



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 3, 2017 – 02:02 PM EDT

PDB ID : 5FYK  
Title : Crystal Structure at 3.7 Å Resolution of Fully Glycosylated HIV-1 Clade B JR-FL SOSIP.664 Prefusion Env Trimer in Complex with Broadly Neutralizing Antibodies PGT122, 35O22 and VRC01  
Authors : Stewart-Jones, G.B.E.; Zhou, T.; Thomas, P.V.; Kwong, P.D.  
Deposited on : unknown  
Resolution : 3.11 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](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

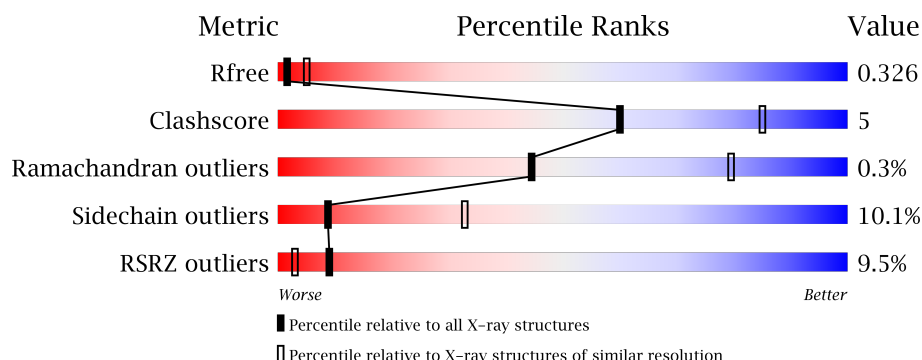
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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.



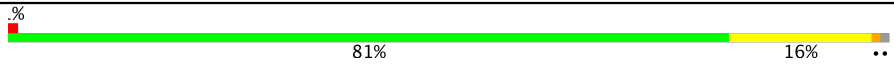
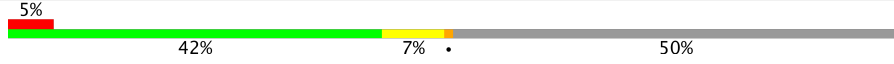

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	161	<div> <div>6%</div> <div> <div>61%</div> <div>27%</div> <div>6%</div> <div>6%</div> </div> </div>
2	D	243	<div> <div>23%</div> <div> <div>90%</div> <div>10%</div> </div> </div>
3	E	216	<div> <div>26%</div> <div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
4	G	475	<div> <div>3%</div> <div> <div>69%</div> <div>23%</div> <div>• 5%</div> </div> </div>
5	H	244	<div> <div>2%</div> <div> <div>82%</div> <div>12%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	L	213	 81% 16%
7	U	240	 42% 7% 50%
7	V	240	 36% 59%

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	1509	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14824 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 JR-FL, GP41 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	151	Total	C	N	O	S	0	0	0
			1195	753	206	228	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q6BC19
B	563	GLU	GLN	conflict	UNP Q6BC19
B	605	CYS	THR	engineered mutation	UNP Q6BC19
B	665	GLY	-	expression tag	UNP Q6BC19
B	666	GLY	-	expression tag	UNP Q6BC19
B	667	LEU	-	expression tag	UNP Q6BC19
B	668	GLU	-	expression tag	UNP Q6BC19
B	669	VAL	-	expression tag	UNP Q6BC19
B	670	LEU	-	expression tag	UNP Q6BC19
B	671	PHE	-	expression tag	UNP Q6BC19
B	672	GLN	-	expression tag	UNP Q6BC19

- Molecule 2 is a protein called 35O22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	243	Total	C	N	O	S	0	0	1
			1833	1165	307	353	8			

- Molecule 3 is a protein called 35O22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called JR-FL, GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total	C	N	O	S	0	0	0
			3571	2248	627	668	28			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	168	LYS	GLU	engineered mutation	UNP Q75760
G	430	ILE	VAL	conflict	UNP Q75760
G	459	CYS	GLY	engineered mutation	UNP Q75760
G	501	CYS	ALA	engineered mutation	UNP Q75760
G	507	GLY	-	expression tag	UNP Q75760
G	508	ARG	-	expression tag	UNP Q75760
G	509	ARG	-	expression tag	UNP Q75760
G	510	ARG	-	expression tag	UNP Q75760
G	511	ARG	-	expression tag	UNP Q75760
G	512	ARG	-	expression tag	UNP Q75760
G	513	ARG	-	expression tag	UNP Q75760

- Molecule 5 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

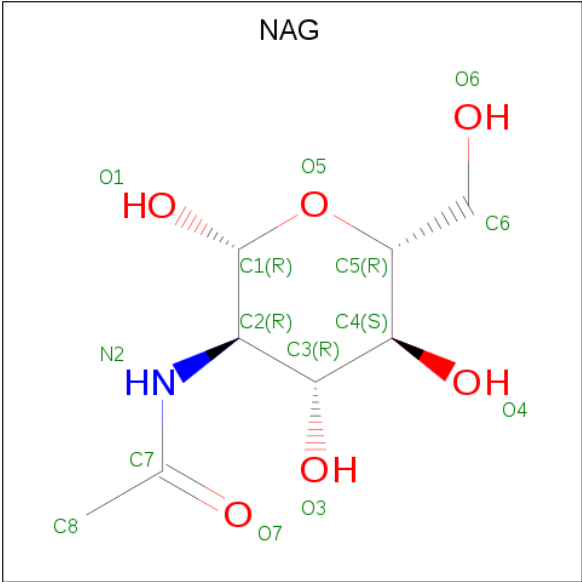
- Molecule 6 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 7 is a protein called VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	119	Total	C	N	O	S	0	0	0
			956	603	173	171	9			
7	V	98	Total	C	N	O	S	0	0	0
			758	479	130	147	2			

