



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2016 – 09:23 PM EDT

PDB ID : 5T3Z
Title : 3.5 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 : 3.50 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

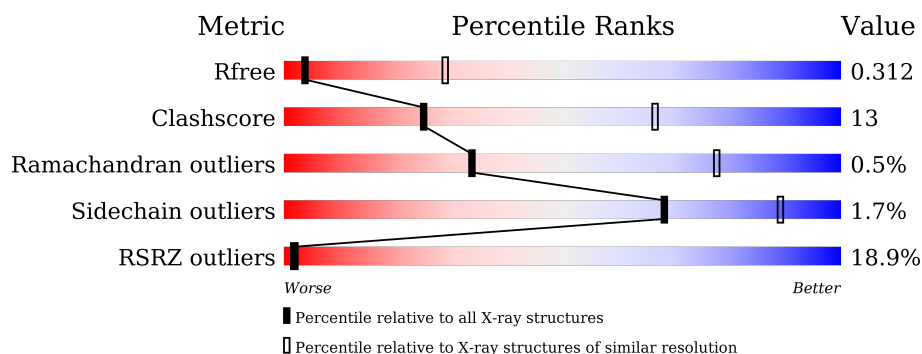
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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>6%</div> <div>58%</div> <div>24%</div> <div>18%</div> </div>
2	G	481	<div> <div>4%</div> <div>67%</div> <div>26%</div> <div>6%</div> </div>
3	H	238	<div> <div>19%</div> <div>66%</div> <div>30%</div> <div>5%</div> </div>
4	L	214	<div> <div>24%</div> <div>74%</div> <div>23%</div> <div>2%</div> </div>
5	D	232	<div> <div>34%</div> <div>62%</div> <div>35%</div> <div>2%</div> </div>
6	E	214	<div> <div>34%</div> <div>71%</div> <div>26%</div> <div>2%</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
8	NAG	G	1970	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12300 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 mutatioin	UNP Q2N0S6
B	605	CYS	THR	engineered mutatioin	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutatioin	UNP Q2N0S6
G	501	CYS	ALA	engineered mutatioin	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			

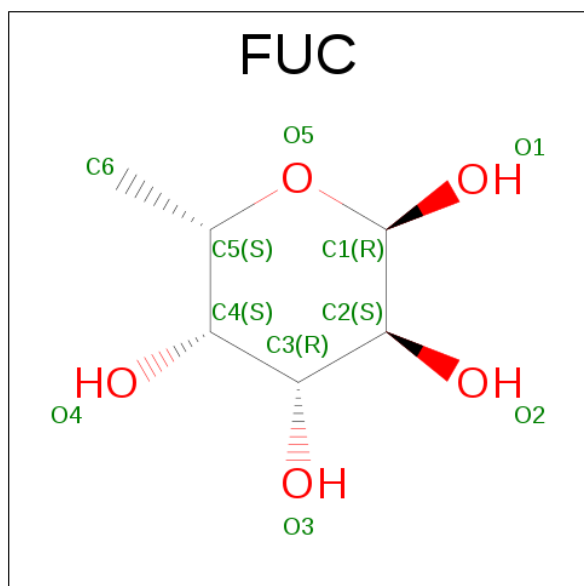
- Molecule 5 is a protein called IOMA Heavy Chain.

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.

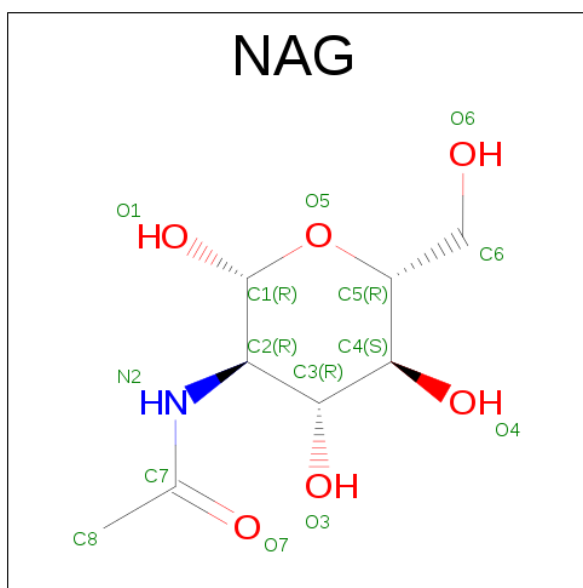
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



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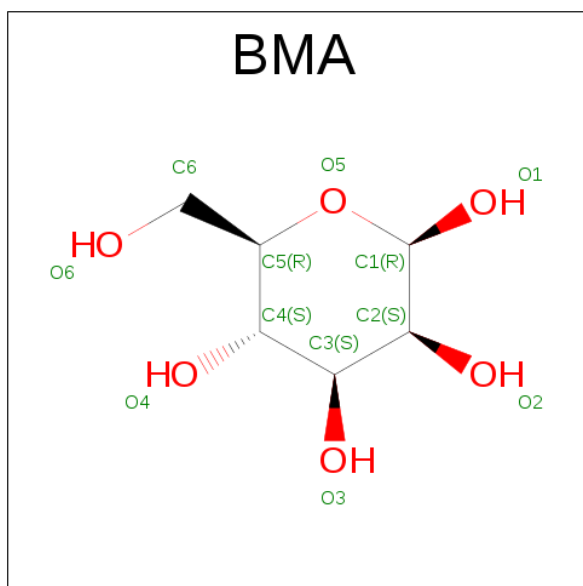
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1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

