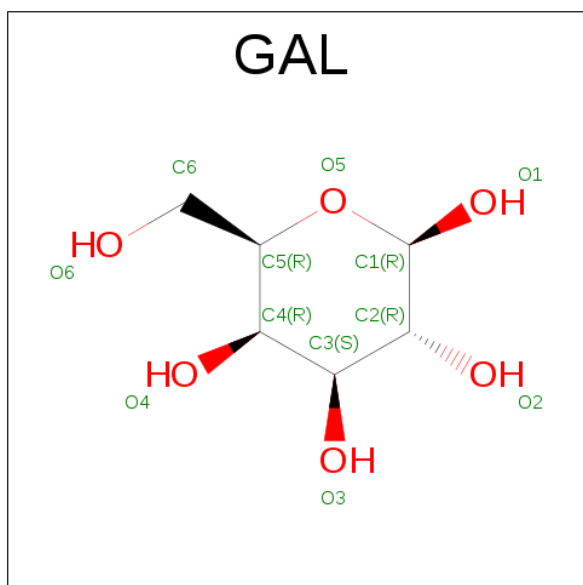
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11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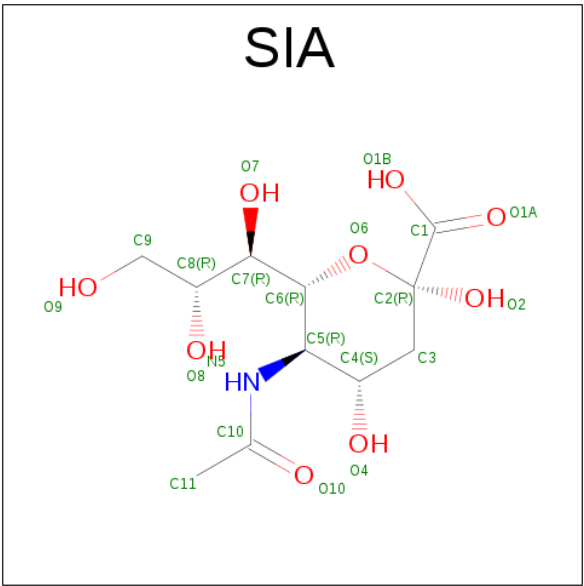
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 11 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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		

- Molecule 12 is O-SIALIC ACID (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).

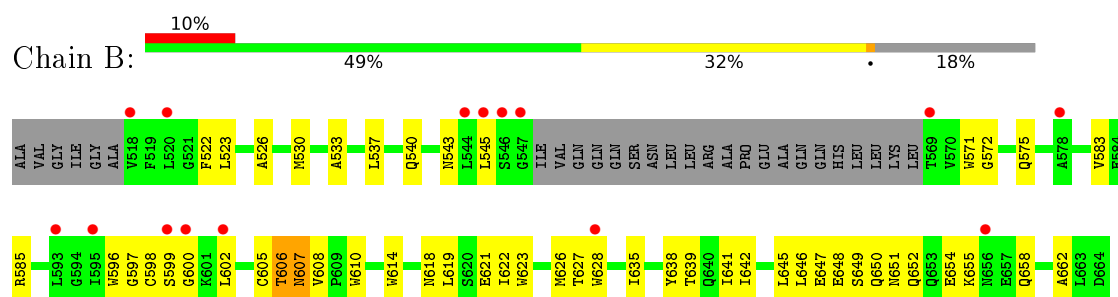


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			20	11	1	8		
12	G	1	Total	C	N	O	0	0
			20	11	1	8		
12	G	1	Total	C	N	O	0	0
			20	11	1	8		