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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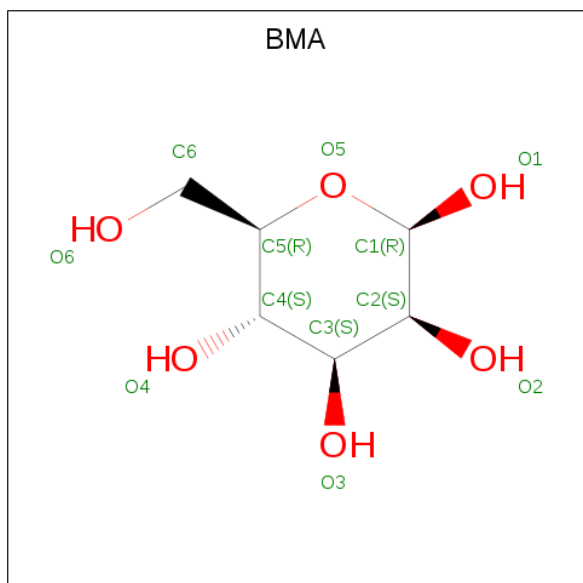
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1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

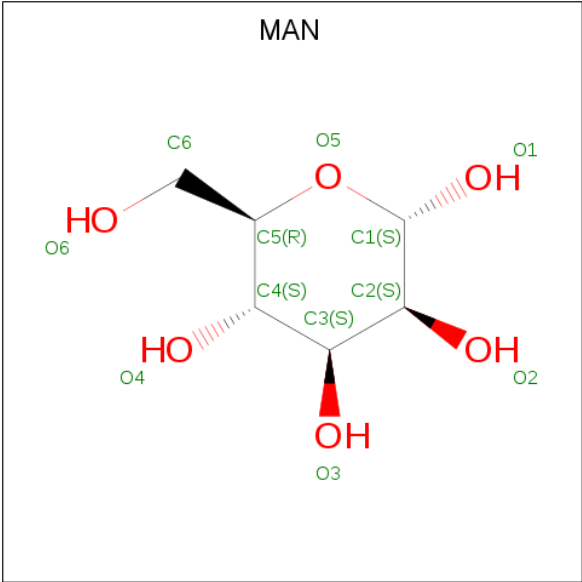
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C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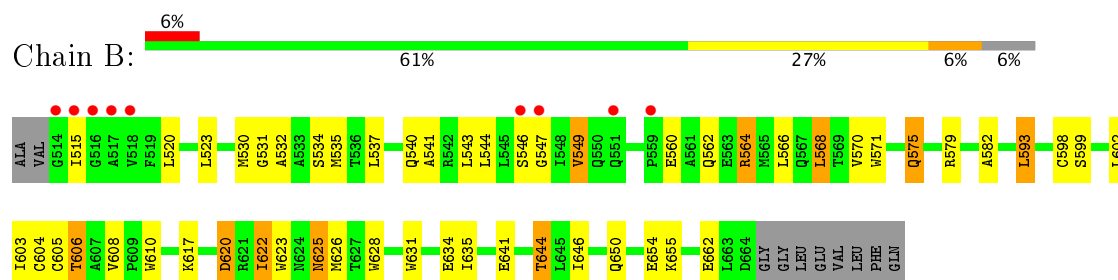
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1	Total	C	O	0	0
			11	6	5		
10	G	1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

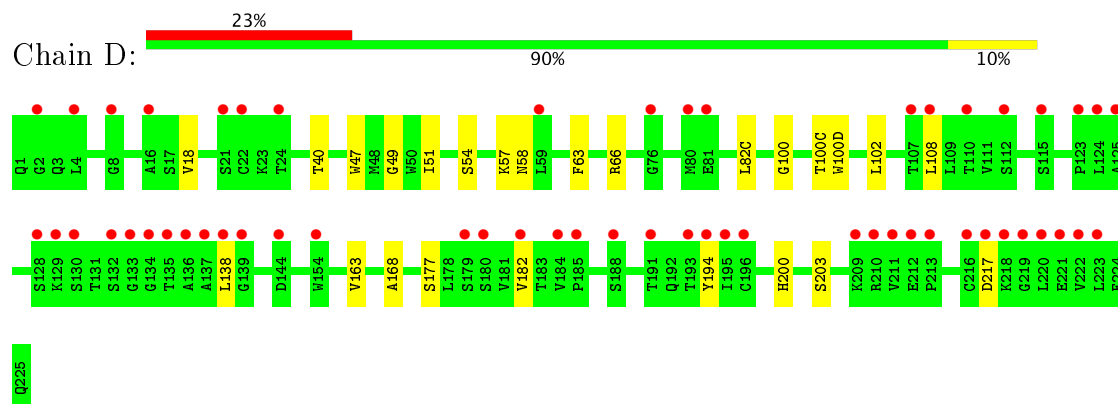
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

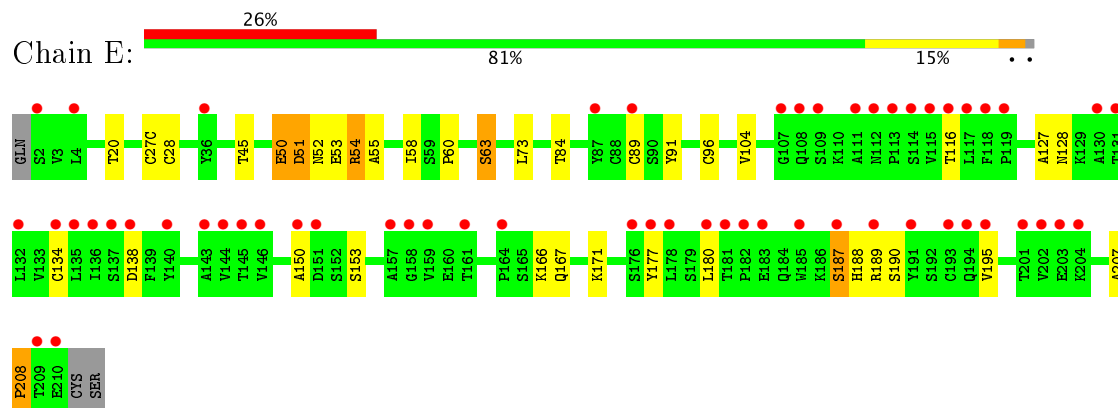
#### • Molecule 1: JR-FL, GP41 ENV ECTODOMAIN