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



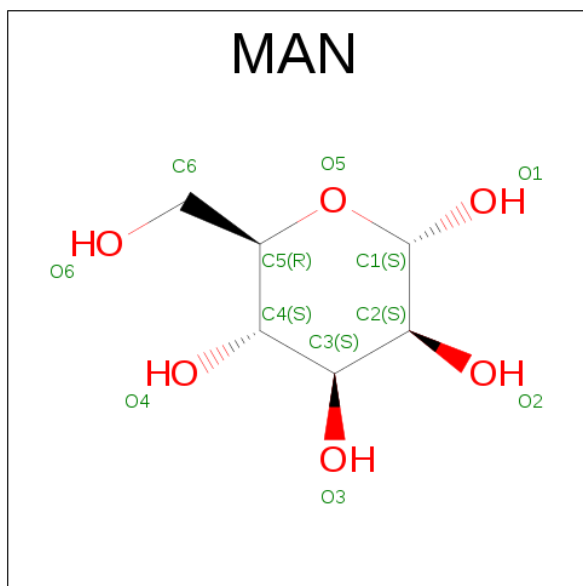
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		

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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		
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		

- Molecule 10 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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		

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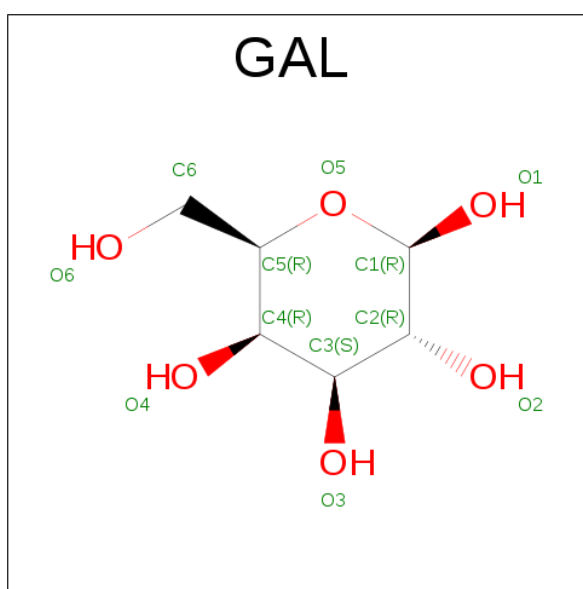
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	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		
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: C₆H₁₂O₆).

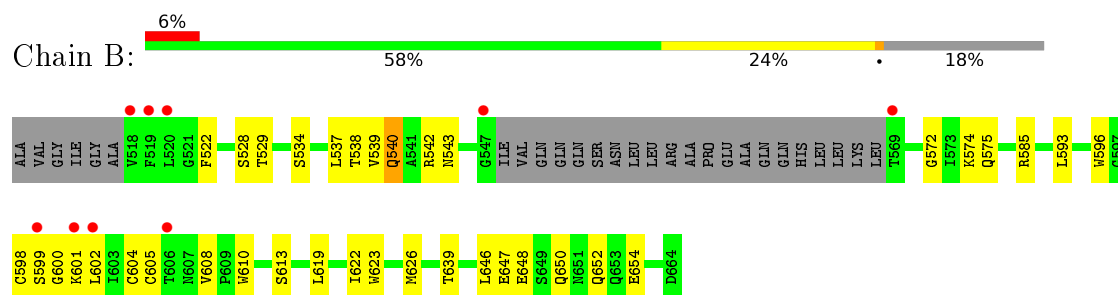


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		

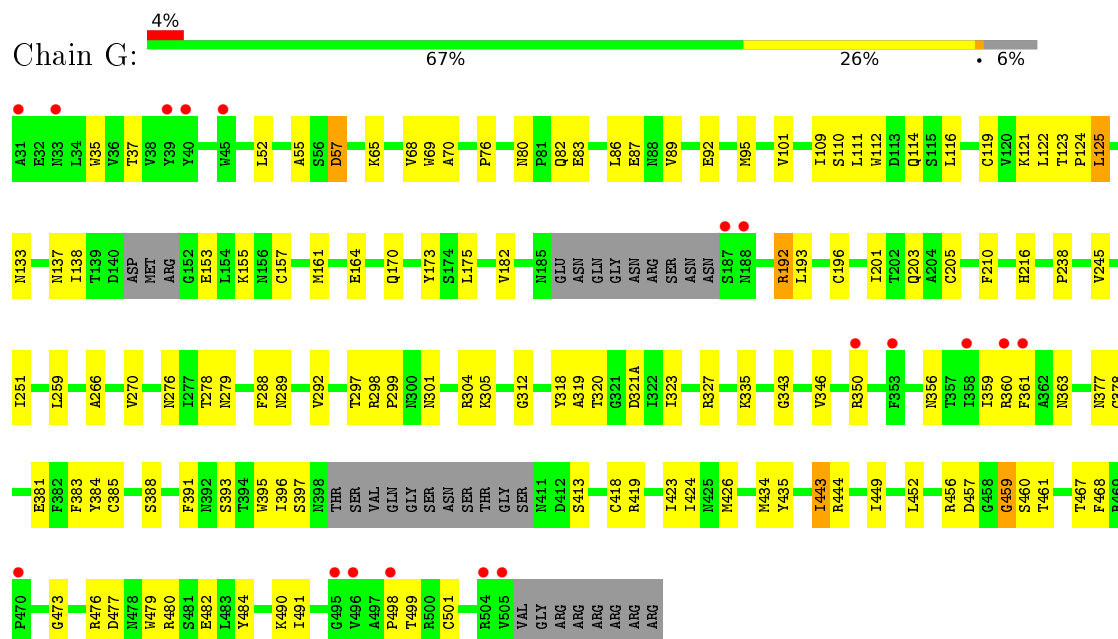
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

