



# Full wwPDB X-ray Structure Validation 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 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

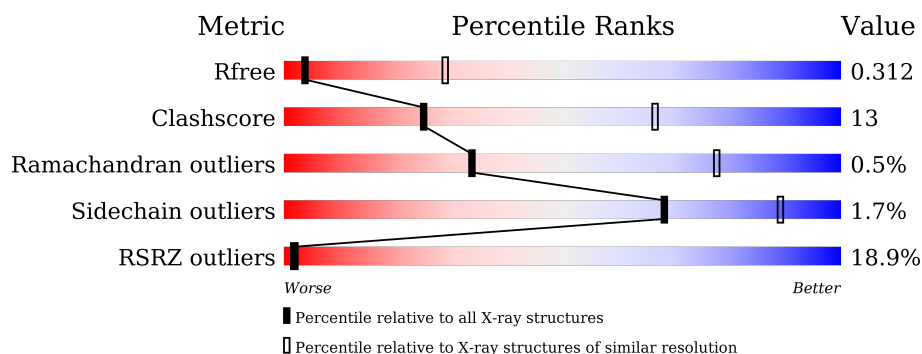
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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  $\geq 3$ , 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>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>.</div> </div>
4	L	214	<div> <div>24%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
5	D	232	<div> <div>34%</div> <div>62%</div> <div>35%</div> <div>..</div> </div>
6	E	214	<div> <div>34%</div> <div>71%</div> <div>26%</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
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			

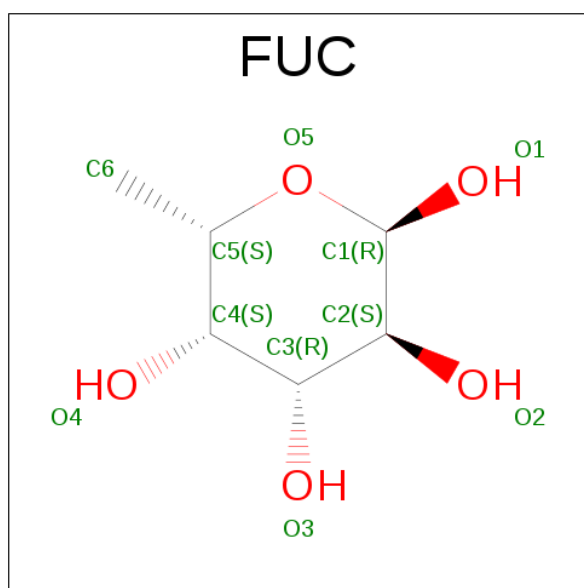
- Molecule 5 is a protein called IOMA Heavy Chain.

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.

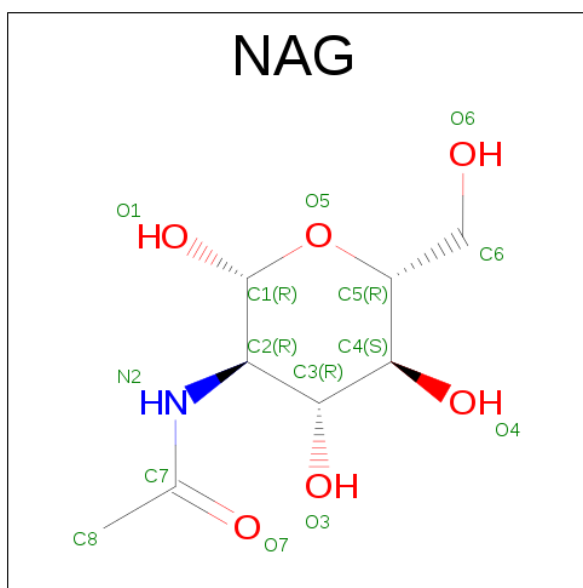
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: 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	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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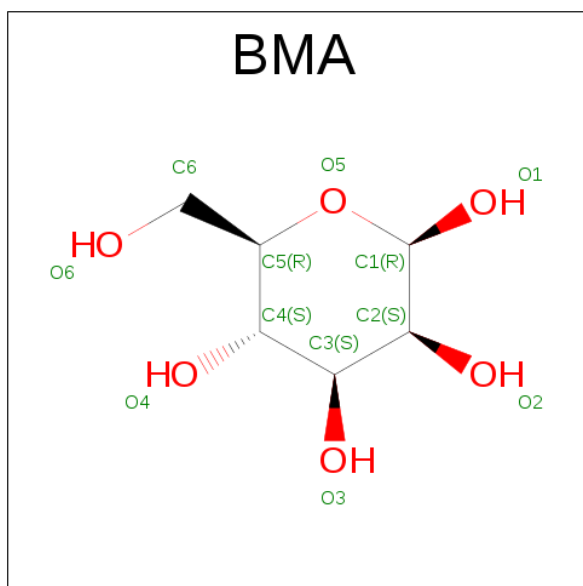
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	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		

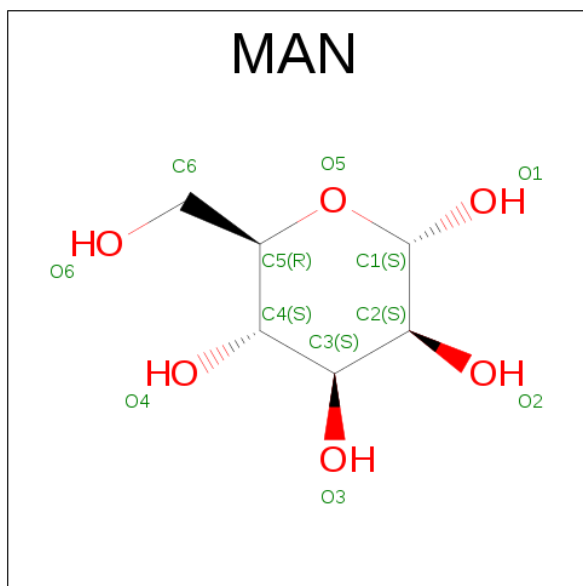
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C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

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

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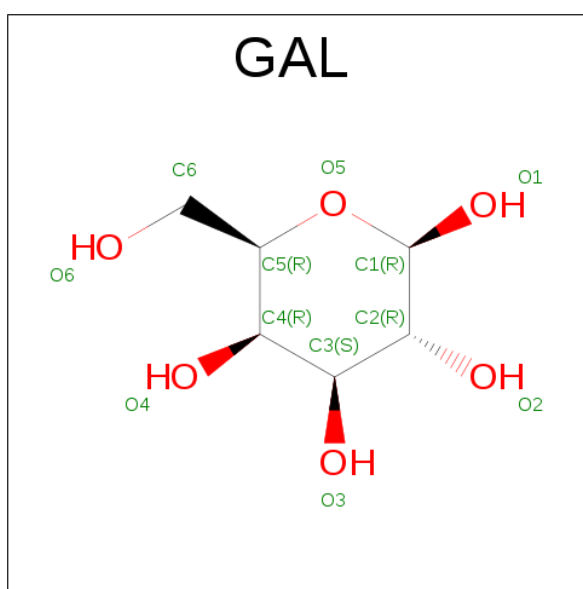
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	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: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