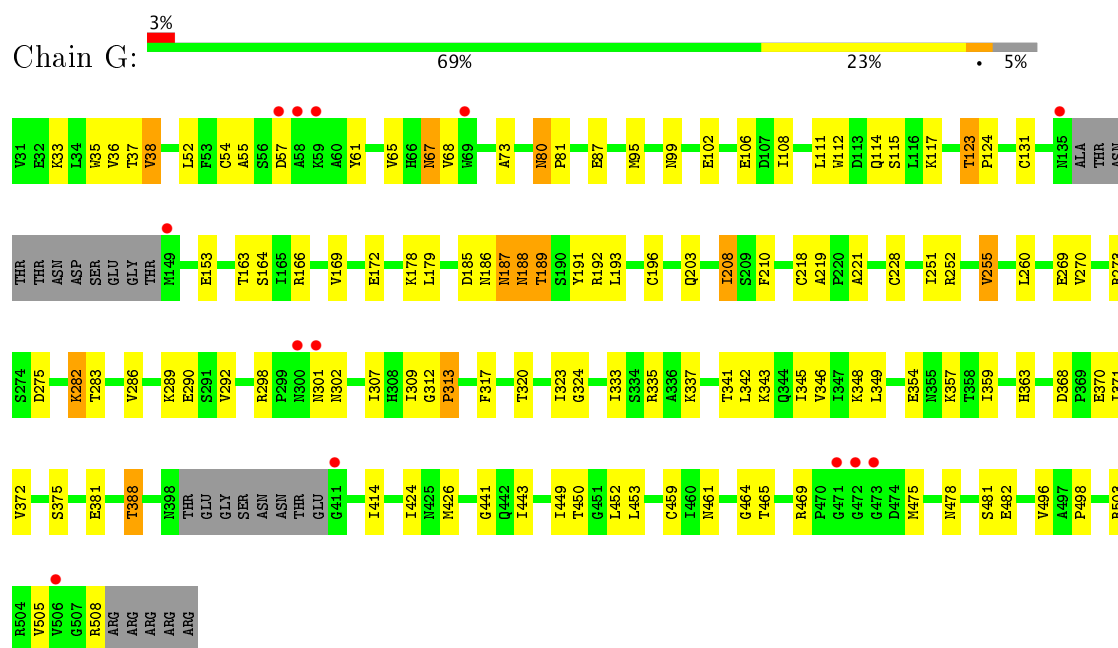
#### • Molecule 2: 35O22

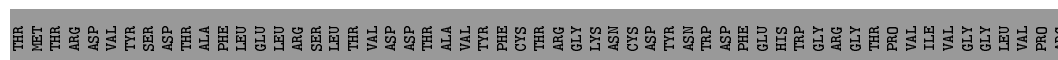


#### • Molecule 3: 35O22



#### • Molecule 4: JR-FL, GP120 ENV ECTODOMAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.78Å 130.78Å 314.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.81 – 3.11 42.81 – 3.11	Depositor EDS
% Data completeness (in resolution range)	58.3 (42.81-3.11) 58.3 (42.81-3.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.246 , 0.303 0.265 , 0.326	Depositor DCC
$R_{free}$ test set	1583 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 122.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	14824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.29	0/1215	0.50	0/1647
2	D	0.25	0/1881	0.43	0/2562
3	E	0.26	0/1658	0.48	0/2266
4	G	0.29	0/3645	0.47	0/4946
5	H	0.24	0/1789	0.47	0/2443
6	L	0.26	0/1632	0.47	0/2236
7	U	0.22	0/981	0.40	0/1328
7	V	0.31	0/778	0.57	1/1058 (0.1%)
All	All	0.27	0/13579	0.47	1/18486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	11	LEU	CB-CG-CD1	5.30	120.02	111.00

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	1195	0	1176	30	0
2	D	1833	0	1806	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1615	0	1541	21	0
4	G	3571	0	3513	60	0
5	H	1742	0	1715	11	0
6	L	1589	0	1530	18	0
7	U	956	0	928	6	0
7	V	758	0	719	4	0
8	B	70	0	63	1	0
8	D	28	0	24	1	0
8	G	490	0	423	8	0
8	H	14	0	13	0	0
8	V	28	0	24	0	0
9	B	11	0	10	0	0
9	D	11	0	8	0	0
9	G	165	0	125	4	0
9	V	11	0	8	0	0
10	D	44	0	38	1	0
10	G	660	0	565	8	0
10	V	33	0	29	0	0
All	All	14824	0	14258	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 155 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)
3:E:50:GLU:HB2	3:E:53:GLU:HB2	1.60	0.83
6:L:106:VAL:HG13	6:L:109:GLN:HE21	1.49	0.76
1:B:546:SER:HA	1:B:549:VAL:HG22	1.72	0.71
1:B:617:LYS:HA	8:B:1668:NAG:H82	1.73	0.71
6:L:106:VAL:O	6:L:109:GLN:NE2	2.28	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	149/161 (92%)	135 (91%)	14 (9%)	0	100	100
2	D	241/243 (99%)	217 (90%)	24 (10%)	0	100	100
3	E	209/216 (97%)	188 (90%)	19 (9%)	2 (1%)	18	57
4	G	445/475 (94%)	397 (89%)	45 (10%)	3 (1%)	25	64
5	H	224/244 (92%)	202 (90%)	22 (10%)	0	100	100
6	L	208/213 (98%)	191 (92%)	17 (8%)	0	100	100
7	U	117/240 (49%)	105 (90%)	12 (10%)	0	100	100
7	V	96/240 (40%)	81 (84%)	15 (16%)	0	100	100
All	All	1689/2032 (83%)	1516 (90%)	168 (10%)	5 (0%)	44	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	187	SER
4	G	313	PRO
4	G	188	ASN
3	E	208	PRO
4	G	65	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	127/134 (95%)	104 (82%)	23 (18%)	2	9
2	D	205/206 (100%)	192 (94%)	13 (6%)	21	56
3	E	186/189 (98%)	171 (92%)	15 (8%)	14	45
4	G	406/427 (95%)	354 (87%)	52 (13%)	5	21
5	H	198/213 (93%)	186 (94%)	12 (6%)	22	58
6	L	178/181 (98%)	161 (90%)	17 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	102/192 (53%)	92 (90%)	10 (10%)	9	35
7	V	81/192 (42%)	73 (90%)	8 (10%)	9	34
All	All	1483/1734 (86%)	1333 (90%)	150 (10%)	9	33

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	187	ASN
4	G	309	ILE
7	U	83	THR
4	G	192	ARG
4	G	260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	188	ASN
6	L	109	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](#)