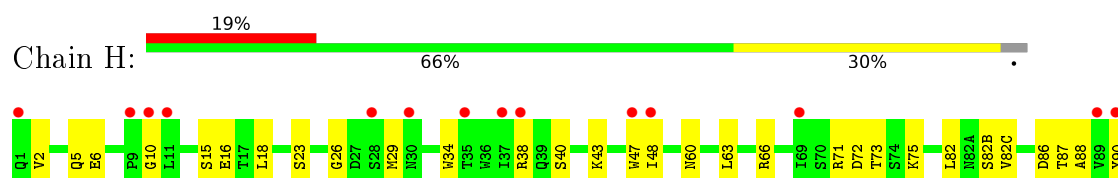
• Molecule 1: Envelope glycoprotein gp160

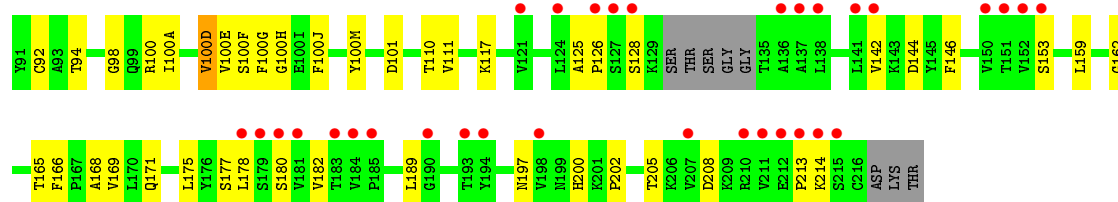


• Molecule 2: Envelope glycoprotein gp160

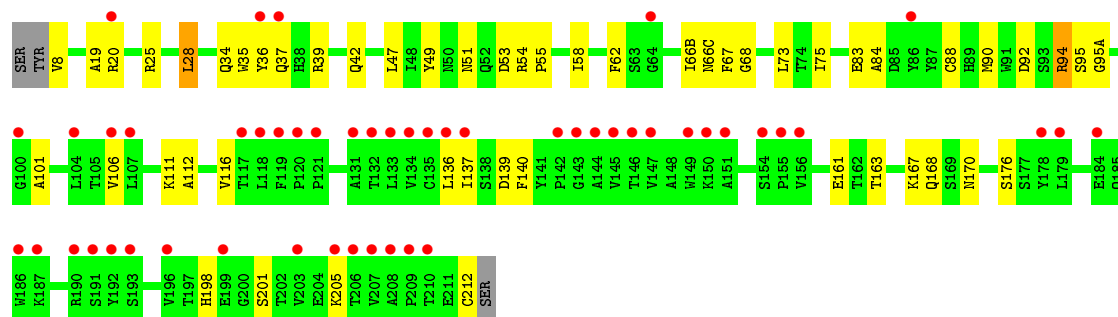
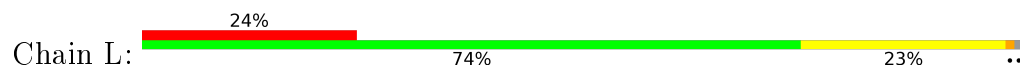


