



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2016 – 05:49 AM EDT

PDB ID : 5D9Q  
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122 and scFv NIH45-46  
Authors : Julien, J.-P.; Stanfield, R.L.; Ward, A.B.; Wilson, I.A.  
Deposited on : 2015-08-18  
Resolution : 4.40 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.

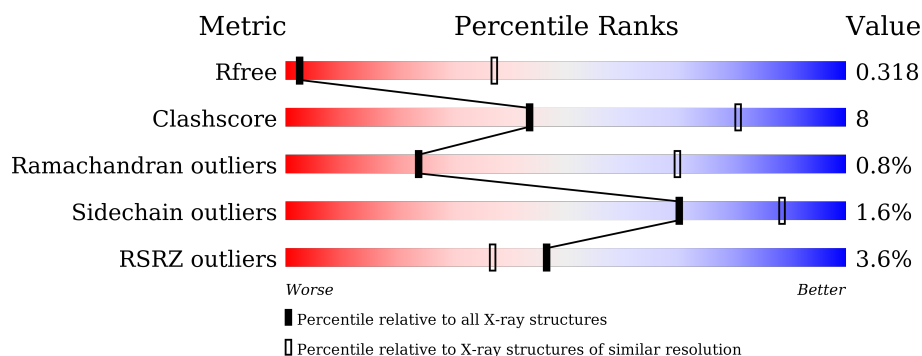
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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (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


The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

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	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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	A	472	 <div> <div></div> <div>69%</div> <div>25%</div> <div>• 5%</div> </div>
1	G	472	 <div> <div></div> <div>70%</div> <div>24%</div> <div>• 5%</div> </div>
1	J	472	 <div> <div></div> <div>67%</div> <div>27%</div> <div>• 5%</div> </div>
2	B	152	 <div> <div></div> <div>60%</div> <div>17%</div> <div>• 20%</div> </div>
2	C	152	 <div> <div></div> <div>57%</div> <div>20%</div> <div>• 20%</div> </div>
2	K	152	 <div> <div></div> <div>57%</div> <div>20%</div> <div>• 20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	211	
3	L	211	
3	M	211	
4	F	235	
4	H	235	
4	N	235	
5	D	241	
5	I	241	
5	O	241	

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
6	NAG	A	607	-	-	-	X
6	NAG	A	616	-	-	-	X
6	NAG	A	662	-	-	-	X
6	NAG	G	616	-	-	-	X
6	NAG	G	625	-	-	-	X
6	NAG	G	641	-	-	-	X
6	NAG	G	662	-	-	-	X
6	NAG	J	641	-	-	-	X
6	NAG	J	662	-	-	-	X
6	NAG	J	667	-	-	-	X
6	NAG	J	669	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31374 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 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	A	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	J	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	460	ALA	SER	conflict	UNP Q2N0S6
G	461	ASN	THR	conflict	UNP Q2N0S6
G	463	THR	SER	conflict	UNP Q2N0S6
G	464	SER	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	460	ALA	SER	conflict	UNP Q2N0S6
A	461	ASN	THR	conflict	UNP Q2N0S6
A	463	THR	SER	conflict	UNP Q2N0S6
A	464	SER	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
J	332	ASN	THR	conflict	UNP Q2N0S6
J	460	ALA	SER	conflict	UNP Q2N0S6
J	461	ASN	THR	conflict	UNP Q2N0S6
J	463	THR	SER	conflict	UNP Q2N0S6
J	464	SER	THR	conflict	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	C	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	K	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
C	559	PRO	ILE	conflict	UNP Q2N0S9
C	605	CYS	THR	conflict	UNP Q2N0S9
K	559	PRO	ILE	conflict	UNP Q2N0S9
K	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called PGT122 light chain,Ig lambda-3 chain C regions.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	E	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	M	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	156	VAL	ALA	conflict	UNP P0CG06
E	156	VAL	ALA	conflict	UNP P0CG06
M	156	VAL	ALA	conflict	UNP P0CG06

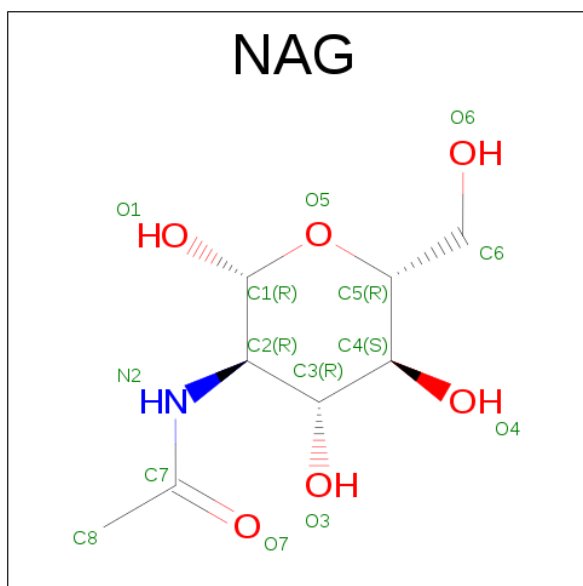
- Molecule 4 is a protein called PGT122 heavy chain,IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	F	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	N	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			

- Molecule 5 is a protein called NIH45-46 single chain Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	I	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	O	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		