130 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	$\# Z  > 2$
8	NAG	B	1665	1,8	14,14,15	0.40	0	15,19,21	0.50	0
8	NAG	B	1666	9,8	14,14,15	0.41	0	15,19,21	1.23	3 (20%)
9	BMA	B	1667	8	11,11,12	1.09	1 (9%)	13,15,17	1.40	3 (23%)
8	NAG	B	1668	1	14,14,15	0.43	0	15,19,21	0.69	1 (6%)
8	NAG	B	1669	1	14,14,15	0.34	0	15,19,21	0.56	0
8	NAG	B	1670	1	14,14,15	0.40	0	15,19,21	0.47	0
8	NAG	D	1226	8,4	14,14,15	0.44	0	15,19,21	0.52	0
8	NAG	D	1227	9,8	14,14,15	0.30	0	15,19,21	0.49	0
9	BMA	D	1228	8,10	11,11,12	0.48	0	13,15,17	0.88	0
10	MAN	D	1229	9	11,11,12	0.92	1 (9%)	13,15,17	0.96	1 (7%)
10	MAN	D	1230	9,10	11,11,12	0.57	0	13,15,17	1.24	1 (7%)
10	MAN	D	1231	10	11,11,12	0.78	0	13,15,17	0.97	1 (7%)
10	MAN	D	1232	10	11,11,12	0.58	0	13,15,17	1.18	2 (15%)
8	NAG	G	1509	4	14,14,15	0.39	0	15,19,21	0.47	0
8	NAG	G	1510	8,4	14,14,15	0.43	0	15,19,21	0.59	0
8	NAG	G	1511	9,8	14,14,15	0.38	0	15,19,21	0.88	1 (6%)
9	BMA	G	1512	8,10	11,11,12	1.11	0	13,15,17	1.31	2 (15%)
10	MAN	G	1513	9,10	11,11,12	0.61	0	13,15,17	1.12	2 (15%)
10	MAN	G	1514	9,10	11,11,12	0.93	1 (9%)	13,15,17	1.38	3 (23%)
10	MAN	G	1515	10	11,11,12	0.81	0	13,15,17	1.57	2 (15%)
10	MAN	G	1516	10	11,11,12	0.74	0	13,15,17	0.99	1 (7%)
10	MAN	G	1517	10	11,11,12	0.60	0	13,15,17	1.02	2 (15%)
10	MAN	G	1518	10	11,11,12	0.65	0	13,15,17	1.01	2 (15%)
8	NAG	G	1519	8,4	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
8	NAG	G	1520	9,8	14,14,15	0.27	0	15,19,21	0.59	0
9	BMA	G	1521	8,10	11,11,12	0.66	0	13,15,17	0.79	0
10	MAN	G	1522	9,10	11,11,12	0.90	0	13,15,17	1.77	3 (23%)
10	MAN	G	1523	10	11,11,12	0.83	0	13,15,17	0.97	1 (7%)
10	MAN	G	1524	10	11,11,12	0.71	0	13,15,17	0.98	1 (7%)
10	MAN	G	1525(A)	10	11,11,12	0.94	1 (9%)	13,15,17	1.68	2 (15%)
8	NAG	G	1526	8,4	14,14,15	0.86	1 (7%)	15,19,21	0.77	0
8	NAG	G	1527	9,8	14,14,15	0.39	0	15,19,21	1.02	1 (6%)
9	BMA	G	1528	8,10	11,11,12	0.50	0	13,15,17	1.01	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	G	1529	9,10	11,11,12	0.79	0	13,15,17	1.08	2 (15%)
10	MAN	G	1530	10	11,11,12	0.68	0	13,15,17	1.25	2 (15%)
10	MAN	G	1531	10	11,11,12	0.59	0	13,15,17	1.12	2 (15%)
10	MAN	G	1532(B)	10	11,11,12	0.65	0	13,15,17	1.08	2 (15%)
8	NAG	G	1533	8,4	14,14,15	0.35	0	15,19,21	0.44	0
8	NAG	G	1534	9,8	14,14,15	0.18	0	15,19,21	0.53	0
9	BMA	G	1535	8,10	11,11,12	0.61	0	13,15,17	0.73	0
10	MAN	G	1536	9	11,11,12	0.65	0	13,15,17	0.97	2 (15%)
8	NAG	G	1537	8,4	14,14,15	0.22	0	15,19,21	0.64	0
8	NAG	G	1538	9,8	14,14,15	0.33	0	15,19,21	0.58	0
9	BMA	G	1539	8,10	11,11,12	0.62	0	13,15,17	0.76	1 (7%)
10	MAN	G	1540	9,10	11,11,12	0.62	0	13,15,17	1.27	1 (7%)
10	MAN	G	1541	9,10	11,11,12	1.06	1 (9%)	13,15,17	1.56	2 (15%)
10	MAN	G	1542	10	11,11,12	0.79	1 (9%)	13,15,17	1.51	1 (7%)
10	MAN	G	1543	10	11,11,12	0.70	0	13,15,17	1.09	2 (15%)
10	MAN	G	1544	10	11,11,12	0.69	0	13,15,17	1.08	2 (15%)
10	MAN	G	1545	10	11,11,12	0.87	1 (9%)	13,15,17	1.04	1 (7%)
8	NAG	G	1546	8,4	14,14,15	0.58	0	15,19,21	0.77	0
8	NAG	G	1547	9,8	14,14,15	0.20	0	15,19,21	0.88	0
9	BMA	G	1548	8,10	11,11,12	1.22	1 (9%)	13,15,17	1.93	3 (23%)
10	MAN	G	1549	9,10	11,11,12	0.71	0	13,15,17	1.01	1 (7%)
10	MAN	G	1550	9,10	11,11,12	1.32	2 (18%)	13,15,17	1.30	2 (15%)
10	MAN	G	1551	10	11,11,12	0.88	1 (9%)	13,15,17	1.23	1 (7%)
10	MAN	G	1552	10	11,11,12	0.64	0	13,15,17	1.40	2 (15%)
10	MAN	G	1553	10	11,11,12	0.70	0	13,15,17	0.98	2 (15%)
8	NAG	G	1554	8,4	14,14,15	0.40	0	15,19,21	0.55	0
8	NAG	G	1555	9,8	14,14,15	0.22	0	15,19,21	0.60	0
9	BMA	G	1556	8,10	11,11,12	1.40	1 (9%)	13,15,17	1.02	1 (7%)
10	MAN	G	1557	9	11,11,12	0.75	1 (9%)	13,15,17	1.12	2 (15%)
10	MAN	G	1558	9	11,11,12	0.82	1 (9%)	13,15,17	1.18	2 (15%)
8	NAG	G	1559	8,4	14,14,15	0.64	1 (7%)	15,19,21	0.90	1 (6%)
8	NAG	G	1560	9,8	14,14,15	0.28	0	15,19,21	0.72	0