• Molecule 3: 10-1074 Heavy Chain

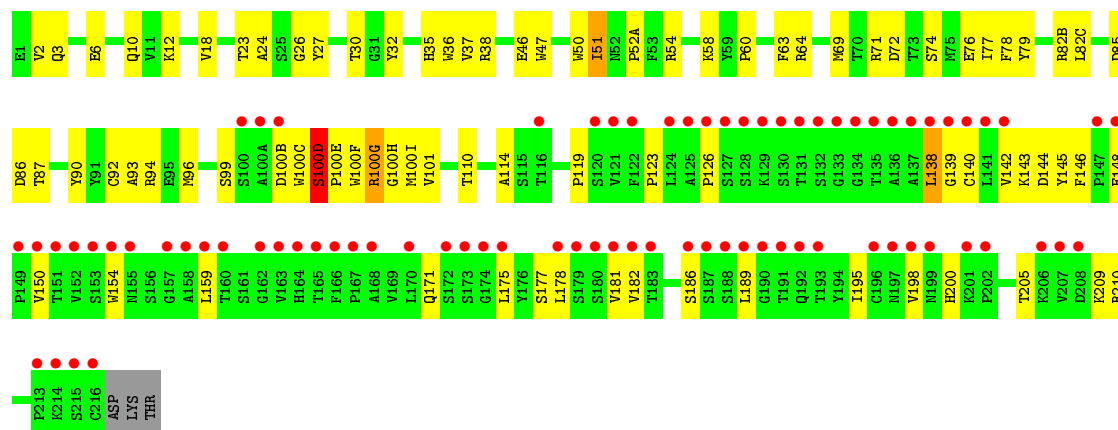




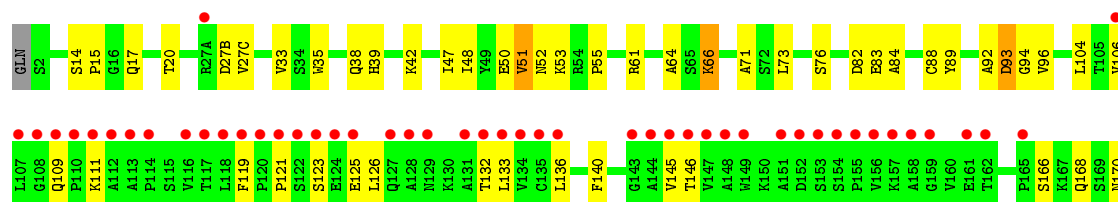
• Molecule 4: 10-1074 Light Chain



• Molecule 5: IOMA Heavy Chain



• Molecule 6: IOMA Light Chain



N171	K172	Y173	A174	A175	S176	S177	Y178	L179	S180	L181	H186	K187	S188	H189	R190	S191	Y192	S193	C194	Q195	V196	T197	H198	E199	G200	S201	T202	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	217.26Å 217.26Å 154.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.63 – 3.50 80.41 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.63-3.50) 94.8 (80.41-3.50)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.275 , 0.298 0.286 , 0.312	Depositor DCC
R_{free} test set	1665 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 155.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.068 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.130 for k,h,-l	Depositor
Outliers	0 of 34367 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12300	wwPDB-VP
Average B, all atoms (Å ²)	211.0	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: FUC, GAL, NAG, BMA, 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	0/3611	0.50	0/4903
3	H	0.25	0/1796	0.47	0/2450
4	L	0.27	0/1649	0.47	0/2250
5	D	0.29	0/1790	0.57	2/2437 (0.1%)
6	E	0.25	0/1596	0.47	0/2175
All	All	0.27	0/11461	0.50	2/15597 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	100(D)	SER	C-N-CD	-7.65	103.77	120.60
5	D	100(D)	SER	C-N-CA	6.00	147.21	122.00

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	24	1
2	G	3538	0	3469	86	0
3	H	1753	0	1719	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1607	0	1550	37	0
5	D	1742	0	1698	73	0
6	E	1558	0	1511	37	0
7	B	10	0	10	1	0
7	G	30	0	30	4	0
8	B	42	0	36	0	0
8	G	546	0	474	11	0
9	B	11	0	10	0	0
9	G	121	0	92	7	0
10	G	297	0	254	13	0
11	G	44	0	40	0	0
All	All	12300	0	11869	306	1

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 13.

The worst 5 of 306 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)
10:G:3635:MAN:H5	5:D:82(B):ARG:HH22	1.24	0.98
5:D:119:PRO:HD2	5:D:205:THR:HB	1.62	0.80
2:G:87:GLU:HB3	8:G:880:NAG:H82	1.67	0.76
2:G:457:ASP:OD2	2:G:467:THR:HB	1.85	0.76
2:G:92:GLU:HA	2:G:238:PRO:HA	1.67	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:SER:O	1:B:652:GLN:NE2[3_555]	2.15	0.05

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%)	109 (89%)	12 (10%)	1 (1%)	24	70
2	G	442/481 (92%)	417 (94%)	22 (5%)	3 (1%)	26	72
3	H	226/238 (95%)	216 (96%)	10 (4%)	0	100	100
4	L	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
5	D	227/232 (98%)	218 (96%)	8 (4%)	1 (0%)	39	81
6	E	208/214 (97%)	198 (95%)	8 (4%)	2 (1%)	19	66
All	All	1434/1532 (94%)	1359 (95%)	68 (5%)	7 (0%)	34	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	57	ASP
2	G	459	GLY
6	E	93	ASP
2	G	138	ILE
5	D	100(D)	SER

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	76
2	G	401/428 (94%)	397 (99%)	4 (1%)	82	93
3	H	202/208 (97%)	199 (98%)	3 (2%)	72	90
4	L	175/178 (98%)	173 (99%)	2 (1%)	80	92
5	D	194/197 (98%)	188 (97%)	6 (3%)	47	81
6	E	173/177 (98%)	171 (99%)	2 (1%)	78	92
All	All	1253/1317 (95%)	1232 (98%)	21 (2%)	68	89

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	100(E)	VAL
4	L	28	LEU
5	D	138	LEU
3	H	100(D)	VAL
5	D	140	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	39	GLN
6	E	109	GLN
5	D	155	ASN
4	L	198	HIS
6	E	38	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](#)