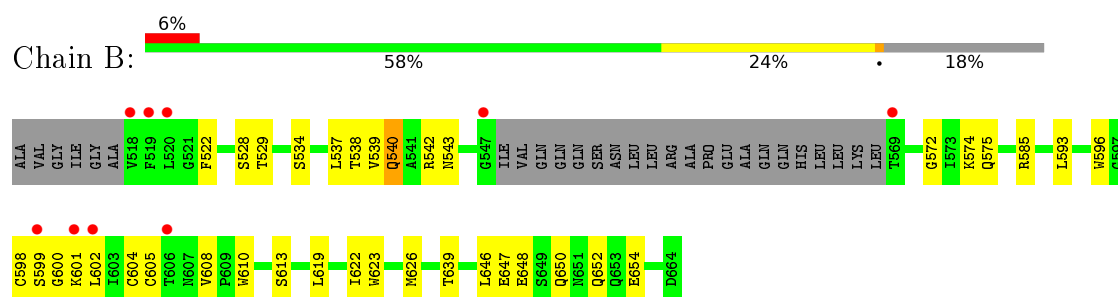


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		
11	G	1	Total	C	O	0	0
			11	6	5		

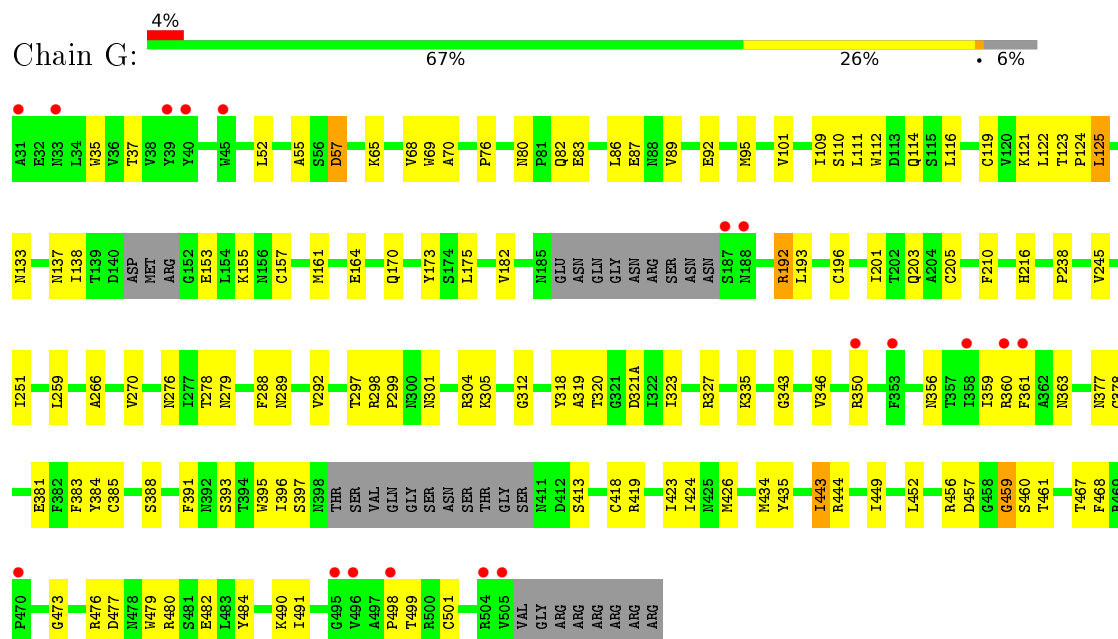
### 3 Residue-property plots

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.

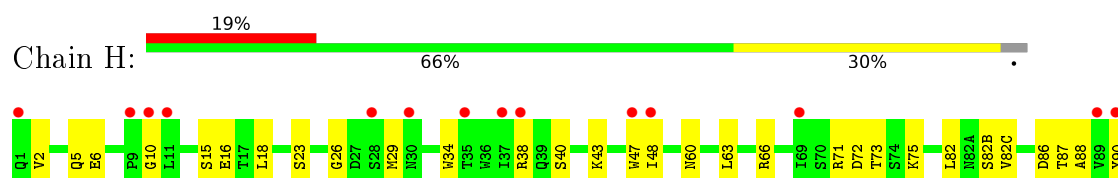
#### • Molecule 1: Envelope glycoprotein gp160

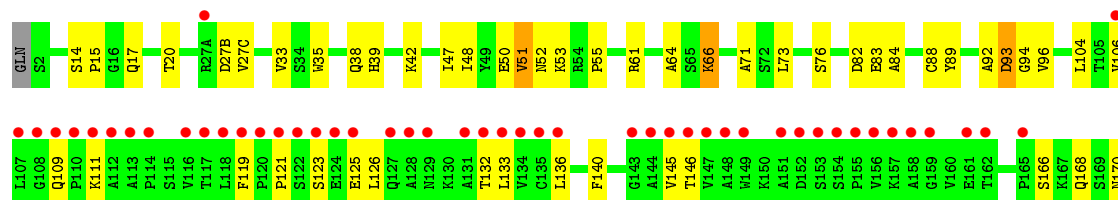


#### • Molecule 2: Envelope glycoprotein gp160



#### • Molecule 3: 10-1074 Heavy Chain





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, $\alpha$ , $\beta$ , $\gamma$	217.26 Å   217.26 Å   154.94 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.49 Å)	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 <sup>2</sup> )	112.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 155.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	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 <sup>2</sup> )	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.*

<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: 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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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.