9	BMA	G	1561	8,10	11,11,12	0.90	1 (9%)	13,15,17	1.02	1 (7%)
10	MAN	G	1562	9,10	11,11,12	0.71	0	13,15,17	1.42	2 (15%)
10	MAN	G	1563	9,10	11,11,12	1.25	1 (9%)	13,15,17	1.21	0
10	MAN	G	1564	10	11,11,12	0.90	0	13,15,17	1.02	1 (7%)
10	MAN	G	1565	10	11,11,12	1.82	4 (36%)	13,15,17	1.26	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	G	1566(A)	10	11,11,12	0.75	0	13,15,17	1.05	1 (7%)
8	NAG	G	1567	8,4	14,14,15	0.31	0	15,19,21	0.53	0
8	NAG	G	1568	9,8	14,14,15	0.20	0	15,19,21	0.78	0
9	BMA	G	1569	8,10	11,11,12	0.91	1 (9%)	13,15,17	0.90	1 (7%)
10	MAN	G	1570	9,10	11,11,12	0.71	1 (9%)	13,15,17	1.47	2 (15%)
10	MAN	G	1571	9,10	11,11,12	0.66	0	13,15,17	1.15	2 (15%)
10	MAN	G	1572	10	11,11,12	0.66	0	13,15,17	0.98	2 (15%)
10	MAN	G	1573	10	11,11,12	0.66	0	13,15,17	1.15	2 (15%)
10	MAN	G	1574	10	11,11,12	0.66	0	13,15,17	1.13	2 (15%)
10	MAN	G	1575	10	11,11,12	0.71	0	13,15,17	1.12	2 (15%)
10	MAN	G	1576(A)	10	11,11,12	0.65	0	13,15,17	0.98	2 (15%)
8	NAG	G	1577	8,4	14,14,15	0.73	1 (7%)	15,19,21	0.80	0
8	NAG	G	1578	9,8	14,14,15	0.18	0	15,19,21	0.44	0
9	BMA	G	1579	8,10	11,11,12	0.93	1 (9%)	13,15,17	1.27	1 (7%)
10	MAN	G	1580	9,10	11,11,12	1.34	2 (18%)	13,15,17	1.99	2 (15%)
10	MAN	G	1581	9,10	11,11,12	0.58	0	13,15,17	1.32	2 (15%)
10	MAN	G	1582	10	11,11,12	0.85	1 (9%)	13,15,17	1.14	2 (15%)
10	MAN	G	1583	10	11,11,12	0.70	0	13,15,17	1.20	2 (15%)
8	NAG	G	1584	8,4	14,14,15	0.23	0	15,19,21	0.45	0
8	NAG	G	1585	9,8	14,14,15	0.27	0	15,19,21	0.82	0
9	BMA	G	1586	8,10	11,11,12	0.80	0	13,15,17	0.98	0
10	MAN	G	1587	9,10	11,11,12	0.63	0	13,15,17	1.17	2 (15%)
10	MAN	G	1588	9,10	11,11,12	0.50	0	13,15,17	1.09	2 (15%)
10	MAN	G	1589	10	11,11,12	0.73	0	13,15,17	1.12	2 (15%)
10	MAN	G	1590	10	11,11,12	0.67	0	13,15,17	1.05	2 (15%)
8	NAG	G	1591	8,4	14,14,15	0.37	0	15,19,21	0.93	2 (13%)
8	NAG	G	1592	9,8	14,14,15	0.48	0	15,19,21	0.78	1 (6%)
9	BMA	G	1593	8,10	11,11,12	1.01	1 (9%)	13,15,17	1.08	1 (7%)
10	MAN	G	1594	9	11,11,12	0.71	0	13,15,17	1.38	2 (15%)
8	NAG	G	1595	8,4	14,14,15	0.33	0	15,19,21	0.71	0
8	NAG	G	1596	9,8	14,14,15	0.56	0	15,19,21	0.78	1 (6%)
9	BMA	G	1597	8,10	11,11,12	0.67	0	13,15,17	0.81	0
10	MAN	G	1598	9	11,11,12	0.75	1 (9%)	13,15,17	1.31	2 (15%)
10	MAN	G	1599	9,10	11,11,12	0.88	0	13,15,17	1.31	2 (15%)
10	MAN	G	1600	10	11,11,12	0.66	0	13,15,17	0.95	1 (7%)
10	MAN	G	1601	10	11,11,12	0.68	0	13,15,17	1.27	2 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	G	1602(B)	10	11,11,12	0.72	0	13,15,17	1.02	2 (15%)
8	NAG	G	1603	8,4	14,14,15	0.38	0	15,19,21	0.60	0
8	NAG	G	1604	9,8	14,14,15	0.44	0	15,19,21	1.43	2 (13%)
9	BMA	G	1605	8,10	11,11,12	0.95	0	13,15,17	1.55	1 (7%)
10	MAN	G	1606	9	11,11,12	0.83	0	13,15,17	0.97	1 (7%)
10	MAN	G	1607	9,10	11,11,12	0.64	0	13,15,17	1.25	2 (15%)
10	MAN	G	1608	10	11,11,12	0.68	0	13,15,17	0.99	2 (15%)
8	NAG	G	1609	8,4	14,14,15	0.25	0	15,19,21	0.46	0
8	NAG	G	1610	8	14,14,15	0.27	0	15,19,21	0.44	0
8	NAG	G	1611	8,4	14,14,15	0.28	0	15,19,21	0.49	0
8	NAG	G	1612	9,8	14,14,15	0.25	0	15,19,21	0.53	0
9	BMA	G	1613	8,10	11,11,12	0.95	0	13,15,17	1.30	2 (15%)
10	MAN	G	1614	9,10	11,11,12	0.71	0	13,15,17	1.57	2 (15%)
10	MAN	G	1615	10	11,11,12	1.94	4 (36%)	13,15,17	1.26	2 (15%)
10	MAN	G	1616(A)	10	11,11,12	0.68	0	13,15,17	1.16	2 (15%)
8	NAG	G	1617	8,4	14,14,15	0.73	1 (7%)	15,19,21	0.78	0
8	NAG	G	1618	8	14,14,15	0.38	0	15,19,21	0.61	0
8	NAG	H	1212	5	14,14,15	0.26	0	15,19,21	0.50	0
8	NAG	V	1107	8,7	14,14,15	0.44	0	15,19,21	0.63	0
8	NAG	V	1108	9,8	14,14,15	0.54	0	15,19,21	1.31	2 (13%)
9	BMA	V	1109	8,10	11,11,12	0.54	0	13,15,17	1.41	1 (7%)
10	MAN	V	1110	9	11,11,12	0.87	0	13,15,17	1.71	2 (15%)
10	MAN	V	1111	9,10	11,11,12	0.96	1 (9%)	13,15,17	1.45	3 (23%)
10	MAN	V	1112	10	11,11,12	0.98	1 (9%)	13,15,17	0.90	1 (7%)