89 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	0.71	0	13,14,16	0.83	0
8	NAG	B	6111	1,7	14,14,15	0.32	0	15,19,21	0.86	0
8	NAG	B	6370	1,8	14,14,15	0.36	0	15,19,21	1.22	1 (6%)
8	NAG	B	6371	9,8	14,14,15	0.26	0	15,19,21	0.92	0
9	BMA	B	6372	8	11,11,12	0.24	0	15,15,17	0.72	0
8	NAG	G	1330	8,2	14,14,15	0.44	0	15,19,21	2.34	6 (40%)
8	NAG	G	1331	8	14,14,15	0.28	0	15,19,21	0.73	0
7	FUC	G	1560	8	10,10,11	1.39	2 (20%)	13,14,16	1.37	1 (7%)
8	NAG	G	1561	8,2,7	14,14,15	0.39	0	15,19,21	1.79	6 (40%)
8	NAG	G	1562	9,8	14,14,15	0.54	0	15,19,21	0.89	0
9	BMA	G	1563	8,10	11,11,12	0.47	0	15,15,17	2.03	4 (26%)
10	MAN	G	1564	9,8	11,11,12	0.40	0	15,15,17	2.01	4 (26%)
8	NAG	G	1565	10	14,14,15	0.25	0	15,19,21	0.99	1 (6%)
8	NAG	G	1566	11,10	14,14,15	0.33	0	15,19,21	0.77	0
11	GAL	G	1567	8	11,11,12	0.47	0	15,15,17	0.93	0
10	MAN	G	1568	9,8	11,11,12	0.66	0	15,15,17	1.94	2 (13%)
8	NAG	G	1569	11,10	14,14,15	0.33	0	15,19,21	0.90	1 (6%)
11	GAL	G	1570	8	11,11,12	0.52	0	15,15,17	1.06	1 (6%)
8	NAG	G	1600	8,2	14,14,15	0.37	0	15,19,21	1.20	2 (13%)
8	NAG	G	1601	9,8	14,14,15	0.37	0	15,19,21	2.15	2 (13%)
9	BMA	G	1602	8,10	11,11,12	0.23	0	15,15,17	1.19	1 (6%)
10	MAN	G	1603	9	11,11,12	0.25	0	15,15,17	0.74	0
10	MAN	G	1604	9	11,11,12	0.28	0	15,15,17	0.77	0
8	NAG	G	1970	8,2	14,14,15	0.51	0	15,19,21	2.28	4 (26%)
8	NAG	G	1971	9,8	14,14,15	0.50	0	15,19,21	1.78	4 (26%)
9	BMA	G	1972	8,10	11,11,12	0.57	0	15,15,17	1.72	2 (13%)
10	MAN	G	1973	9,8	11,11,12	0.49	0	15,15,17	1.50	3 (20%)
8	NAG	G	1974	11,10	14,14,15	0.29	0	15,19,21	0.64	0
11	GAL	G	1975	8	11,11,12	0.54	0	15,15,17	1.07	0
10	MAN	G	1976	9,8	11,11,12	0.26	0	15,15,17	1.13	1 (6%)
8	NAG	G	1977	10	14,14,15	0.27	0	15,19,21	0.66	0
8	NAG	G	2340	8,2	14,14,15	0.36	0	15,19,21	0.78	1 (6%)
8	NAG	G	2341	8	14,14,15	0.28	0	15,19,21	0.76	0
8	NAG	G	2620	8,2	14,14,15	0.35	0	15,19,21	0.74	0
8	NAG	G	2621	9,8	14,14,15	0.33	0	15,19,21	1.24	3 (20%)
9	BMA	G	2622	8,10	11,11,12	0.29	0	15,15,17	1.03	1 (6%)
10	MAN	G	2623	9,10	11,11,12	0.23	0	15,15,17	0.78	0
10	MAN	G	2624	10	11,11,12	0.25	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	G	2625	9,10	11,11,12	0.47	0	15,15,17	0.99	1 (6%)
10	MAN	G	2626	10	11,11,12	0.46	0	15,15,17	1.09	1 (6%)
7	FUC	G	2760	8	10,10,11	0.58	0	13,14,16	0.85	0
8	NAG	G	2761	8,2,7	14,14,15	0.51	0	15,19,21	1.32	1 (6%)
8	NAG	G	2762	9,8	14,14,15	0.30	0	15,19,21	1.13	2 (13%)
9	BMA	G	2763	8,10	11,11,12	0.28	0	15,15,17	1.39	2 (13%)
10	MAN	G	2764	9,8	11,11,12	0.48	0	15,15,17	1.79	3 (20%)
8	NAG	G	2765	11,10	14,14,15	0.26	0	15,19,21	0.55	0
11	GAL	G	2766	8	11,11,12	0.45	0	15,15,17	0.95	0
10	MAN	G	2767	9	11,11,12	0.47	0	15,15,17	1.07	1 (6%)
8	NAG	G	2950	8,2	14,14,15	0.28	0	15,19,21	0.57	0
8	NAG	G	2951	8	14,14,15	0.28	0	15,19,21	0.57	0
8	NAG	G	3010	8,2	14,14,15	0.34	0	15,19,21	0.84	1 (6%)
8	NAG	G	3011	9,8	14,14,15	0.32	0	15,19,21	0.60	0
9	BMA	G	3012	8,10	11,11,12	0.24	0	15,15,17	1.50	2 (13%)
10	MAN	G	3013	9,8	11,11,12	0.20	0	15,15,17	1.17	1 (6%)
8	NAG	G	3014	10	14,14,15	0.27	0	15,19,21	0.73	0
10	MAN	G	3015	9	11,11,12	0.86	0	15,15,17	1.34	3 (20%)
8	NAG	G	3320	8,2	14,14,15	0.33	0	15,19,21	0.79	1 (6%)
8	NAG	G	3321	9,8	14,14,15	0.27	0	15,19,21	1.22	2 (13%)