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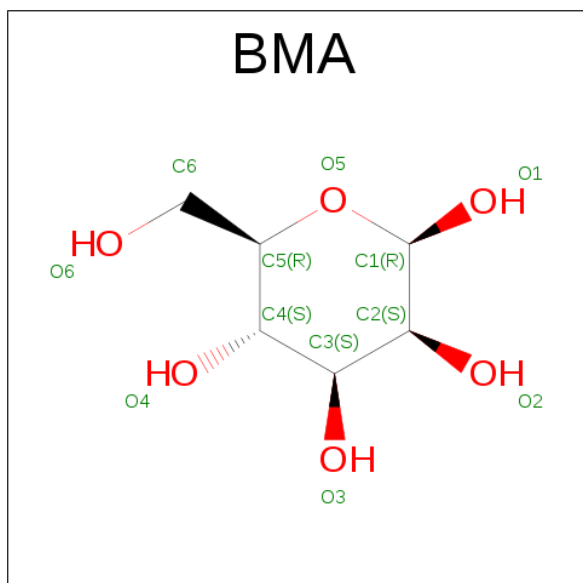
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



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

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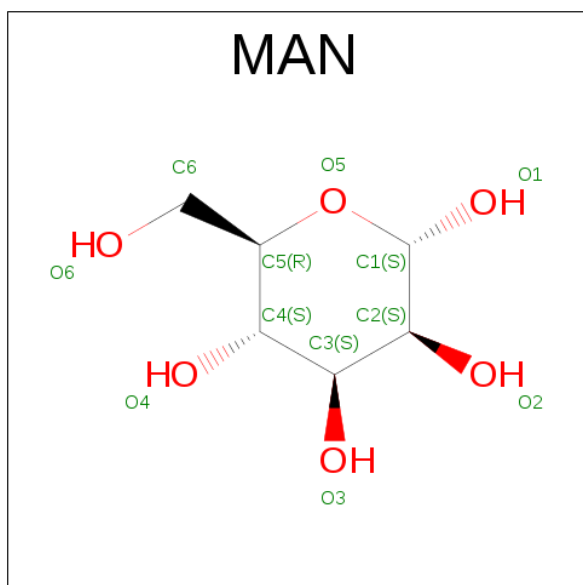
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7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

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

- Molecule 8 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
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		

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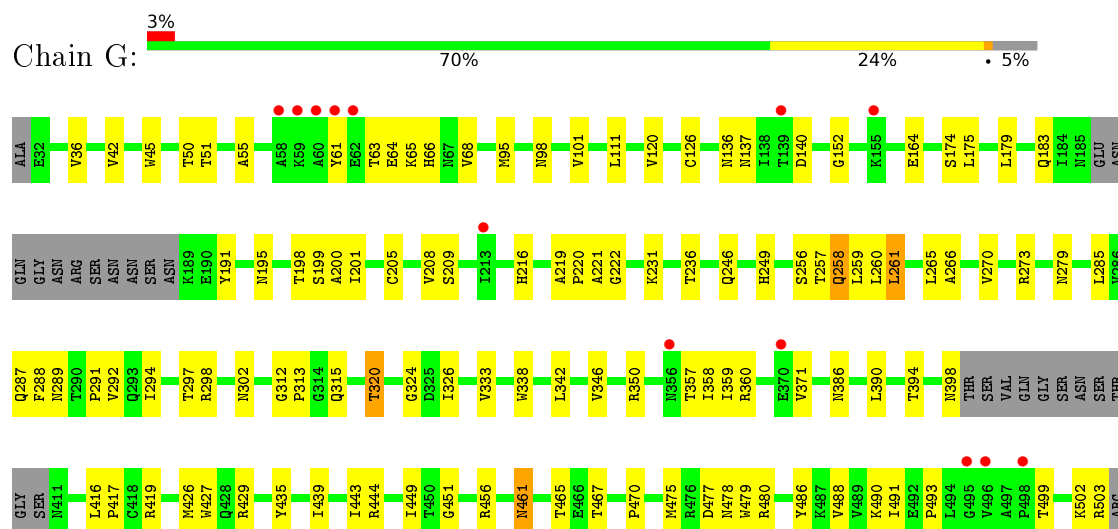
*Continued from previous page...*

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

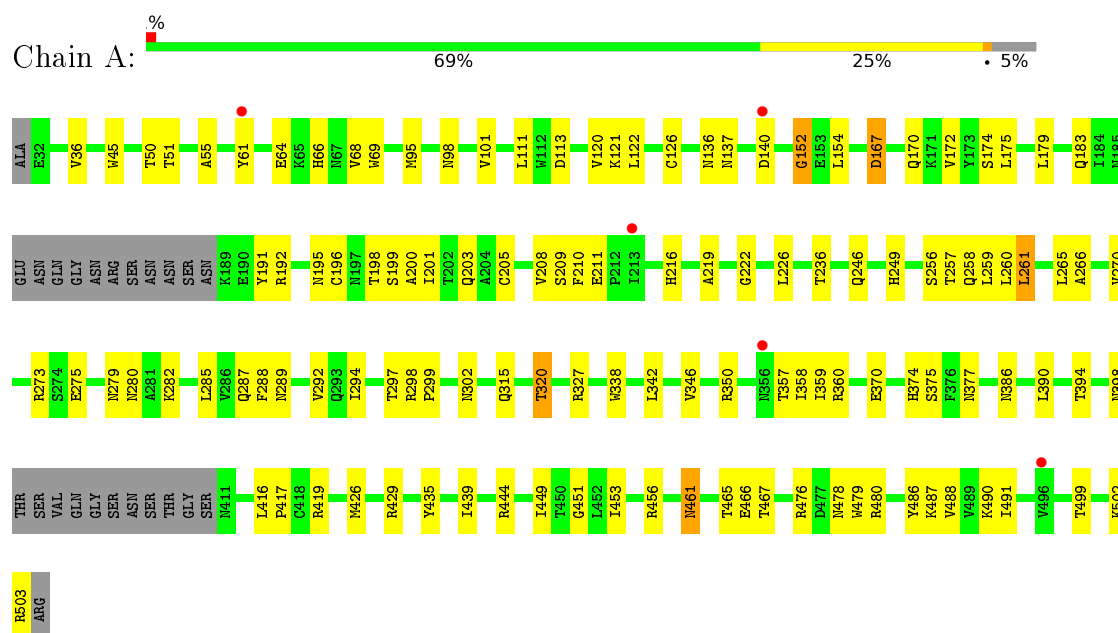
### 3 Residue-property plots [i](#)