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
8	NAG	B	1665	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1666	9,8	-	0/6/23/26	0/1/1/1
9	BMA	B	1667	8	-	0/2/19/22	0/1/1/1
8	NAG	B	1668	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1669	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1670	1	-	0/6/23/26	0/1/1/1
8	NAG	D	1226	8,4	-	0/6/23/26	0/1/1/1
8	NAG	D	1227	9,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	D	1228	8,10	-	0/2/19/22	0/1/1/1
10	MAN	D	1229	9	-	0/2/19/22	0/1/1/1
10	MAN	D	1230	9,10	-	0/2/19/22	0/1/1/1
10	MAN	D	1231	10	-	0/2/19/22	0/1/1/1
10	MAN	D	1232	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1509	4	-	0/6/23/26	0/1/1/1
8	NAG	G	1510	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1511	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1512	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1513	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1514	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1515	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1516	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1517	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1518	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1519	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1520	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1521	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1522	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1523	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1524	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1525(A)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1526	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1527	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1528	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1529	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1530	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1531	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1532(B)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1533	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1534	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1535	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1536	9	-	0/2/19/22	0/1/1/1
8	NAG	G	1537	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1538	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1539	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1540	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1541	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1542	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1543	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1544	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1545	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	G	1546	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1547	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1548	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1549	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1550	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1551	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1552	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1553	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1554	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1555	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1556	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1557	9	-	0/2/19/22	0/1/1/1
10	MAN	G	1558	9	-	0/2/19/22	0/1/1/1
8	NAG	G	1559	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1560	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1561	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1562	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1563	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1564	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1565	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1566(A)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1567	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1568	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1569	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1570	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1571	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1572	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1573	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1574	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1575	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1576(A)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1577	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1578	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1579	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1580	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1581	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1582	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1583	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1584	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1585	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1586	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1587	9,10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	G	1588	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1589	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1590	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1591	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1592	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1593	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1594	9	-	0/2/19/22	0/1/1/1
8	NAG	G	1595	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1596	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1597	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1598	9	-	0/2/19/22	0/1/1/1
10	MAN	G	1599	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1600	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1601	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1602(B)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1603	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1604	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1605	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1606	9	-	0/2/19/22	0/1/1/1
10	MAN	G	1607	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1608	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1609	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1610	8	-	0/6/23/26	0/1/1/1
8	NAG	G	1611	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1612	9,8	-	0/6/23/26	0/1/1/1
9	BMA	G	1613	8,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1614	9,10	-	0/2/19/22	0/1/1/1
10	MAN	G	1615	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1616(A)	10	-	0/2/19/22	0/1/1/1
8	NAG	G	1617	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	1618	8	-	0/6/23/26	0/1/1/1
8	NAG	H	1212	5	-	0/6/23/26	0/1/1/1
8	NAG	V	1107	8,7	-	0/6/23/26	0/1/1/1
8	NAG	V	1108	9,8	-	0/6/23/26	0/1/1/1
9	BMA	V	1109	8,10	-	0/2/19/22	0/1/1/1
10	MAN	V	1110	9	-	0/2/19/22	0/1/1/1
10	MAN	V	1111	9,10	-	0/2/19/22	0/1/1/1
10	MAN	V	1112	10	-	0/2/19/22	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1526	NAG	O5-C1	-3.11	1.38	1.43
10	G	1615	MAN	O5-C1	-2.93	1.38	1.43
8	G	1577	NAG	O5-C1	-2.59	1.39	1.43
10	D	1229	MAN	O5-C1	-2.42	1.39	1.43
8	G	1617	NAG	O5-C1	-2.39	1.39	1.43