All (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
8:G:1566:NAG:H81	8:G:1569:NAG:H82	1.71	0.73
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.71	0.72
5:D:96:MET:HG3	5:D:100(H):GLY:HA3	1.69	0.72
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.72	0.71
2:G:95:MET:HB3	2:G:484:TYR:HA	1.73	0.71
1:B:605:CYS:HA	2:G:37:THR:HG22	1.74	0.70
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.26	0.68
5:D:87:THR:HG23	5:D:110:THR:HA	1.76	0.68
6:E:27(B):ASP:HB3	6:E:92:ALA:HB2	1.76	0.66
2:G:350:ARG:NH2	2:G:396:ILE:O	2.28	0.66
4:L:83:GLU:HG2	4:L:106:VAL:H	1.61	0.66
5:D:60:PRO:HG2	5:D:63:PHE:HD2	1.61	0.66
3:H:88:ALA:HB3	3:H:90:TYR:HE1	1.61	0.65
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.61	0.65
8:G:1600:NAG:H61	8:G:1601:NAG:H82	1.79	0.65
2:G:473:GLY:O	5:D:54:ARG:NH1	2.30	0.65
3:H:15:SER:HA	3:H:82(B):SER:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:298:ARG:HB3	2:G:443:ILE:HB	1.80	0.64
5:D:12:LYS:HG3	5:D:18:VAL:HG21	1.80	0.64
10:G:3635:MAN:H5	5:D:82(B):ARG:NH2	2.06	0.63
4:L:39:ARG:NH1	4:L:83:GLU:O	2.30	0.63
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.28	0.62
9:G:3632:BMA:H3	10:G:3633:MAN:H5	1.81	0.62
2:G:460:SER:OG	2:G:461:THR:N	2.33	0.62
2:G:35:TRP:O	2:G:498:PRO:HA	1.99	0.62
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.23	0.62
6:E:133:LEU:HD12	6:E:179:LEU:HD23	1.83	0.61
5:D:72:ASP:OD1	5:D:74:SER:OG	2.16	0.61
2:G:321(A):ASP:HB2	7:G:1560:FUC:C6	2.30	0.61
4:L:83:GLU:OE2	4:L:167:LYS:NZ	2.26	0.61
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.81	0.61
5:D:32:TYR:HB3	5:D:94:ARG:HD2	1.82	0.60
2:G:321(A):ASP:HB2	7:G:1560:FUC:H61	1.82	0.60
10:G:3328:MAN:O3	4:L:51:ASN:ND2	2.33	0.60
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.84	0.60
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.82	0.60
5:D:60:PRO:HD2	5:D:63:PHE:HB2	1.83	0.60
1:B:613:SER:HB2	7:B:6110:FUC:H5	1.83	0.59
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.34	0.59
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.82	0.59
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.34	0.59
6:E:66:LYS:HA	6:E:71:ALA:HA	1.84	0.59
2:G:192:ARG:NH1	2:G:193:LEU:O	2.35	0.59
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.84	0.59
2:G:499:THR:HG23	2:G:501:CYS:H	1.68	0.59
2:G:456:ARG:HG2	2:G:457:ASP:H	1.68	0.59
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.85	0.58
5:D:2:VAL:HG11	5:D:94:ARG:HH12	1.68	0.58
6:E:92:ALA:O	6:E:94:GLY:N	2.29	0.58
2:G:83:GLU:HG3	2:G:245:VAL:HG22	1.86	0.58
2:G:259:LEU:HD23	2:G:452:LEU:HD21	1.84	0.58
2:G:182:VAL:HG23	2:G:192:ARG:HD3	1.84	0.58
3:H:200:HIS:HB3	3:H:205:THR:HB	1.85	0.58
3:H:6:GLU:N	3:H:6:GLU:OE1	2.36	0.58
2:G:292:VAL:HB	2:G:449:ILE:HB	1.85	0.58
3:H:10:GLY:HA3	3:H:202:PRO:HG3	1.85	0.58
9:G:2763:BMA:H2	10:G:2764:MAN:H5	1.85	0.58
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.85	0.57
2:G:70:ALA:HA	2:G:111:LEU:HD21	1.86	0.57
2:G:363:ASN:HB3	2:G:388:SER:HA	1.87	0.57
5:D:36:TRP:HB2	5:D:69:MET:HE1	1.85	0.57
1:B:598:CYS:C	1:B:600:GLY:H	2.08	0.57
1:B:648:GLU:O	1:B:652:GLN:HB3	2.05	0.57
10:G:1564:MAN:O3	8:G:1565:NAG:O5	2.20	0.57
2:G:304:ARG:HD3	2:G:318:TYR:HB3	1.85	0.57
2:G:424:ILE:HG22	2:G:426:MET:H	1.69	0.57
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.69	0.57
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.87	0.56
3:H:100(D):VAL:HG22	3:H:100(G):PHE:H	1.71	0.56
4:L:19:ALA:HB3	4:L:75:ILE:HB	1.88	0.56
2:G:266:ALA:N	2:G:288:PHE:O	2.27	0.56
6:E:61:ARG:NH1	6:E:82:ASP:OD2	2.39	0.56
5:D:100(E):PRO:HB3	5:D:100(G):ARG:NH1	2.21	0.55
5:D:46:GLU:HB3	5:D:63:PHE:HZ	1.72	0.55
5:D:146:PHE:H	5:D:200:HIS:CE1	2.25	0.55
4:L:163:THR:HG1	4:L:176:SER:H	1.55	0.55
3:H:117:LYS:HD3	3:H:175:LEU:HD22	1.88	0.54
4:L:19:ALA:N	4:L:75:ILE:O	2.28	0.54
5:D:139:GLY:HA2	5:D:154:TRP:HH2	1.72	0.54
5:D:23:THR:HG22	5:D:77:ILE:HG23	1.89	0.54
2:G:335:LYS:H	2:G:413:SER:HA	1.72	0.54
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.90	0.54
5:D:38:ARG:HD3	5:D:63:PHE:HE1	1.72	0.54
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.43	0.54
2:G:384:TYR:O	2:G:419:ARG:N	2.40	0.54
2:G:69:TRP:CG	2:G:70:ALA:N	2.75	0.53
5:D:186:SER:HA	5:D:189:LEU:HG	1.91	0.53
5:D:60:PRO:O	5:D:64:ARG:HB2	2.09	0.53
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.90	0.53
4:L:94:ARG:HH21	4:L:94:ARG:HB3	1.73	0.53
3:H:94:THR:OG1	3:H:101:ASP:OD1	2.27	0.53
2:G:161:MET:N	2:G:170:GLN:O	2.30	0.52
4:L:28:LEU:HA	4:L:67:PHE:HZ	1.75	0.52
3:H:72:ASP:HB3	3:H:75:LYS:HB2	1.91	0.52
6:E:145:VAL:HG12	6:E:146:THR:N	2.25	0.52
2:G:476:ARG:HA	2:G:479:TRP:CD1	2.45	0.52