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

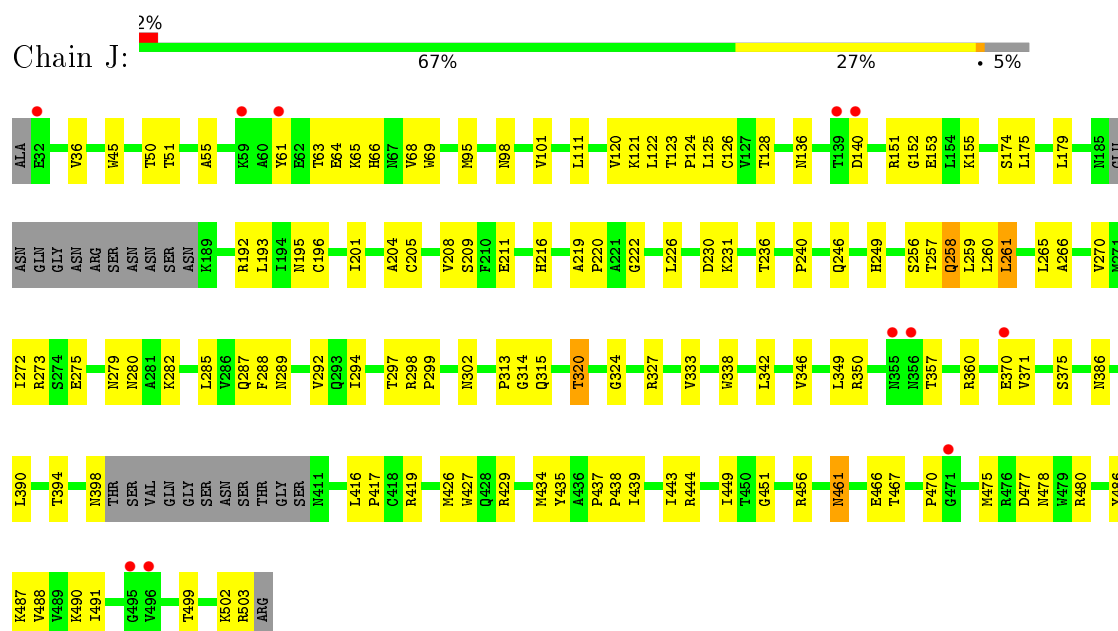
#### • Molecule 1: Envelope glycoprotein gp120



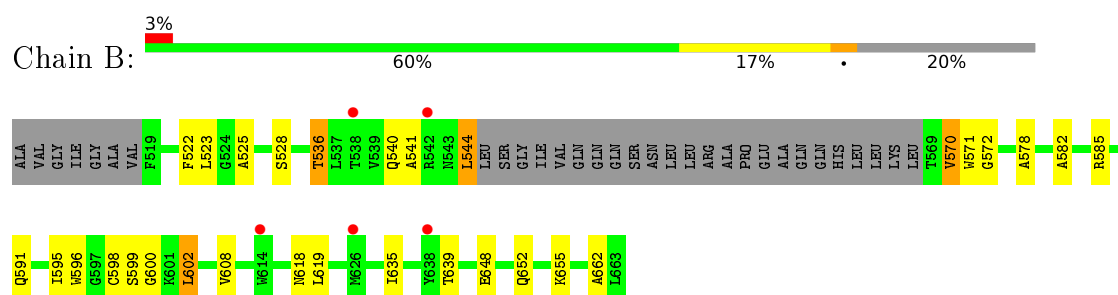
#### • Molecule 1: Envelope glycoprotein gp120



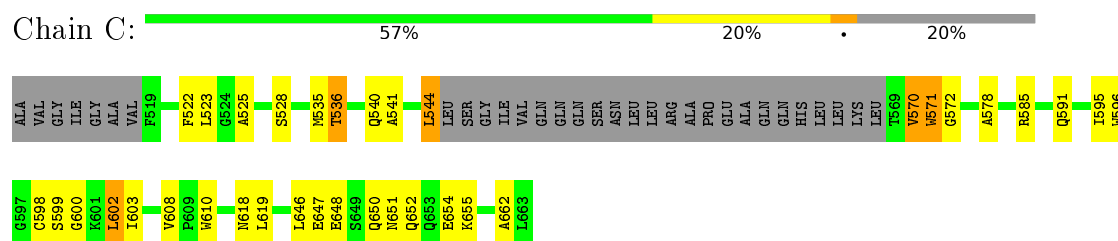
#### • Molecule 1: Envelope glycoprotein gp120



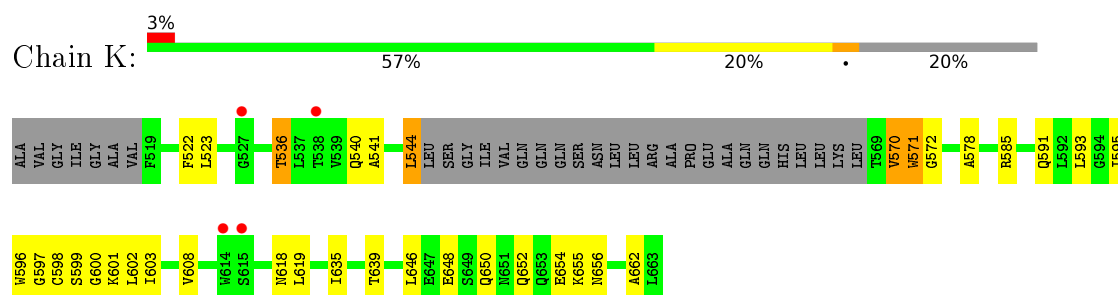
- Molecule 2: Envelope glycoprotein gp41