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	1551	MAN	O2-C2-C3	-3.68	102.95	110.17
10	G	1562	MAN	O2-C2-C3	-3.31	103.68	110.17
8	G	1519	NAG	O5-C1-C2	-2.64	107.80	111.47
10	G	1601	MAN	O2-C2-C3	-2.60	105.07	110.17
9	G	1548	BMA	C3-C4-C5	-2.55	105.72	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1668	NAG	1	0
8	D	1226	NAG	1	0
10	D	1229	MAN	1	0
8	G	1533	NAG	1	0
8	G	1534	NAG	1	0
9	G	1539	BMA	1	0
10	G	1541	MAN	1	0
10	G	1550	MAN	1	0
8	G	1554	NAG	1	0
8	G	1555	NAG	1	0
9	G	1556	BMA	1	0
10	G	1557	MAN	1	0
8	G	1559	NAG	2	0
10	G	1572	MAN	1	0
8	G	1577	NAG	1	0
8	G	1578	NAG	1	0
9	G	1579	BMA	2	0
10	G	1580	MAN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	1582	MAN	1	0
10	G	1594	MAN	1	0
8	G	1609	NAG	1	0
8	G	1610	NAG	2	0
8	G	1617	NAG	1	0
8	G	1618	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	95:SER	C	95(A):GLY	N	3.44