9	BMA	G	3322	8,10	11,11,12	0.30	0	15,15,17	1.05	1 (6%)
10	MAN	G	3323	9,10	11,11,12	0.26	0	15,15,17	0.75	0
10	MAN	G	3324	10	11,11,12	0.28	0	15,15,17	1.37	3 (20%)
10	MAN	G	3325	10	11,11,12	0.28	0	15,15,17	0.85	0
10	MAN	G	3326	10	11,11,12	0.26	0	15,15,17	0.72	0
10	MAN	G	3327	9,10	11,11,12	0.23	0	15,15,17	1.12	2 (13%)
10	MAN	G	3328	10	11,11,12	0.32	0	15,15,17	1.51	3 (20%)
10	MAN	G	3329	10	11,11,12	0.28	0	15,15,17	0.85	1 (6%)
8	NAG	G	3390	2	14,14,15	0.28	0	15,19,21	0.70	0
8	NAG	G	3550	2	14,14,15	0.30	0	15,19,21	0.57	0
8	NAG	G	3630	8,2	14,14,15	0.42	0	15,19,21	1.01	1 (6%)
8	NAG	G	3631	9,8	14,14,15	0.38	0	15,19,21	1.57	4 (26%)
9	BMA	G	3632	8,10	11,11,12	0.61	0	15,15,17	1.93	2 (13%)
10	MAN	G	3633	9	11,11,12	1.34	2 (18%)	15,15,17	1.79	3 (20%)
10	MAN	G	3634	9,10	11,11,12	0.81	0	15,15,17	1.93	5 (33%)
10	MAN	G	3635	10	11,11,12	0.51	0	15,15,17	1.22	1 (6%)
10	MAN	G	3636	10	11,11,12	0.82	0	15,15,17	1.93	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	G	3860	8,2	14,14,15	0.36	0	15,19,21	0.98	1 (6%)
8	NAG	G	3861	9,8	14,14,15	0.38	0	15,19,21	1.02	0
9	BMA	G	3862	8,10	11,11,12	0.46	0	15,15,17	1.47	2 (13%)
10	MAN	G	3863	9	11,11,12	0.31	0	15,15,17	0.94	0
10	MAN	G	3864	9	11,11,12	1.16	2 (18%)	15,15,17	2.37	3 (20%)
7	FUC	G	3920	8	10,10,11	0.97	0	13,14,16	1.30	2 (15%)
8	NAG	G	3921	8,2,7	14,14,15	0.30	0	15,19,21	1.07	2 (13%)
8	NAG	G	3922	9,8	14,14,15	0.28	0	15,19,21	0.84	0
9	BMA	G	3923	8	11,11,12	0.26	0	15,15,17	0.72	0
8	NAG	G	4480	8,2	14,14,15	0.28	0	15,19,21	0.72	0
8	NAG	G	4481	9,8	14,14,15	0.29	0	15,19,21	1.07	2 (13%)
9	BMA	G	4482	8	11,11,12	0.32	0	15,15,17	0.60	0
8	NAG	G	880	8,2	14,14,15	0.27	0	15,19,21	0.79	1 (6%)
8	NAG	G	881	8	14,14,15	0.26	0	15,19,21	0.60	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
8	NAG	B	6370	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	6371	9,8	-	0/6/23/26	0/1/1/1
9	BMA	B	6372	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	8	-	0/6/23/26	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	1600	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	1601	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	1602	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1603	9	-	0/2/19/22	0/1/1/1
10	MAN	G	1604	9	-	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	-	0/2/19/22	0/1/1/1
10	MAN	G	1976	9,8	-	0/2/19/22	0/1/1/1
8	NAG	G	1977	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	-	0/2/19/22	0/1/1/1
10	MAN	G	2767	9	-	0/2/19/22	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	-	0/2/19/22	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	2	-	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	-	0/2/19/22	0/1/1/1
10	MAN	G	3634	9,10	-	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	10	-	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	-	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	-	0/2/19/22	0/1/1/1
8	NAG	G	880	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	881	8	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1560	FUC	O2-C2	-2.27	1.38	1.43
7	G	1560	FUC	C1-C2	2.04	1.57	1.52
10	G	3864	MAN	C1-C2	2.14	1.57	1.52
10	G	3633	MAN	C1-C2	2.81	1.59	1.52
10	G	3864	MAN	O5-C1	3.09	1.48	1.43