5:D:150:VAL:HB	5:D:178:LEU:HD21	1.91	0.52
6:E:166:SER:O	6:E:168:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:MET:O	2:G:170:GLN:N	2.36	0.52
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.92	0.52
5:D:38:ARG:HD3	5:D:63:PHE:CE1	2.45	0.52
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.90	0.52
6:E:47:ILE:O	6:E:55:PRO:HD2	2.10	0.52
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.50	0.52
4:L:39:ARG:HB2	4:L:42:GLN:HB2	1.92	0.51
2:G:133:ASN:OD1	2:G:155:LYS:NZ	2.41	0.51
2:G:101:VAL:HG13	2:G:479:TRP:HB2	1.92	0.51
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.93	0.51
4:L:116:VAL:HG22	4:L:137:ILE:HG23	1.92	0.51
2:G:385:CYS:HA	2:G:418:CYS:HA	1.91	0.51
3:H:142:VAL:HB	3:H:178:LEU:HG	1.92	0.51
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.93	0.51
5:D:24:ALA:HB1	5:D:27:TYR:HE1	1.76	0.50
5:D:99:SER:OG	5:D:100(B):ASP:O	2.29	0.50
2:G:276:ASN:OD1	2:G:278:THR:OG1	2.29	0.50
6:E:92:ALA:C	6:E:94:GLY:H	2.11	0.50
1:B:538:THR:O	1:B:542:ARG:NH1	2.45	0.50
6:E:83:GLU:HG3	6:E:104:LEU:O	2.12	0.50
3:H:38:ARG:HH12	3:H:86:ASP:HA	1.75	0.50
6:E:61:ARG:HB3	6:E:76:SER:O	2.11	0.50
2:G:210:PHE:HB2	2:G:377:ASN:ND2	2.26	0.50
6:E:145:VAL:HG12	6:E:146:THR:H	1.76	0.50
8:G:3321:NAG:H2	3:H:100(D):VAL:HA	1.93	0.50
5:D:38:ARG:HB3	5:D:90:TYR:CD2	2.47	0.50
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.93	0.49
5:D:93:ALA:HB1	5:D:100(I):MET:HB3	1.94	0.49
2:G:305:LYS:O	2:G:319:ALA:N	2.35	0.49
2:G:116:LEU:HD21	2:G:434:MET:HG3	1.94	0.49
3:H:40:SER:HB3	3:H:43:LYS:HD2	1.94	0.49
4:L:20:ARG:HA	4:L:73:LEU:O	2.12	0.49
1:B:608:VAL:HG21	1:B:646:LEU:HD23	1.94	0.49
5:D:94:ARG:O	5:D:100(I):MET:HA	2.12	0.49
2:G:201:ILE:HD13	2:G:423:ILE:HG23	1.94	0.49
3:H:5:GLN:O	3:H:23:SER:N	2.41	0.49
5:D:10:GLN:HB3	5:D:12:LYS:NZ	2.28	0.49
6:E:170:ASN:O	6:E:171:ASN:HB2	2.13	0.49
9:G:1972:BMA:O5	10:G:1976:MAN:H5	2.12	0.49
4:L:39:ARG:HD2	4:L:84:ALA:HB2	1.94	0.49
3:H:125:ALA:HB3	3:H:214:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.48	0.49
5:D:38:ARG:NH1	5:D:85:ASP:O	2.41	0.49
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.78	0.48
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.77	0.48
3:H:100(H):GLY:HA2	3:H:100(J):PHE:CE2	2.48	0.48
3:H:171:GLN:NE2	3:H:177:SER:OG	2.45	0.48
5:D:72:ASP:O	5:D:76:GLU:N	2.45	0.48
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.78	0.48
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.48	0.48
4:L:66(B):ILE:O	4:L:66(C):ASN:HB2	2.13	0.48
5:D:58:LYS:HE3	5:D:58:LYS:HB2	1.75	0.48
2:G:298:ARG:NH1	2:G:381:GLU:HG3	2.28	0.48
10:G:3327:MAN:O6	3:H:100:ARG:NH2	2.46	0.48
2:G:57:ASP:O	2:G:76:PRO:HA	2.13	0.48
4:L:34:GLN:HB3	4:L:36:TYR:CE2	2.49	0.48
1:B:622:ILE:O	1:B:626:MET:HB2	2.13	0.47
5:D:86:ASP:O	5:D:90:TYR:OH	2.30	0.47
8:G:1970:NAG:O3	8:G:1971:NAG:N2	2.46	0.47
3:H:168:ALA:HB2	3:H:178:LEU:HB3	1.96	0.47
1:B:539:VAL:HG22	1:B:542:ARG:HH22	1.79	0.47
6:E:47:ILE:HG22	6:E:48:ILE:HG12	1.96	0.47
6:E:39:HIS:HD2	6:E:84:ALA:HB2	1.79	0.47
5:D:145:TYR:HE1	5:D:148:GLU:HA	1.78	0.47
6:E:123:SER:HA	6:E:126:LEU:HB2	1.96	0.47
4:L:111:LYS:HG3	4:L:198:HIS:HE1	1.78	0.47
3:H:47:TRP:HD1	3:H:48:ILE:H	1.63	0.47
5:D:146:PHE:H	5:D:200:HIS:HE1	1.61	0.47
5:D:47:TRP:CE3	5:D:60:PRO:HG3	2.49	0.47
5:D:46:GLU:HB3	5:D:63:PHE:CZ	2.50	0.47
2:G:137:ASN:HB2	4:L:95(A):GLY:HA2	1.97	0.47
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.50	0.47
2:G:396:ILE:HG22	2:G:397:SER:H	1.80	0.47
1:B:522:PHE:CE1	1:B:543:ASN:HB2	2.50	0.46
1:B:522:PHE:CE1	1:B:540:GLN:HA	2.50	0.46
5:D:100(C):TRP:O	5:D:100(D):SER:HB2	2.15	0.46
2:G:259:LEU:HD22	2:G:449:ILE:HG21	1.97	0.46
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.97	0.46
6:E:38:GLN:O	6:E:84:ALA:HB1	2.15	0.46
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.79	0.46
2:G:298:ARG:CB	2:G:443:ILE:HB	2.43	0.46
1:B:650:GLN:NE2	1:B:654:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LYS:HG3	2:G:52:LEU:O	2.16	0.46
10:G:3634:MAN:O2	5:D:82(B):ARG:NH2	2.49	0.46
4:L:112:ALA:HB3	4:L:140:PHE:HA	1.97	0.46
7:G:1560:FUC:O2	8:G:1562:NAG:H4	2.16	0.46
4:L:54:ARG:HG2	4:L:58:ILE:HB	1.98	0.46
9:G:3632:BMA:H3	10:G:3633:MAN:H3	1.96	0.46
3:H:66:ARG:HD2	3:H:82(B):SER:HB2	1.98	0.46
8:G:2340:NAG:H62	8:G:2341:NAG:C7	2.46	0.45
6:E:33:VAL:HB	6:E:51:VAL:HG22	1.98	0.45
4:L:49:TYR:O	4:L:53:ASP:HB2	2.15	0.45
2:G:251:ILE:HG23	2:G:482:GLU:HG3	1.97	0.45
2:G:301:ASN:HB3	2:G:323:ILE:HB	1.98	0.45
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.82	0.45
4:L:116:VAL:O	4:L:205:LYS:HE3	2.16	0.45
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.51	0.45