## 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, 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	151/161 (93%)	0.29	9 (5%) 23 9	39, 104, 223, 254	0
2	D	243/243 (100%)	1.12	56 (23%) 1 0	133, 213, 281, 315	0
3	E	213/216 (98%)	1.25	57 (26%) 1 0	131, 210, 284, 309	0
4	G	451/475 (94%)	0.11	13 (2%) 52 28	43, 110, 187, 295	0
5	H	228/244 (93%)	-0.03	5 (2%) 62 41	105, 156, 197, 247	0
6	L	210/213 (98%)	-0.17	3 (1%) 75 57	85, 136, 179, 212	0
7	U	119/240 (49%)	0.46	11 (9%) 10 3	130, 167, 232, 248	0
7	V	98/240 (40%)	0.49	9 (9%) 10 3	136, 204, 240, 342	0
All	All	1713/2032 (84%)	0.40	163 (9%) 9 3	39, 154, 264, 342	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	146	VAL	11.0
1	B	514	GLY	10.8
3	E	144	VAL	10.0
2	D	138	LEU	9.6
2	D	221	GLU	8.9

### 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, 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	1509	14/15	0.81	0.42	1.78	135,144,144,146	0
8	NAG	B	1669	14/15	0.87	0.35	1.41	123,136,154,157	0
8	NAG	G	1567	14/15	0.93	0.22	0.64	126,131,134,135	0
8	NAG	D	1227	14/15	0.89	0.19	0.20	101,103,108,112	0
8	NAG	B	1665	14/15	0.75	0.33	0.20	190,199,211,214	0
8	NAG	G	1591	14/15	0.87	0.23	-0.28	144,155,163,169	0
8	NAG	D	1226	14/15	0.94	0.20	-0.42	95,98,101,102	0
9	BMA	D	1228	11/12	0.93	0.17	-0.45	110,116,128,134	0
10	MAN	D	1230	11/12	0.84	0.14	-0.79	137,140,142,143	0
8	NAG	G	1538	14/15	0.88	0.16	-0.94	101,105,113,123	0
8	NAG	G	1537	14/15	0.92	0.16	-0.96	69,75,81,93	0
10	MAN	G	1570	11/12	0.91	0.17	-1.09	101,105,114,122	0
8	NAG	G	1609	14/15	0.85	0.12	-1.15	145,150,154,156	0
10	MAN	G	1572	11/12	0.92	0.15	-1.34	129,132,135,138	0
8	NAG	G	1510	14/15	0.93	0.16	-1.37	97,110,125,135	0
8	NAG	B	1666	14/15	0.82	0.23	-1.45	197,200,201,202	0
8	NAG	G	1554	14/15	0.91	0.16	-1.85	168,170,185,189	0
8	NAG	G	1568	14/15	0.90	0.13	-2.10	106,117,119,122	0
8	NAG	G	1546	14/15	0.87	0.16	-2.64	133,143,150,153	0
9	BMA	G	1548	11/12	0.89	0.07	-	166,168,169,172	0
10	MAN	G	1543	11/12	0.67	0.56	-	196,201,203,203	0
10	MAN	G	1600	11/12	0.82	0.27	-	231,234,234,234	0
8	NAG	G	1547	14/15	0.89	0.18	-	156,161,164,165	0
10	MAN	G	1563	11/12	0.49	0.19	-	190,193,220,221	0
10	MAN	G	1553	11/12	0.82	0.27	-	201,203,204,204	0
8	NAG	G	1519	14/15	0.85	0.12	-	134,146,157,172	0
10	MAN	G	1594	11/12	0.81	0.28	-	214,215,216,216	0
10	MAN	G	1552	11/12	0.86	0.22	-	163,164,164,165	0
10	MAN	G	1606	11/12	0.90	0.31	-	193,194,197,198	0
8	NAG	B	1668	14/15	0.80	0.54	-	147,156,161,162	0
10	MAN	G	1581	11/12	0.71	0.17	-	211,212,215,216	0
10	MAN	G	1601	11/12	0.79	0.42	-	242,248,250,250	0
8	NAG	G	1511	14/15	0.89	0.15	-	148,154,163,172	0
10	MAN	G	1616(A)	11/12	0.82	0.21	-	203,204,205,205	0
10	MAN	G	1599	11/12	0.66	0.23	-	225,235,237,240	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MAN	G	1607	11/12	0.80	0.25	-	198,200,202,203	0
10	MAN	G	1514	11/12	0.76	0.16	-	204,215,219,222	0
10	MAN	D	1231	11/12	0.87	0.22	-	135,137,139,141	0
8	NAG	G	1604	14/15	0.68	0.20	-	189,193,195,197	0
10	MAN	G	1515	11/12	0.84	0.26	-	210,212,217,218	0
10	MAN	G	1558	11/12	0.69	0.39	-	198,201,203,204	0
9	BMA	G	1605	11/12	0.58	0.28	-	198,199,199,200	0
9	BMA	G	1539	11/12	0.93	0.10	-	131,133,154,162	0
10	MAN	D	1229	11/12	0.94	0.19	-	122,125,125,126	0
9	BMA	G	1613	11/12	0.82	0.21	-	167,179,247,247	0
8	NAG	G	1520	14/15	0.77	0.34	-	186,195,198,203	0
10	MAN	G	1573	11/12	0.96	0.07	-	146,148,153,155	0
10	MAN	G	1589	11/12	0.79	0.51	-	257,261,265,265	0
9	BMA	G	1586	11/12	0.80	0.23	-	201,213,232,237	0
10	MAN	G	1551	11/12	0.87	0.40	-	192,197,198,200	0
8	NAG	G	1559	14/15	0.89	0.38	-	177,182,192,202	0
10	MAN	G	1530	11/12	0.63	0.23	-	242,244,247,248	0
8	NAG	G	1534	14/15	0.90	0.15	-	133,140,149,156	0
10	MAN	G	1549	11/12	0.91	0.08	-	172,174,178,185	0
10	MAN	G	1614	11/12	0.85	0.24	-	180,183,191,194	0
10	MAN	V	1111	11/12	0.45	0.47	-	258,261,263,263	0
8	NAG	G	1555	14/15	0.86	0.24	-	171,173,177,180	0
8	NAG	B	1670	14/15	0.36	0.56	-	170,182,187,189	0
8	NAG	H	1212	14/15	0.88	0.22	-	121,132,140,149	0
9	BMA	G	1593	11/12	0.72	0.15	-	187,190,214,215	0
9	BMA	B	1667	11/12	0.77	0.25	-	200,201,204,205	0
8	NAG	V	1108	14/15	0.82	0.28	-	241,247,250,252	0
10	MAN	G	1615	11/12	0.88	0.24	-	195,197,203,203	0
10	MAN	G	1523	11/12	0.73	0.40	-	223,225,227,228	0
8	NAG	G	1577	14/15	0.80	0.33	-	188,193,196,198	0
10	MAN	G	1582	11/12	0.71	0.44	-	214,216,219,219	0
10	MAN	G	1588	11/12	0.89	0.28	-	199,199,200,200	0
8	NAG	G	1618	14/15	0.80	0.30	-	194,199,200,200	0
10	MAN	G	1541	11/12	0.88	0.18	-	170,176,181,189	0
8	NAG	G	1585	14/15	0.84	0.25	-	188,192,200,206	0
10	MAN	G	1522	11/12	0.80	0.22	-	220,221,223,225	0
8	NAG	G	1603	14/15	0.84	0.21	-	183,189,193,193	0
10	MAN	G	1587	11/12	0.84	0.56	-	245,248,250,254	0
10	MAN	G	1574	11/12	0.86	0.15	-	144,146,147,148	0
10	MAN	G	1557	11/12	0.84	0.18	-	194,197,201,204	0
10	MAN	G	1524	11/12	0.78	0.41	-	226,228,229,229	0
10	MAN	G	1564	11/12	0.78	0.26	-	198,199,203,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	BMA	G	1521	11/12	0.72	0.33	-	207,215,218,219	0
10	MAN	G	1598	11/12	0.81	0.50	-	219,226,230,230	0
9	BMA	G	1528	11/12	0.64	0.35	-	230,233,238,240	0
10	MAN	G	1517	11/12	0.89	0.32	-	211,212,214,214	0
9	BMA	G	1556	11/12	0.71	0.30	-	183,195,211,211	0
10	MAN	G	1518	11/12	0.80	0.36	-	217,220,220,220	0
10	MAN	G	1583	11/12	0.77	0.26	-	214,215,217,217	0
9	BMA	G	1535	11/12	0.81	0.20	-	163,166,172,173	0
10	MAN	G	1580	11/12	0.84	0.16	-	206,207,210,212	0
10	MAN	G	1529	11/12	0.65	0.21	-	241,244,248,249	0
10	MAN	G	1566(A)	11/12	0.88	0.33	-	222,223,225,225	0
10	MAN	G	1602(B)	11/12	0.70	0.35	-	244,245,248,249	0
10	MAN	G	1608	11/12	0.70	0.35	-	202,205,206,206	0
10	MAN	V	1110	11/12	0.79	0.18	-	241,242,247,249	0
10	MAN	G	1576(A)	11/12	0.85	0.21	-	157,157,158,158	0
8	NAG	G	1584	14/15	0.83	0.15	-	159,165,172,180	0
10	MAN	G	1590	11/12	0.83	0.48	-	201,203,204,204	0
10	MAN	G	1540	11/12	0.92	0.11	-	144,146,149,151	0
8	NAG	G	1612	14/15	0.86	0.20	-	151,155,159,163	0
8	NAG	G	1533	14/15	0.96	0.16	-	85,91,104,119	0
8	NAG	G	1617	14/15	0.88	0.27	-	160,178,183,188	0
10	MAN	G	1513	11/12	0.92	0.21	-	196,200,206,208	0
9	BMA	G	1561	11/12	0.72	0.15	-	184,188,191,192	0
8	NAG	G	1592	14/15	0.79	0.17	-	178,182,186,189	0
8	NAG	G	1560	14/15	0.77	0.25	-	170,179,181,183	0
8	NAG	G	1527	14/15	0.71	0.29	-	206,212,217,224	0
8	NAG	G	1611	14/15	0.89	0.10	-	113,125,132,141	0
8	NAG	V	1107	14/15	0.83	0.44	-	235,241,244,245	0
8	NAG	G	1526	14/15	0.53	0.26	-	183,195,198,203	0
9	BMA	V	1109	11/12	0.70	0.26	-	252,254,257,258	0
10	MAN	G	1536	11/12	0.73	0.30	-	171,174,174,175	0
10	MAN	G	1516	11/12	0.76	0.25	-	223,224,225,225	0
10	MAN	G	1544	11/12	0.88	0.24	-	177,179,181,181	0
8	NAG	G	1596	14/15	0.86	0.19	-	156,166,175,187	0
10	MAN	G	1545	11/12	0.75	0.47	-	178,184,190,190	0
9	BMA	G	1512	11/12	0.81	0.12	-	181,189,197,200	0
10	MAN	D	1232	11/12	0.87	0.15	-	140,144,145,146	0
9	BMA	G	1579	11/12	0.73	0.18	-	206,208,212,213	0
10	MAN	G	1571	11/12	0.85	0.12	-	134,141,145,148	0
10	MAN	G	1565	11/12	0.84	0.21	-	220,221,245,245	0
10	MAN	G	1542	11/12	0.92	0.17	-	155,162,170,174	0
8	NAG	G	1578	14/15	0.78	0.43	-	203,206,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	G	1595	14/15	0.90	0.30	-	110,117,127,140	0
10	MAN	G	1531	11/12	0.90	0.32	-	242,244,245,245	0
10	MAN	G	1550	11/12	0.89	0.09	-	163,167,172,172	0
8	NAG	G	1610	14/15	0.90	0.21	-	161,163,165,165	0
10	MAN	G	1525(A)	11/12	0.84	0.33	-	226,226,227,228	0
10	MAN	G	1532(B)	11/12	0.84	0.29	-	242,245,248,248	0
9	BMA	G	1569	11/12	0.96	0.14	-	112,117,124,130	0
9	BMA	G	1597	11/12	0.83	0.12	-	199,207,214,220	0
10	MAN	V	1112	11/12	0.40	0.51	-	246,250,254,256	0
10	MAN	G	1575	11/12	0.89	0.22	-	143,151,152,152	0
10	MAN	G	1562	11/12	0.78	0.21	-	193,194,196,197	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.