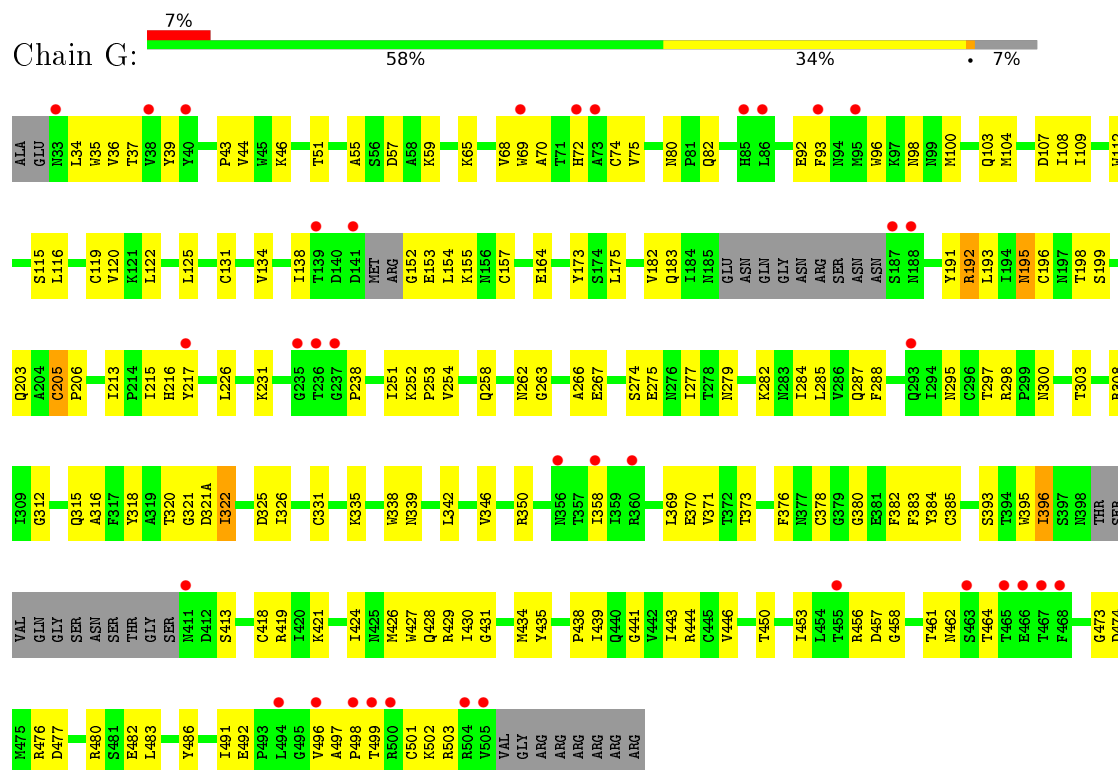
3 Residue-property plots

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

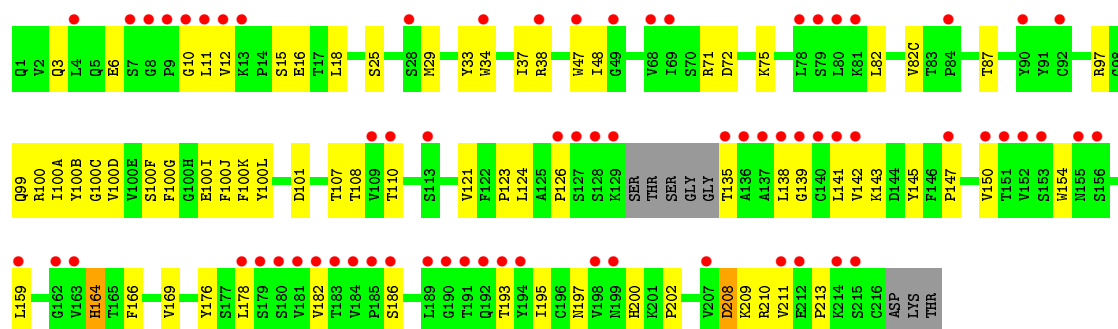


- Molecule 2: Envelope glycoprotein gp160

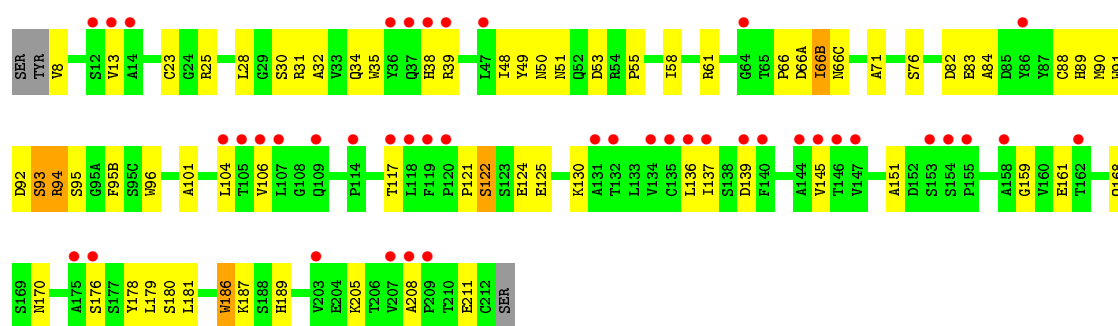


- Molecule 3: 10-1074 Heavy Chain

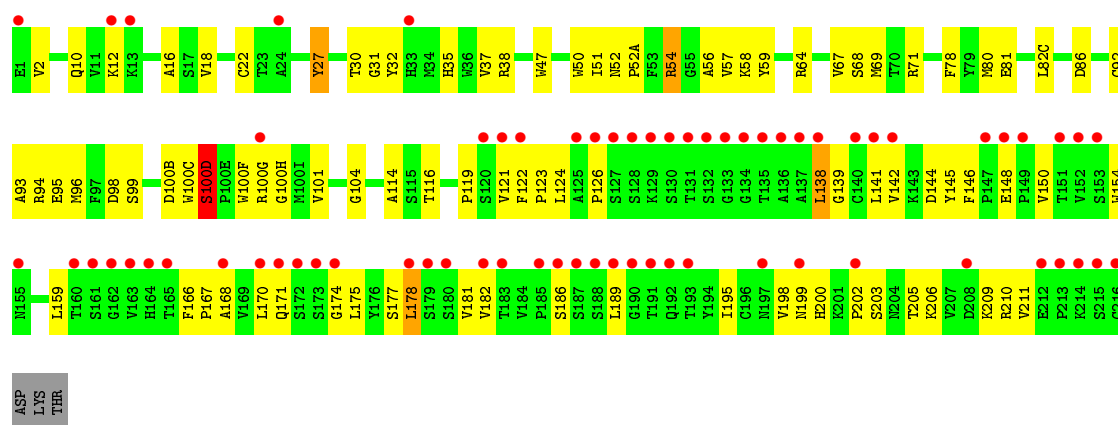




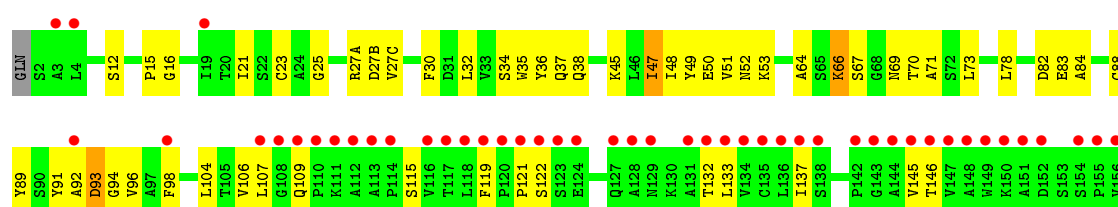
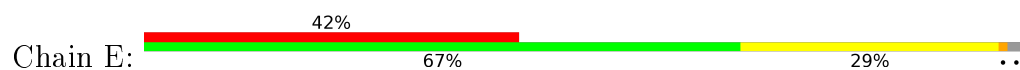
• Molecule 4: 10-1074 Light Chain



• Molecule 5: IOMA Heavy Chain



• Molecule 6: IOMA Light Chain



K157	K158	G159	V160	E161	T162	T163	T164	P165	M170	N171	K172	Y173	A174	A175	S176	S177	Y178	L179	S180	L181	T182	P183	E184	Q185	W186	K187	S188	H189	R190	S191	Y192	S193	C194	Q195	V196	T197	H198	E199	G200	S201	E204	K205	T206	V207	A208	P209	T210	GLU	CYS	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	132.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 326.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

² 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.

The worst 5 of 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

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

5 of 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

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

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	164	HIS

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Mol	Chain	Res	Type
4	L	93	SER
6	E	47	ILE
3	H	208	ASP
4	L	94	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	171	GLN
6	E	109	GLN
5	D	35	HIS
3	H	60	ASN
4	L	52	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	2764	MAN	O5-C1-C2	-4.20	104.18	110.89

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	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

The worst 5 of 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

6.2 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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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.