2:G:119:CYS:SG	2:G:205:CYS:N	2.87	0.45
6:E:27(B):ASP:OD1	6:E:27(C):VAL:N	2.44	0.45
8:G:1970:NAG:O3	8:G:1971:NAG:C7	2.65	0.45
5:D:96:MET:HG2	5:D:101:VAL:CG2	2.47	0.45
2:G:361:PHE:HB3	2:G:391:PHE:HB3	1.99	0.45
5:D:181:VAL:HG12	6:E:136:LEU:HD13	1.99	0.45
3:H:71:ARG:HH21	3:H:73:THR:HG22	1.80	0.45
3:H:87:THR:OG1	3:H:111:VAL:N	2.48	0.45
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.98	0.45
5:D:143:LYS:HG2	5:D:144:ASP:H	1.82	0.45
2:G:452:LEU:HA	2:G:452:LEU:HD23	1.85	0.45
2:G:65:LYS:HB2	2:G:68:VAL:HG13	1.99	0.45
2:G:155:LYS:O	2:G:175:LEU:HA	2.17	0.44
2:G:270:VAL:HG12	2:G:289:ASN:H	1.82	0.44
2:G:122:LEU:O	2:G:125:LEU:HB2	2.18	0.44
3:H:165:THR:HA	3:H:180:SER:HA	1.99	0.44
5:D:126:PRO:HD3	5:D:138:LEU:HB3	1.99	0.44
5:D:18:VAL:HB	5:D:82(C):LEU:HD11	1.99	0.44
5:D:6:GLU:OE2	5:D:92:CYS:N	2.51	0.44
6:E:52:ASN:HB3	6:E:64:ALA:O	2.17	0.44
4:L:92:ASP:OD1	4:L:95:SER:N	2.42	0.44
4:L:67:PHE:HB3	4:L:68:GLY:H	1.47	0.44
6:E:111:LYS:NZ	6:E:199:GLU:OE2	2.37	0.44
3:H:87:THR:HG23	3:H:110:THR:HA	2.00	0.44
5:D:100(C):TRP:HB3	5:D:100(D):SER:O	2.18	0.44
5:D:119:PRO:HG3	5:D:200:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:36:TRP:HB2	5:D:69:MET:CE	2.47	0.44
2:G:384:TYR:N	2:G:419:ARG:O	2.47	0.44
2:G:164:GLU:HA	2:G:312:GLY:O	2.18	0.43
9:G:1972:BMA:H3	10:G:1973:MAN:H5	1.99	0.43
1:B:572:GLY:O	1:B:575:GLN:NE2	2.52	0.43
9:G:3862:BMA:H61	10:G:3864:MAN:H3	1.99	0.43
2:G:359:ILE:O	2:G:395:TRP:N	2.49	0.43
5:D:38:ARG:HH12	5:D:86:ASP:HA	1.84	0.43
6:E:125:GLU:OE2	6:E:132:THR:OG1	2.31	0.43
6:E:20:THR:HA	6:E:73:LEU:O	2.18	0.43
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.53	0.43
2:G:360:ARG:NH2	2:G:467:THR:OG1	2.51	0.43
3:H:60:ASN:HB3	3:H:63:LEU:HD13	1.99	0.43
6:E:197:THR:HA	6:E:202:THR:HA	2.00	0.43
3:H:6:GLU:HG3	3:H:92:CYS:SG	2.58	0.43
1:B:593:LEU:HD21	1:B:601:LYS:HA	2.01	0.43
2:G:343:GLY:HA2	2:G:346:VAL:HG12	2.00	0.43
3:H:98:GLY:N	3:H:100(M):TYR:O	2.42	0.43
3:H:88:ALA:HB3	3:H:90:TYR:CE1	2.49	0.43
2:G:109:ILE:O	2:G:112:TRP:HB3	2.19	0.42
2:G:175:LEU:O	2:G:320:THR:OG1	2.36	0.42
9:G:3632:BMA:H2	10:G:3633:MAN:H3	2.00	0.42
1:B:585:ARG:HH22	2:G:490:LYS:HD2	1.85	0.42
1:B:646:LEU:O	1:B:650:GLN:HB2	2.19	0.42
1:B:585:ARG:NH2	2:G:491:ILE:O	2.43	0.42
1:B:528:SER:HA	8:G:880:NAG:O7	2.19	0.42
2:G:361:PHE:CD2	2:G:393:SER:HB2	2.54	0.42
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.52	0.42
5:D:35:HIS:ND1	5:D:50:TRP:HB3	2.34	0.42
4:L:19:ALA:O	4:L:75:ILE:N	2.37	0.42
5:D:38:ARG:NH1	5:D:86:ASP:HA	2.34	0.42
2:G:157:CYS:O	2:G:173:TYR:HA	2.20	0.42
3:H:189:LEU:HA	3:H:189:LEU:HD23	1.80	0.42
4:L:198:HIS:N	4:L:201:SER:O	2.46	0.42
1:B:598:CYS:C	1:B:600:GLY:N	2.71	0.42
5:D:114:ALA:HB3	5:D:146:PHE:CD2	2.55	0.42
5:D:38:ARG:HB3	5:D:90:TYR:CE2	2.54	0.42
2:G:321(A):ASP:HB2	7:G:1560:FUC:H63	2.01	0.42
2:G:55:ALA:N	2:G:216:HIS:O	2.53	0.42
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.53	0.42
5:D:119:PRO:HD3	5:D:200:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:144:ASP:OD1	3:H:171:GLN:NE2	2.42	0.41
2:G:80:ASN:O	2:G:82:GLN:N	2.53	0.41
5:D:69:MET:HA	5:D:79:TYR:O	2.20	0.41
8:G:3631:NAG:O7	8:G:3860:NAG:O3	2.30	0.41
2:G:456:ARG:HG3	2:G:468:PHE:CE2	2.55	0.41
3:H:117:LYS:HB3	3:H:146:PHE:N	2.36	0.41
5:D:51:ILE:HG12	5:D:69:MET:HB3	2.03	0.41
6:E:121:PRO:HD2	6:E:186:TRP:CH2	2.55	0.41
5:D:126:PRO:HA	6:E:119:PHE:HE1	1.86	0.41
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.56	0.41
3:H:153:SER:OG	3:H:197:ASN:HB2	2.20	0.41
3:H:18:LEU:HB3	3:H:82:LEU:HB3	2.03	0.41
1:B:537:LEU:HB3	1:B:602:LEU:HD22	2.02	0.41
5:D:142:VAL:O	5:D:177:SER:HA	2.21	0.41
4:L:25:ARG:HH22	4:L:90:MET:H	1.68	0.41
1:B:529:THR:HB	1:B:623:TRP:O	2.20	0.41
5:D:139:GLY:HA2	5:D:154:TRP:CH2	2.55	0.41
6:E:35:TRP:CZ3	6:E:88:CYS:HB3	2.55	0.41
5:D:150:VAL:HG11	5:D:198:VAL:HG13	2.02	0.41
5:D:2:VAL:HA	5:D:26:GLY:HA3	2.03	0.41
3:H:29:MET:HA	3:H:34:TRP:CZ2	2.55	0.41
2:G:121:LYS:HB2	2:G:121:LYS:HE3	1.81	0.41
2:G:299:PRO:HG2	2:G:327:ARG:HB2	2.02	0.41
3:H:101:ASP:OD1	3:H:101:ASP:N	2.42	0.41
3:H:162:GLY:O	3:H:182:VAL:HA	2.21	0.41
3:H:169:VAL:HG12	3:H:177:SER:HB2	2.03	0.41
4:L:168:GLN:HB2	4:L:170:ASN:OD1	2.21	0.41
3:H:128:SER:OG	4:L:212:CYS:O	2.38	0.40
4:L:62:PHE:CD2	4:L:75:ILE:HG12	2.56	0.40
6:E:14:SER:HB3	6:E:17:GLN:HG3	2.03	0.40
6:E:89:TYR:CE1	6:E:96:VAL:HG13	2.56	0.40
2:G:65:LYS:HA	2:G:65:LYS:HD3	1.90	0.40
5:D:143:LYS:HE3	5:D:171:GLN:NE2	2.37	0.40
5:D:24:ALA:HB1	5:D:27:TYR:CE1	2.56	0.40
6:E:140:PHE:CE2	6:E:173:TYR:HB2	2.55	0.40
2:G:110:SER:O	2:G:114:GLN:HG2	2.20	0.40
2:G:123:THR:N	2:G:124:PRO:HD2	2.36	0.40
2:G:459:GLY:O	2:G:460:SER:C	2.59	0.40