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	1564	MAN	C1-C2-C3	-5.39	103.02	109.55
8	G	1970	NAG	O4-C4-C3	-5.19	98.66	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	1563	BMA	O3-C3-C2	-4.63	101.52	110.01
8	G	2761	NAG	O4-C4-C5	-4.20	98.15	109.23
10	G	2764	MAN	O5-C1-C2	-4.15	104.25	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	6110	FUC	1	0
7	G	1560	FUC	4	0
8	G	1562	NAG	1	0
10	G	1564	MAN	1	0
8	G	1565	NAG	1	0
8	G	1566	NAG	1	0
8	G	1569	NAG	1	0
8	G	1600	NAG	1	0
8	G	1601	NAG	1	0
8	G	1970	NAG	2	0
8	G	1971	NAG	2	0
9	G	1972	BMA	2	0
10	G	1973	MAN	1	0
10	G	1976	MAN	1	0
8	G	2340	NAG	1	0
8	G	2341	NAG	1	0
9	G	2763	BMA	1	0
10	G	2764	MAN	1	0
8	G	3321	NAG	1	0
10	G	3327	MAN	1	0
10	G	3328	MAN	1	0
8	G	3631	NAG	1	0
9	G	3632	BMA	3	0
10	G	3633	MAN	3	0
10	G	3634	MAN	1	0
10	G	3635	MAN	2	0
8	G	3860	NAG	1	0
9	G	3862	BMA	1	0
10	G	3864	MAN	1	0
8	G	880	NAG	2	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%)	0.41	9 (7%) 19 15	134, 197, 240, 278	0
2	G	450/481 (93%)	0.56	18 (4%) 42 33	70, 138, 243, 334	0
3	H	230/238 (96%)	1.28	46 (20%) 1 2	106, 228, 348, 427	0
4	L	211/214 (98%)	1.37	51 (24%) 1 1	119, 258, 380, 414	0
5	D	229/232 (98%)	2.28	78 (34%) 0 0	89, 177, 439, 480	0
6	E	210/214 (98%)	2.02	73 (34%) 0 0	109, 243, 408, 445	0
All	All	1456/1532 (95%)	1.26	275 (18%) 2 2	70, 189, 390, 480	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	133	GLY	18.7
5	D	127	SER	18.0
6	E	210	THR	17.3
5	D	126	PRO	17.2
4	L	209	PRO	16.9