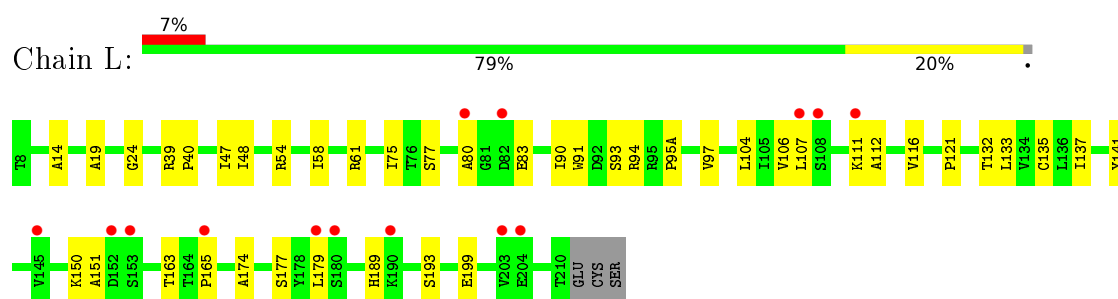
- Molecule 2: Envelope glycoprotein gp41



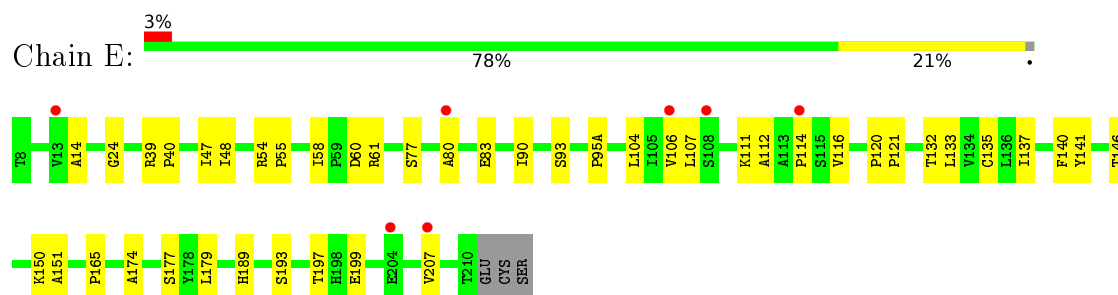
- Molecule 2: Envelope glycoprotein gp41



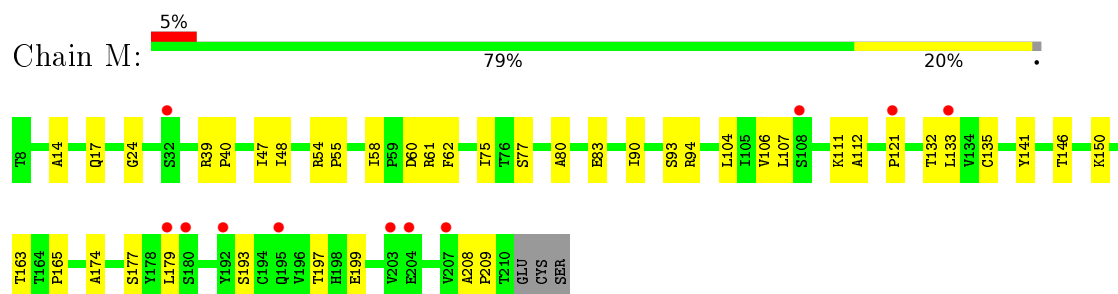
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



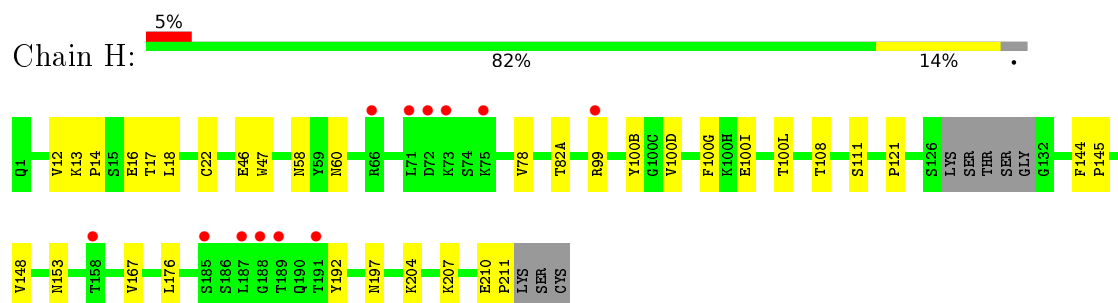
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



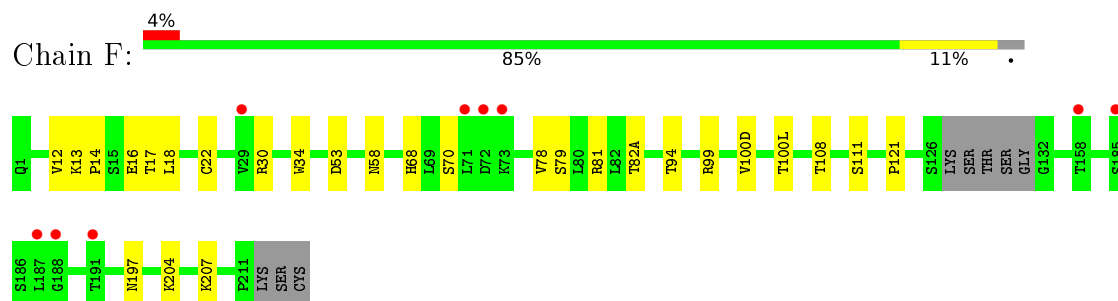
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