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

All (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
1	B	599	SER
6	E	51	VAL

### 5.3.2 Protein sidechains [i](#)

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

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	540	GLN
1	B	604	CYS
1	B	619	LEU
1	B	639	THR
2	G	125	LEU
2	G	192	ARG
2	G	356	ASN
2	G	443	ILE
3	H	100(D)	VAL
3	H	100(E)	VAL
3	H	100(F)	SER
4	L	28	LEU
4	L	94	ARG
5	D	3	GLN
5	D	51	ILE
5	D	71	ARG
5	D	100(G)	ARG
5	D	138	LEU
5	D	140	CYS
6	E	42	LYS
6	E	66	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	650	GLN
4	L	198	HIS

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Mol	Chain	Res	Type
5	D	33	HIS
5	D	39	GLN
5	D	155	ASN
6	E	38	GLN
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 ⓘ

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%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
10	G	3633	MAN	O5-C1	3.18	1.48	1.43

All (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
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
10	G	3864	MAN	O5-C1-C2	-4.11	104.32	110.89
8	G	1970	NAG	O3-C3-C2	-4.05	100.71	109.37
9	G	3012	BMA	O3-C3-C2	-4.02	102.64	110.01
8	G	1970	NAG	O4-C4-C5	-3.95	98.81	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	1972	BMA	O5-C1-C2	-3.90	104.66	110.89
8	G	1561	NAG	O4-C4-C3	-3.89	101.59	110.36
8	B	6370	NAG	O4-C4-C3	-3.88	101.62	110.36
8	G	3631	NAG	O4-C4-C5	-3.81	99.18	109.23
8	G	1971	NAG	O4-C4-C3	-3.64	102.14	110.36
10	G	3633	MAN	O5-C1-C2	-3.52	105.27	110.89
10	G	1973	MAN	O5-C1-C2	-3.51	105.29	110.89
8	G	1971	NAG	O4-C4-C5	-3.35	100.41	109.23
10	G	3328	MAN	O5-C1-C2	-3.07	105.98	110.89
10	G	3328	MAN	O2-C2-C1	-3.03	103.18	109.23
10	G	3636	MAN	C3-C4-C5	-2.98	104.92	110.23
10	G	3324	MAN	C1-C2-C3	-2.92	106.01	109.55
8	G	1600	NAG	O4-C4-C3	-2.92	103.78	110.36
8	G	2621	NAG	O4-C4-C5	-2.89	101.61	109.23
8	G	3631	NAG	O4-C4-C3	-2.78	104.09	110.36
9	G	3632	BMA	O5-C1-C2	-2.73	106.52	110.89
10	G	2764	MAN	O2-C2-C1	-2.73	103.77	109.23
8	G	2762	NAG	O4-C4-C3	-2.69	104.30	110.36
8	G	1561	NAG	C1-O5-C5	-2.64	108.26	112.14
8	G	3321	NAG	O4-C4-C5	-2.62	102.33	109.23
10	G	3013	MAN	O5-C1-C2	-2.60	106.73	110.89
10	G	1976	MAN	O5-C1-C2	-2.56	106.80	110.89
10	G	2626	MAN	O5-C1-C2	-2.55	106.81	110.89
8	G	1330	NAG	O5-C5-C4	-2.55	105.92	110.13
10	G	1973	MAN	O2-C2-C3	-2.53	105.08	110.19
8	G	3630	NAG	O4-C4-C3	-2.53	104.66	110.36
9	G	3862	BMA	O3-C3-C2	-2.52	105.38	110.01
8	G	4481	NAG	O4-C4-C5	-2.50	102.64	109.23
9	G	2763	BMA	C3-C4-C5	-2.48	105.80	110.23
10	G	3634	MAN	O3-C3-C2	-2.48	105.46	110.01
8	G	2340	NAG	O4-C4-C5	-2.46	102.75	109.23
10	G	3324	MAN	O5-C1-C2	-2.46	106.97	110.89
10	G	3328	MAN	O2-C2-C3	-2.45	105.25	110.19
9	G	3322	BMA	O3-C3-C2	-2.41	105.59	110.01
8	G	2762	NAG	O4-C4-C5	-2.40	102.89	109.23
8	G	880	NAG	O4-C4-C3	-2.40	104.94	110.36
8	G	1330	NAG	C4-C3-C2	-2.38	107.65	111.34
8	G	2621	NAG	O4-C4-C3	-2.33	105.11	110.36
8	G	3321	NAG	O4-C4-C3	-2.31	105.16	110.36
10	G	1564	MAN	O2-C2-C1	-2.27	104.70	109.23
9	G	1563	BMA	C6-C5-C4	-2.23	107.40	112.99
10	G	3636	MAN	O5-C1-C2	-2.22	107.35	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	1602	BMA	O3-C3-C2	-2.22	105.94	110.01
8	G	3320	NAG	C2-N2-C7	-2.21	120.22	123.11
9	G	1563	BMA	C2-C3-C4	-2.18	107.24	111.05
8	G	3921	NAG	O4-C4-C3	-2.18	105.44	110.36
10	G	1564	MAN	O5-C1-C2	-2.18	107.42	110.89
8	G	1971	NAG	O3-C3-C2	-2.12	104.84	109.37
8	G	1561	NAG	C3-C4-C5	-2.11	106.46	110.23
10	G	3324	MAN	O2-C2-C3	-2.11	105.93	110.19
8	G	4481	NAG	C2-N2-C7	-2.10	120.38	123.11
10	G	3634	MAN	C2-C3-C4	-2.10	107.39	111.05
10	G	3329	MAN	O5-C1-C2	-2.07	107.58	110.89
10	G	3327	MAN	O5-C1-C2	-2.05	107.62	110.89
8	G	1561	NAG	O4-C4-C5	-2.02	103.91	109.23
10	G	3015	MAN	C2-C3-C4	-2.01	107.54	111.05
8	G	3921	NAG	C6-C5-C4	-2.00	107.97	112.99
8	G	2621	NAG	C2-N2-C7	2.01	125.72	123.11
11	G	1570	GAL	C1-O5-C5	2.02	115.11	112.14
10	G	3634	MAN	O4-C4-C5	2.02	114.56	109.23
10	G	3015	MAN	C1-C2-C3	2.03	112.01	109.55
8	G	1330	NAG	C3-C4-C5	2.07	113.92	110.23
8	G	1561	NAG	O5-C5-C6	2.07	111.77	107.34
8	G	3010	NAG	C1-O5-C5	2.11	115.24	112.14
8	G	3631	NAG	O5-C5-C4	2.11	113.63	110.13
9	G	2763	BMA	C1-C2-C3	2.11	112.11	109.55
9	G	2622	BMA	C1-C2-C3	2.16	112.17	109.55
10	G	2625	MAN	C1-C2-C3	2.17	112.18	109.55
8	G	1561	NAG	C4-C3-C2	2.17	114.71	111.34
7	G	3920	FUC	O5-C5-C4	2.19	113.37	109.58
8	G	3631	NAG	O5-C5-C6	2.22	112.10	107.34
10	G	3636	MAN	O5-C5-C6	2.29	112.24	107.34
8	G	1569	NAG	C1-O5-C5	2.33	115.57	112.14
8	G	3860	NAG	C1-O5-C5	2.34	115.57	112.14
8	G	1600	NAG	C1-O5-C5	2.41	115.68	112.14
9	G	3012	BMA	C1-C2-C3	2.44	112.51	109.55
10	G	2767	MAN	O5-C5-C6	2.50	112.69	107.34
8	G	1970	NAG	O5-C5-C4	2.51	114.30	110.13
10	G	3015	MAN	O5-C5-C6	2.56	112.81	107.34
7	G	1560	FUC	C1-C2-C3	2.58	112.68	109.55
10	G	3327	MAN	C1-C2-C3	2.72	112.84	109.55
10	G	1973	MAN	C1-O5-C5	2.74	116.17	112.14
8	G	1565	NAG	C1-O5-C5	2.76	116.19	112.14
10	G	3634	MAN	O4-C4-C3	2.78	116.62	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1601	NAG	C8-C7-N2	2.93	121.71	116.10
7	G	3920	FUC	O2-C2-C1	3.02	115.28	109.23
10	G	3635	MAN	C1-C2-C3	3.07	113.27	109.55
10	G	3636	MAN	O3-C3-C4	3.07	117.28	110.36
10	G	3633	MAN	C1-O5-C5	3.18	116.82	112.14
9	G	1972	BMA	O3-C3-C4	3.26	117.70	110.36
8	G	1971	NAG	C4-C3-C2	3.34	116.53	111.34
10	G	1568	MAN	O3-C3-C2	3.41	116.25	110.01
9	G	3862	BMA	C1-C2-C3	3.42	113.69	109.55
10	G	2764	MAN	C1-O5-C5	3.43	117.19	112.14
8	G	1330	NAG	O4-C4-C3	3.63	118.54	110.36
10	G	1564	MAN	O4-C4-C5	3.65	118.85	109.23
8	G	1330	NAG	C1-O5-C5	3.98	117.99	112.14
10	G	3633	MAN	C1-C2-C3	4.00	114.40	109.55
10	G	3636	MAN	O3-C3-C2	4.17	117.66	110.01
9	G	1563	BMA	C1-C2-C3	4.64	115.17	109.55
10	G	3864	MAN	C1-O5-C5	5.02	119.52	112.14
10	G	3634	MAN	C1-C2-C3	5.23	115.89	109.55
9	G	3632	BMA	O3-C3-C2	5.29	119.69	110.01
8	G	1330	NAG	O4-C4-C5	5.73	124.32	109.23
10	G	1568	MAN	O2-C2-C3	5.86	121.98	110.19
10	G	3864	MAN	C1-C2-C3	6.06	116.89	109.55
8	G	1601	NAG	C2-N2-C7	7.04	132.26	123.11