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
8	NAG	G	1970	14/15	0.75	0.45	6.77	153,162,180,183	0
8	NAG	G	880	14/15	0.72	0.24	0.33	222,222,222,222	0
10	MAN	G	3329	11/12	0.79	0.30	-0.07	144,149,154,155	0
8	NAG	G	2620	14/15	0.92	0.31	-0.37	102,113,131,136	0
8	NAG	G	4480	14/15	0.85	0.28	-0.41	173,191,202,205	0
10	MAN	G	3328	11/12	0.94	0.22	-0.45	125,129,142,149	0
8	NAG	G	1600	14/15	0.78	0.32	-0.59	140,164,173,185	0
8	NAG	G	2340	14/15	0.84	0.25	-0.73	186,200,216,224	0
8	NAG	G	2950	14/15	0.82	0.27	-0.74	164,179,205,214	0
8	NAG	G	3321	14/15	0.95	0.29	-0.77	102,118,139,145	0
8	NAG	G	2621	14/15	0.90	0.27	-0.78	153,169,190,196	0
8	NAG	G	3320	14/15	0.89	0.27	-1.05	121,132,150,155	0
8	NAG	G	1330	14/15	0.91	0.29	-1.12	189,204,216,219	0
10	MAN	G	3327	11/12	0.90	0.20	-1.17	132,137,155,175	0
8	NAG	G	1561	14/15	0.85	0.20	-2.11	148,161,214,215	0
9	BMA	B	6372	11/12	0.78	0.25	-	241,241,241,241	0
8	NAG	G	3550	14/15	0.60	0.25	-	279,296,303,305	0
10	MAN	G	1603	11/12	0.62	0.30	-	293,293,293,293	0
10	MAN	G	3325	11/12	0.80	0.35	-	266,266,266,266	0
8	NAG	G	2951	14/15	0.83	0.33	-	199,213,224,232	0
10	MAN	G	1568	11/12	0.81	0.17	-	236,236,236,236	0
10	MAN	G	3633	11/12	0.62	0.31	-	237,237,237,237	0
10	MAN	G	3323	11/12	0.87	0.24	-	151,168,174,183	0
10	MAN	G	2623	11/12	0.70	0.33	-	251,268,274,283	0
10	MAN	G	1973	11/12	0.74	0.23	-	255,255,255,255	0
8	NAG	G	881	14/15	0.69	0.51	-	244,244,244,244	0
11	GAL	G	1975	11/12	0.34	0.41	-	306,310,319,322	0
8	NAG	G	1971	14/15	0.73	0.36	-	177,197,200,200	0
8	NAG	G	3860	14/15	0.91	0.31	-	153,164,182,187	0
10	MAN	G	2625	11/12	0.88	0.24	-	223,223,223,223	0
8	NAG	G	1569	14/15	0.78	0.19	-	263,263,263,263	0
10	MAN	G	2626	11/12	0.63	0.35	-	223,223,223,223	0
8	NAG	G	4481	14/15	0.87	0.25	-	214,236,262,289	0
8	NAG	G	3011	14/15	0.80	0.24	-	207,207,207,207	0
7	FUC	G	1560	10/11	0.88	0.21	-	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	GAL	G	2766	11/12	0.59	0.28	-	290,290,290,290	0
9	BMA	G	3012	11/12	0.75	0.15	-	231,231,231,231	0
9	BMA	G	1972	11/12	0.75	0.27	-	198,205,209,214	0
10	MAN	G	3324	11/12	0.80	0.34	-	237,252,258,260	0
10	MAN	G	3863	11/12	0.59	0.28	-	242,242,242,242	0
8	NAG	G	2341	14/15	0.76	0.36	-	227,229,232,233	0
9	BMA	G	3632	11/12	0.59	0.21	-	243,243,243,243	0
8	NAG	G	1977	14/15	0.79	0.28	-	210,223,227,229	0
8	NAG	G	3630	14/15	0.86	0.32	-	171,180,204,223	0
10	MAN	G	3636	11/12	0.63	0.25	-	215,215,215,215	0
7	FUC	B	6110	10/11	0.65	0.39	-	256,256,256,256	0
10	MAN	G	3015	11/12	0.53	0.50	-	236,236,236,236	0
9	BMA	G	3322	11/12	0.96	0.26	-	98,115,130,132	0
8	NAG	G	1565	14/15	0.69	0.43	-	275,275,275,275	0
9	BMA	G	2763	11/12	0.75	0.13	-	265,272,276,281	0
11	GAL	G	1570	11/12	0.79	0.23	-	275,275,275,275	0
8	NAG	G	1331	14/15	0.57	0.37	-	242,242,242,242	0
8	NAG	B	6111	14/15	0.65	0.38	-	246,258,311,313	0
9	BMA	G	1602	11/12	0.76	0.16	-	273,273,273,273	0
9	BMA	G	1563	11/12	0.74	0.13	-	237,237,237,237	0
10	MAN	G	1976	11/12	0.67	0.24	-	216,224,229,230	0
10	MAN	G	2624	11/12	0.66	0.44	-	257,259,268,273	0
8	NAG	G	2765	14/15	0.79	0.22	-	285,299,303,305	0
10	MAN	G	3864	11/12	0.75	0.33	-	245,245,245,245	0
9	BMA	G	4482	11/12	0.71	0.34	-	244,280,310,364	0
10	MAN	G	1564	11/12	0.88	0.11	-	263,263,263,263	0
10	MAN	G	1604	11/12	0.62	0.33	-	293,293,293,293	0
7	FUC	G	2760	10/11	0.52	0.57	-	225,225,225,225	0
10	MAN	G	2767	11/12	0.40	0.39	-	277,277,277,277	0
8	NAG	G	3921	14/15	0.80	0.22	-	214,224,242,245	0
8	NAG	G	3922	14/15	0.80	0.19	-	233,254,256,257	0
9	BMA	G	3862	11/12	0.60	0.21	-	249,249,249,249	0
10	MAN	G	3013	11/12	0.78	0.32	-	245,245,245,245	0
8	NAG	G	3010	14/15	0.88	0.30	-	167,167,167,167	0
9	BMA	G	2622	11/12	0.79	0.30	-	193,211,226,228	0
8	NAG	G	1601	14/15	0.84	0.20	-	208,221,233,240	0
8	NAG	B	6370	14/15	0.85	0.19	-	238,256,268,270	0
10	MAN	G	3634	11/12	0.77	0.16	-	227,227,227,227	0
8	NAG	G	3390	14/15	0.64	0.42	-	221,239,246,251	0
8	NAG	G	2761	14/15	0.65	0.40	-	204,214,231,234	0
8	NAG	G	3014	14/15	0.70	0.25	-	223,223,223,223	0
11	GAL	G	1567	11/12	0.63	0.27	-	278,278,278,278	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	G	1974	14/15	0.70	0.38	-	284,297,302,304	0
8	NAG	B	6371	14/15	0.85	0.19	-	246,246,246,246	0
8	NAG	G	3631	14/15	0.75	0.36	-	227,233,241,245	0
8	NAG	G	1562	14/15	0.73	0.23	-	179,199,212,212	0
8	NAG	G	3861	14/15	0.94	0.22	-	180,196,217,222	0
10	MAN	G	3635	11/12	0.70	0.20	-	218,218,218,218	0
9	BMA	G	3923	11/12	0.78	0.24	-	227,234,238,243	0
10	MAN	G	3326	11/12	0.83	0.29	-	186,188,197,203	0
10	MAN	G	2764	11/12	0.83	0.18	-	302,302,302,302	0
8	NAG	G	1566	14/15	0.81	0.18	-	273,273,273,273	0
7	FUC	G	3920	10/11	0.71	0.33	-	250,255,265,273	0
8	NAG	G	2762	14/15	0.51	0.40	-	226,246,249,249	0

6.5 Other polymers [i](#)

There are no such residues in this entry.