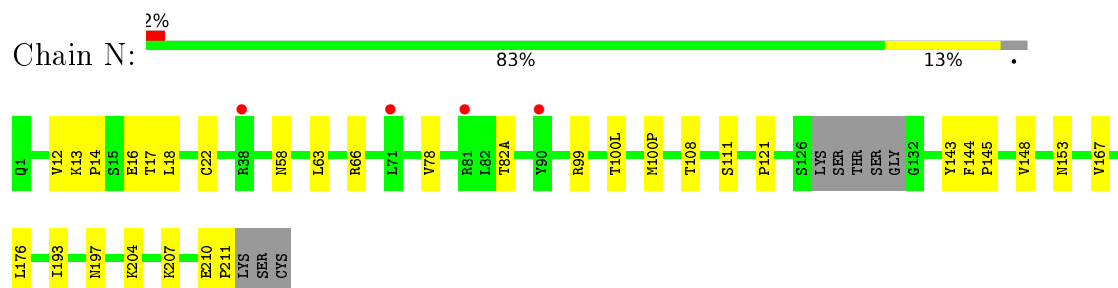
- Molecule 4: PGT122 heavy chain,IgG H chain



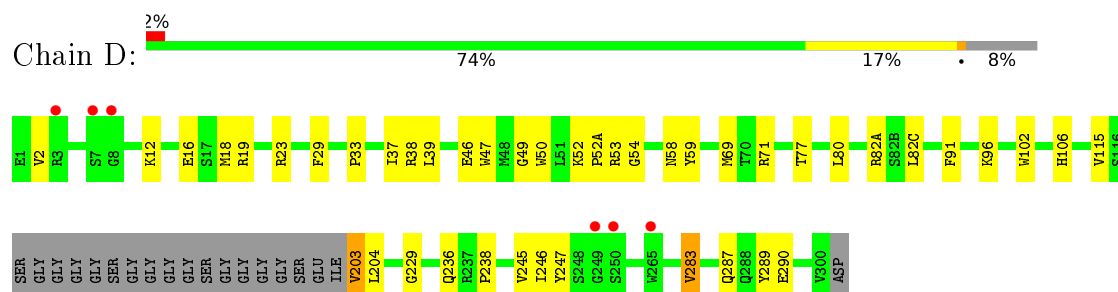
- Molecule 4: PGT122 heavy chain,IgG H chain



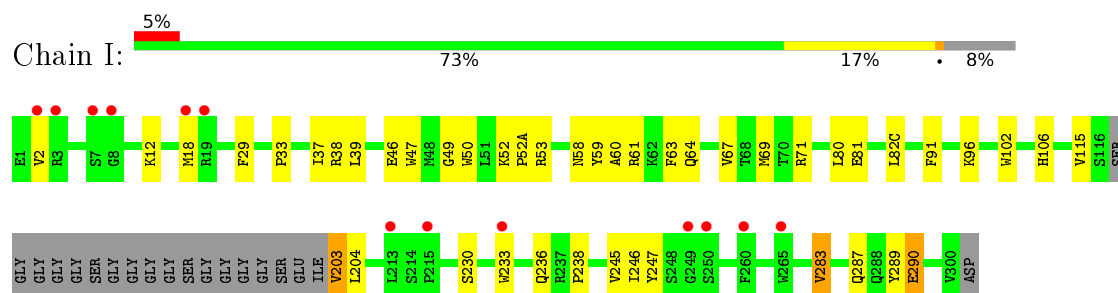
- Molecule 4: PGT122 heavy chain,IgG H chain



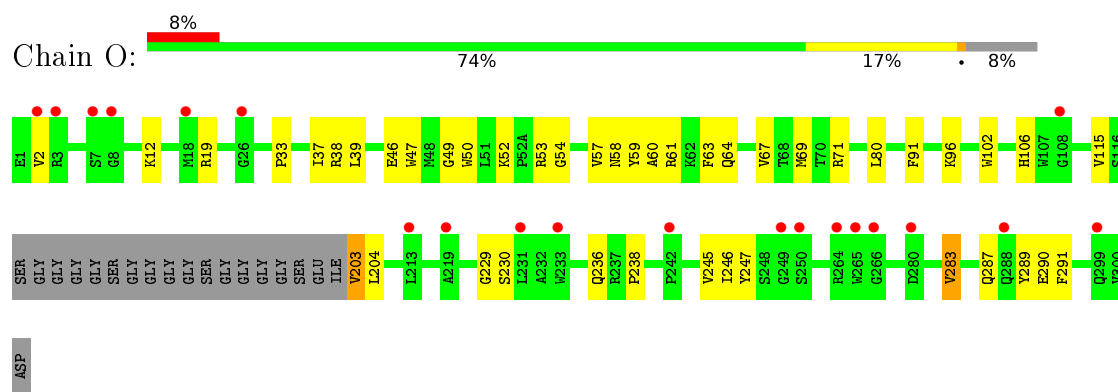
- Molecule 5: NIH45-46 single chain Fv



- Molecule 5: NIH45-46 single chain Fv



- Molecule 5: NIH45-46 single chain Fv



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.76Å 254.35Å 283.55Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	39.89 – 4.40 39.89 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.89-4.40) 100.0 (39.89-4.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.290 , 0.320 0.294 , 0.318	Depositor DCC
$R_{free}$ test set	1008 reflections (1.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	144.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 99.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	31374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, PCA, 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	A	0.28	0/3602	0.48	0/4891
1	G	0.27	0/3602	0.47	0/4891
1	J	0.27	0/3602	0.48	0/4891
2	B	0.26	0/986	0.44	0/1337
2	C	0.26	0/986	0.45	0/1337
2	K	0.27	0/986	0.44	0/1337
3	E	0.24	0/1619	0.42	0/2217
3	L	0.24	0/1619	0.41	0/2217
3	M	0.25	0/1619	0.42	0/2217
4	F	0.26	0/1785	0.45	0/2437
4	H	0.26	0/1785	0.44	0/2437
4	N	0.25	0/1785	0.44	0/2437
5	D	0.24	0/1792	0.41	0/2428
5	I	0.25	0/1792	0.41	0/2428
5	O	0.24	0/1792	0.41	0/2428
All	All	0.26	0/29352	0.45	0/39930

There are no bond length outliers.