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 ⓘ

### 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%)	0.41	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

All (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
5	D	216	CYS	16.4
6	E	155	PRO	15.4
6	E	108	GLY	14.7
5	D	134	GLY	14.1
5	D	135	THR	13.6
3	H	127	SER	12.8
6	E	134	VAL	12.7
5	D	128	SER	12.6
4	L	145	VAL	11.9
3	H	212	GLU	11.9
5	D	125	ALA	11.7
6	E	117	THR	11.6
5	D	215	SER	11.4
5	D	165	THR	11.2

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Mol	Chain	Res	Type	RSRZ
6	E	133	LEU	11.2
5	D	199	ASN	10.8
6	E	147	VAL	10.8
5	D	140	CYS	10.7
6	E	190	ARG	10.5
4	L	192	TYR	10.5
3	H	136	ALA	10.1
6	E	208	ALA	9.8
4	L	118	LEU	9.1
3	H	138	LEU	9.1
5	D	192	GLN	8.9
3	H	152	VAL	8.7
6	E	136	LEU	8.7
6	E	206	THR	8.6
6	E	107	LEU	8.6
5	D	129	LYS	8.6
4	L	144	ALA	8.4
5	D	130	SER	8.0
5	D	141	LEU	8.0
4	L	132	THR	7.9
5	D	120	SER	7.5
6	E	143	GLY	7.3
5	D	151	THR	7.2
3	H	213	PRO	7.1
3	H	184	VAL	7.1
5	D	191	THR	7.1
3	H	183	THR	7.1
4	L	117	THR	7.0
6	E	135	CYS	7.0
3	H	194	TYR	6.8
6	E	118	LEU	6.8
5	D	147	PRO	6.8
5	D	189	LEU	6.7
5	D	152	VAL	6.7
4	L	206	THR	6.7
5	D	122	PHE	6.6
6	E	119	PHE	6.6
4	L	119	PHE	6.5
6	E	145	VAL	6.5
2	G	187	SER	6.5
5	D	121	VAL	6.4
3	H	179	SER	6.2

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Mol	Chain	Res	Type	RSRZ
5	D	148	GLU	6.2
6	E	127	GLN	6.2
5	D	160	THR	6.0
5	D	197	ASN	6.0
6	E	158	ALA	6.0
5	D	137	ALA	6.0
5	D	202	PRO	5.8
5	D	139	GLY	5.7
3	H	30	ASN	5.6
5	D	208	ASP	5.5
5	D	124	LEU	5.5
3	H	185	PRO	5.4
5	D	183	THR	5.4
5	D	149	PRO	5.4
3	H	126	PRO	5.4
3	H	137	ALA	5.3
4	L	191	SER	5.3
6	E	209	PRO	5.3
2	G	505	VAL	5.3
5	D	166	PHE	5.2
6	E	207	VAL	5.2
3	H	153	SER	5.2
5	D	201	LYS	5.2
3	H	181	VAL	5.2
4	L	207	VAL	5.2
5	D	167	PRO	5.1
5	D	162	GLY	5.1
6	E	148	ALA	5.1
6	E	120	PRO	5.1
6	E	196	VAL	5.0
6	E	113	ALA	5.0
5	D	153	SER	5.0
4	L	156	VAL	5.0
3	H	142	VAL	5.0
5	D	179	SER	5.0
6	E	156	VAL	4.9
6	E	111	LYS	4.9
1	B	518	VAL	4.8
6	E	176	SER	4.8
5	D	136	ALA	4.7
4	L	208	ALA	4.7
6	E	189	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
5	D	132	SER	4.7
5	D	180	SER	4.7
6	E	159	GLY	4.7
5	D	193	THR	4.7
5	D	157	GLY	4.6
6	E	132	THR	4.6
6	E	122	SER	4.6
5	D	206	LYS	4.6
3	H	141	LEU	4.6
6	E	146	THR	4.5
4	L	134	VAL	4.5
6	E	179	LEU	4.5
6	E	109	GLN	4.5
4	L	107	LEU	4.5
6	E	149	TRP	4.5
5	D	178	LEU	4.5
5	D	154	TRP	4.4
1	B	602	LEU	4.3
3	H	214	LYS	4.3
3	H	150	VAL	4.2
5	D	138	LEU	4.2
4	L	133	LEU	4.2
6	E	114	PRO	4.2
3	H	198	VAL	4.1
3	H	124	LEU	4.1
3	H	151	THR	4.1
4	L	186	TRP	4.1
3	H	90	TYR	4.1
2	G	504	ARG	4.1
6	E	194	CYS	4.1
5	D	190	GLY	4.0
6	E	112	ALA	4.0
4	L	199	GLU	4.0
3	H	37	ILE	4.0
6	E	157	LYS	4.0
6	E	154	SER	4.0
6	E	191	SER	4.0
5	D	150	VAL	3.9
6	E	128	ALA	3.9
6	E	144	ALA	3.9
1	B	519	PHE	3.9
6	E	131	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	H	38	ARG	3.8
1	B	547	GLY	3.7
6	E	195	GLN	3.7
5	D	158	ALA	3.6
5	D	155	ASN	3.6
3	H	190	GLY	3.6
4	L	120	PRO	3.6
4	L	150	LYS	3.6
6	E	175	ALA	3.6
4	L	187	LYS	3.6
3	H	28	SER	3.6
2	G	40	TYR	3.6
3	H	211	VAL	3.6
5	D	187	SER	3.5
6	E	205	LYS	3.5
4	L	104	LEU	3.5
2	G	353	PHE	3.5
4	L	210	THR	3.5
6	E	188	SER	3.5
2	G	39	TYR	3.5
3	H	178	LEU	3.4
3	H	215	SER	3.4
3	H	9	PRO	3.4
5	D	173	SER	3.3
5	D	182	VAL	3.2
6	E	171	ASN	3.2
4	L	136	LEU	3.2
4	L	155	PRO	3.2
1	B	520	LEU	3.2
4	L	203	VAL	3.2
5	D	168	ALA	3.1
4	L	154	SER	3.1
4	L	190	ARG	3.1
5	D	214	LYS	3.1
5	D	198	VAL	3.1
6	E	165	PRO	3.0
5	D	172	SER	3.0
3	H	69	ILE	3.0
4	L	100	GLY	3.0
2	G	496	VAL	3.0
4	L	151	ALA	3.0
4	L	137	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
6	E	180	SER	3.0
6	E	193	SER	3.0
5	D	100	SER	3.0
4	L	106	VAL	3.0
2	G	358	ILE	2.9
3	H	210	ARG	2.9
5	D	131	THR	2.9
2	G	360	ARG	2.9
3	H	180	SER	2.9
4	L	149	TRP	2.9
4	L	142	PRO	2.9
3	H	1	GLN	2.9
3	H	128	SER	2.9
2	G	498	PRO	2.8
4	L	121	PRO	2.8
3	H	193	THR	2.8
5	D	170	LEU	2.8
5	D	159	LEU	2.8
4	L	146	THR	2.8
6	E	162	THR	2.8
5	D	164	HIS	2.8
3	H	207	VAL	2.8
4	L	205	LYS	2.8
4	L	20	ARG	2.8
5	D	116	THR	2.8
6	E	187	LYS	2.7
6	E	192	TYR	2.7
6	E	116	VAL	2.7
2	G	361	PHE	2.7
4	L	135	CYS	2.7
4	L	179	LEU	2.7
1	B	569	THR	2.7
4	L	86	TYR	2.7
4	L	64	GLY	2.7
5	D	181	VAL	2.6
1	B	599	SER	2.6
4	L	178	TYR	2.6
5	D	142	VAL	2.6
6	E	152	ASP	2.6
4	L	147	VAL	2.6
2	G	31	ALA	2.6
5	D	213	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
6	E	110	PRO	2.5
6	E	27(A)	ARG	2.5
6	E	124	GLU	2.5
6	E	181	LEU	2.5
6	E	106	VAL	2.5
2	G	45	TRP	2.5
3	H	121	VAL	2.5
6	E	161	GLU	2.5
6	E	178	TYR	2.5
5	D	196	CYS	2.4
5	D	174	GLY	2.4
2	G	188	ASN	2.4
6	E	129	ASN	2.4
5	D	163	VAL	2.3
2	G	33	ASN	2.3
3	H	35	THR	2.3
4	L	36	TYR	2.3
5	D	186	SER	2.3
5	D	175	LEU	2.3
4	L	193	SER	2.3
6	E	123	SER	2.3
3	H	47	TRP	2.3
3	H	89	VAL	2.3
3	H	10	GLY	2.2
5	D	188	SER	2.2
2	G	495	GLY	2.2
3	H	48	ILE	2.2
2	G	350	ARG	2.2
2	G	470	PRO	2.2
5	D	100(B)	ASP	2.2
5	D	100(A)	ALA	2.2
4	L	196	VAL	2.1
4	L	37	GLN	2.1
4	L	143	GLY	2.1
6	E	153	SER	2.1
6	E	200	GLY	2.1
4	L	184	GLU	2.1
6	E	125	GLU	2.1
5	D	207	VAL	2.1
4	L	131	ALA	2.1
1	B	601	LYS	2.1
3	H	11	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	606	THR	2.0
6	E	121	PRO	2.0
6	E	177	SER	2.0
6	E	151	ALA	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
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

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

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

There are no such residues in this entry.