There are no bond angle outliers.

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	A	3528	0	3456	84	0
1	G	3528	0	3456	79	0
1	J	3528	0	3456	89	0
2	B	968	0	944	23	0
2	C	968	0	944	30	0
2	K	968	0	944	29	0
3	E	1577	0	1518	24	0
3	L	1577	0	1518	25	0
3	M	1577	0	1518	25	0
4	F	1738	0	1711	16	0
4	H	1738	0	1711	21	0
4	N	1738	0	1711	21	0
5	D	1753	0	1678	28	0
5	I	1753	0	1678	30	0
5	O	1753	0	1678	27	0
6	A	448	0	394	7	0
6	B	28	0	26	0	0
6	C	28	0	26	0	0
6	G	448	0	394	8	0
6	J	448	0	394	6	0
6	K	28	0	26	0	0
7	A	88	0	65	0	0
7	G	88	0	65	0	0
7	J	88	0	65	0	0
8	A	330	0	285	0	0
8	G	330	0	285	3	0
8	J	330	0	285	2	0
All	All	31374	0	30231	496	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 8.

The worst 5 of 496 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)
4:N:197:ASN:HD22	4:N:204:LYS:HG2	1.48	0.78
4:H:14:PRO:HG3	4:H:111:SER:HB3	1.67	0.77
1:J:68:VAL:HG22	1:J:209:SER:HB3	1.67	0.76
3:E:39:ARG:HD3	3:E:40:PRO:HD2	1.68	0.76
1:J:279:ASN:OD1	5:O:102:TRP:NE1	2.15	0.76

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	A	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	21	67
1	G	442/472 (94%)	410 (93%)	28 (6%)	4 (1%)	21	67
1	J	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	21	67
2	B	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	56
2	C	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	56
2	K	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	56
3	E	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	34	77
3	L	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	34	77
3	M	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	34	77
4	F	223/235 (95%)	214 (96%)	9 (4%)	0	100	100
4	H	223/235 (95%)	213 (96%)	10 (4%)	0	100	100
4	N	223/235 (95%)	212 (95%)	11 (5%)	0	100	100
5	D	218/241 (90%)	205 (94%)	11 (5%)	2 (1%)	21	67
5	I	218/241 (90%)	206 (94%)	9 (4%)	3 (1%)	14	59
5	O	218/241 (90%)	205 (94%)	10 (5%)	3 (1%)	14	59
All	All	3618/3933 (92%)	3371 (93%)	218 (6%)	29 (1%)	24	70

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	140	ASP
5	D	53	ARG
1	A	140	ASP
5	I	53	ARG
1	J	140	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/419 (95%)	393 (98%)	6 (2%)	72	89
1	G	399/419 (95%)	394 (99%)	5 (1%)	76	89
1	J	399/419 (95%)	394 (99%)	5 (1%)	76	89
2	B	104/128 (81%)	100 (96%)	4 (4%)	40	74
2	C	104/128 (81%)	100 (96%)	4 (4%)	40	74
2	K	104/128 (81%)	100 (96%)	4 (4%)	40	74
3	E	177/180 (98%)	175 (99%)	2 (1%)	80	90
3	L	177/180 (98%)	175 (99%)	2 (1%)	80	90
3	M	177/180 (98%)	175 (99%)	2 (1%)	80	90
4	F	197/205 (96%)	196 (100%)	1 (0%)	92	96
4	H	197/205 (96%)	196 (100%)	1 (0%)	92	96
4	N	197/205 (96%)	196 (100%)	1 (0%)	92	96
5	D	183/190 (96%)	179 (98%)	4 (2%)	60	84
5	I	183/190 (96%)	179 (98%)	4 (2%)	60	84
5	O	183/190 (96%)	178 (97%)	5 (3%)	52	80
All	All	3180/3366 (94%)	3130 (98%)	50 (2%)	70	88

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	536	THR
3	E	111	LYS
5	O	71	ARG
2	C	544	LEU
2	C	571	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	HIS
4	F	76	ASN
4	N	153	ASN
1	A	428	GLN
4	F	153	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
5	PCA	D	1	5	7,8,9	1.66	1 (14%)	9,10,12	2.05	5 (55%)
5	PCA	I	1	5	7,8,9	1.68	1 (14%)	9,10,12	2.10	6 (66%)
5	PCA	O	1	5	7,8,9	1.67	1 (14%)	9,10,12	2.09	5 (55%)

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
5	PCA	D	1	5	-	0/0/11/13	0/1/1/1
5	PCA	I	1	5	-	0/0/11/13	0/1/1/1
5	PCA	O	1	5	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	PCA	CD-N	4.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1	PCA	CD-N	4.31	1.46	1.33
5	I	1	PCA	CD-N	4.35	1.47	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	PCA	CB-CA-C	-3.03	108.30	112.80
5	O	1	PCA	CB-CA-C	-2.95	108.42	112.80
5	O	1	PCA	OE-CD-CG	-2.81	121.29	126.85
5	I	1	PCA	OE-CD-CG	-2.78	121.36	126.85
5	D	1	PCA	OE-CD-CG	-2.76	121.40	126.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

216 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	$\# Z  > 2$
6	NAG	A	601	1,6	14,14,15	0.26	0	15,19,21	0.38	0
6	NAG	A	602	7,6	14,14,15	0.52	0	15,19,21	1.28	1 (6%)
7	BMA	A	603	8,6	11,11,12	0.64	0	15,15,17	0.68	0
8	MAN	A	604	7	11,11,12	0.88	1 (9%)	15,15,17	1.35	4 (26%)
8	MAN	A	605	7	11,11,12	0.91	0	15,15,17	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	606	1	14,14,15	0.21	0	15,19,21	0.34	0
6	NAG	A	607	1,6	14,14,15	0.46	0	15,19,21	0.35	0
6	NAG	A	608	7,6	14,14,15	0.27	0	15,19,21	0.23	0
7	BMA	A	609	8,6	11,11,12	0.63	0	15,15,17	0.71	0
8	MAN	A	610	7	11,11,12	0.76	1 (9%)	15,15,17	0.98	1 (6%)
6	NAG	A	611	1,6	14,14,15	0.20	0	15,19,21	0.40	0
6	NAG	A	612	7,6	14,14,15	0.24	0	15,19,21	0.24	0
7	BMA	A	613	8,6	11,11,12	0.61	0	15,15,17	0.50	0
8	MAN	A	614	7	11,11,12	0.81	0	15,15,17	1.00	1 (6%)
8	MAN	A	615	7	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
6	NAG	A	616	1,6	14,14,15	0.25	0	15,19,21	0.43	0
6	NAG	A	617	6	14,14,15	0.45	0	15,19,21	1.24	1 (6%)
6	NAG	A	618	1,6	14,14,15	0.53	0	15,19,21	0.56	0
6	NAG	A	619	7,6	14,14,15	0.28	0	15,19,21	0.30	0
7	BMA	A	620	8,6	11,11,12	0.65	0	15,15,17	1.63	2 (13%)
8	MAN	A	621	7	11,11,12	0.71	0	15,15,17	1.34	3 (20%)
8	MAN	A	622	8,7	11,11,12	1.17	1 (9%)	15,15,17	1.35	2 (13%)
8	MAN	A	623	8	11,11,12	0.78	0	15,15,17	1.29	2 (13%)
8	MAN	A	624	8	11,11,12	0.70	0	15,15,17	1.43	3 (20%)
6	NAG	A	625	1,6	14,14,15	0.80	1 (7%)	15,19,21	0.70	0
6	NAG	A	626	7,6	14,14,15	0.43	0	15,19,21	0.32	0
7	BMA	A	627	8,6	11,11,12	0.65	0	15,15,17	1.19	2 (13%)
8	MAN	A	628	8,7	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
8	MAN	A	629	8	11,11,12	0.85	0	15,15,17	1.11	1 (6%)
8	MAN	A	630	8	11,11,12	0.93	0	15,15,17	1.03	1 (6%)
8	MAN	A	631	8,7	11,11,12	1.12	2 (18%)	15,15,17	1.31	2 (13%)
8	MAN	A	632	8	11,11,12	0.94	0	15,15,17	1.21	1 (6%)
8	MAN	A	633	8	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
8	MAN	A	634	8	11,11,12	0.59	0	15,15,17	1.30	2 (13%)
8	MAN	A	635	8	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
6	NAG	A	636	1,6	14,14,15	0.70	1 (7%)	15,19,21	0.60	0
6	NAG	A	637	7,6	14,14,15	0.29	0	15,19,21	0.30	0
7	BMA	A	638	8,6	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
8	MAN	A	639	7	11,11,12	0.70	0	15,15,17	1.27	2 (13%)
8	MAN	A	640	7	11,11,12	0.78	0	15,15,17	1.04	2 (13%)
6	NAG	A	641	1	14,14,15	0.20	0	15,19,21	0.26	0
6	NAG	A	642	1,6	14,14,15	0.30	0	15,19,21	0.45	0
6	NAG	A	643	6	14,14,15	0.24	0	15,19,21	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	644	1,6	14,14,15	0.60	1 (7%)	15,19,21	0.73	0
6	NAG	A	645	7,6	14,14,15	0.48	0	15,19,21	0.25	0
7	BMA	A	646	8,6	11,11,12	0.62	0	15,15,17	0.85	0
8	MAN	A	647	7	11,11,12	0.67	0	15,15,17	1.17	1 (6%)
8	MAN	A	648	8,7	11,11,12	0.98	0	15,15,17	1.28	2 (13%)
8	MAN	A	649	8	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
8	MAN	A	650	8	11,11,12	0.71	0	15,15,17	1.32	2 (13%)
6	NAG	A	651	1,6	14,14,15	0.39	0	15,19,21	0.31	0
6	NAG	A	652	7,6	14,14,15	0.34	0	15,19,21	0.41	0
7	BMA	A	653	8,6	11,11,12	0.74	0	15,15,17	1.14	2 (13%)
8	MAN	A	654	8,7	11,11,12	0.80	0	15,15,17	0.98	2 (13%)
8	MAN	A	655	8	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
8	MAN	A	656	8	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
8	MAN	A	657	8,7	11,11,12	0.74	0	15,15,17	1.35	2 (13%)
8	MAN	A	658	8	11,11,12	0.83	1 (9%)	15,15,17	0.86	1 (6%)
8	MAN	A	659	8	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
8	MAN	A	660	8	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
6	NAG	A	661	1	14,14,15	0.21	0	15,19,21	0.33	0
6	NAG	A	662	1	14,14,15	0.31	0	15,19,21	0.34	0
6	NAG	A	663	1,6	14,14,15	0.26	0	15,19,21	0.59	0
6	NAG	A	664	6	14,14,15	0.21	0	15,19,21	0.31	0
6	NAG	A	665	1,6	14,14,15	0.25	0	15,19,21	0.27	0
6	NAG	A	666	6	14,14,15	0.35	0	15,19,21	0.38	0
6	NAG	A	667	1,6	14,14,15	0.19	0	15,19,21	0.48	0
6	NAG	A	668	6	14,14,15	0.27	0	15,19,21	0.29	0
6	NAG	A	669	1,6	14,14,15	0.71	1 (7%)	15,19,21	0.62	0
6	NAG	A	670	6	14,14,15	0.26	0	15,19,21	0.32	0
6	NAG	B	701	2	14,14,15	0.17	0	15,19,21	0.44	0
6	NAG	B	702	2	14,14,15	0.17	0	15,19,21	0.37	0
6	NAG	C	701	2	14,14,15	0.20	0	15,19,21	0.39	0
6	NAG	C	702	2	14,14,15	0.19	0	15,19,21	0.35	0
6	NAG	G	601	1,6	14,14,15	0.30	0	15,19,21	0.38	0
6	NAG	G	602	7,6	14,14,15	0.56	0	15,19,21	1.28	1 (6%)
7	BMA	G	603	8,6	11,11,12	0.60	0	15,15,17	0.67	0
8	MAN	G	604	7	11,11,12	0.79	0	15,15,17	1.27	2 (13%)
8	MAN	G	605	7	11,11,12	0.92	0	15,15,17	1.01	1 (6%)
6	NAG	G	606	1	14,14,15	0.22	0	15,19,21	0.33	0
6	NAG	G	607	1,6	14,14,15	0.53	0	15,19,21	0.30	0
6	NAG	G	608	7,6	14,14,15	0.27	0	15,19,21	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	G	609	8,6	11,11,12	0.61	0	15,15,17	0.69	0
8	MAN	G	610	7	11,11,12	0.91	1 (9%)	15,15,17	0.95	1 (6%)
6	NAG	G	611	1,6	14,14,15	0.22	0	15,19,21	0.40	0
6	NAG	G	612	7,6	14,14,15	0.23	0	15,19,21	0.24	0
7	BMA	G	613	8,6	11,11,12	0.61	0	15,15,17	0.55	0
8	MAN	G	614	7	11,11,12	0.72	0	15,15,17	1.08	1 (6%)
8	MAN	G	615	7	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
6	NAG	G	616	1,6	14,14,15	0.24	0	15,19,21	0.42	0
6	NAG	G	617	6	14,14,15	0.49	0	15,19,21	1.23	1 (6%)
6	NAG	G	618	1,6	14,14,15	0.48	0	15,19,21	0.58	0
6	NAG	G	619	7,6	14,14,15	0.35	0	15,19,21	0.30	0
7	BMA	G	620	8,6	11,11,12	0.64	0	15,15,17	1.46	1 (6%)
8	MAN	G	621	7	11,11,12	0.68	0	15,15,17	1.28	3 (20%)
8	MAN	G	622	8,7	11,11,12	1.23	2 (18%)	15,15,17	1.32	2 (13%)
8	MAN	G	623	8	11,11,12	0.75	0	15,15,17	1.30	2 (13%)
8	MAN	G	624	8	11,11,12	0.64	0	15,15,17	1.29	2 (13%)
6	NAG	G	625	1,6	14,14,15	0.64	1 (7%)	15,19,21	0.66	0
6	NAG	G	626	7,6	14,14,15	0.38	0	15,19,21	0.29	0
7	BMA	G	627	8,6	11,11,12	0.67	0	15,15,17	1.26	2 (13%)
8	MAN	G	628	8,7	11,11,12	0.63	0	15,15,17	1.29	2 (13%)
8	MAN	G	629	8	11,11,12	0.88	1 (9%)	15,15,17	1.06	2 (13%)
8	MAN	G	630	8	11,11,12	0.89	0	15,15,17	1.07	1 (6%)
8	MAN	G	631	8,7	11,11,12	1.19	2 (18%)	15,15,17	1.38	3 (20%)
8	MAN	G	632	8	11,11,12	1.03	1 (9%)	15,15,17	1.15	1 (6%)
8	MAN	G	633	8	11,11,12	0.78	0	15,15,17	1.16	1 (6%)
8	MAN	G	634	8	11,11,12	0.61	0	15,15,17	1.36	2 (13%)
8	MAN	G	635	8	11,11,12	0.73	0	15,15,17	1.19	2 (13%)
6	NAG	G	636	1,6	14,14,15	0.78	1 (7%)	15,19,21	0.60	0
6	NAG	G	637	7,6	14,14,15	0.32	0	15,19,21	0.34	0
7	BMA	G	638	8,6	11,11,12	0.64	0	15,15,17	1.05	1 (6%)
8	MAN	G	639	7	11,11,12	0.71	0	15,15,17	1.19	2 (13%)
8	MAN	G	640	7	11,11,12	0.87	0	15,15,17	1.02	1 (6%)
6	NAG	G	641	1	14,14,15	0.25	0	15,19,21	0.29	0
6	NAG	G	642	1,6	14,14,15	0.38	0	15,19,21	0.41	0
6	NAG	G	643	6	14,14,15	0.20	0	15,19,21	0.28	0
6	NAG	G	644	1,6	14,14,15	0.67	1 (7%)	15,19,21	0.74	0
6	NAG	G	645	7,6	14,14,15	0.43	0	15,19,21	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	G	646	8,6	11,11,12	0.63	0	15,15,17	0.80	0
8	MAN	G	647	7	11,11,12	0.70	0	15,15,17	1.23	2 (13%)
8	MAN	G	648	8,7	11,11,12	1.04	1 (9%)	15,15,17	1.20	1 (6%)
8	MAN	G	649	8	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
8	MAN	G	650	8	11,11,12	0.68	0	15,15,17	1.33	1 (6%)
6	NAG	G	651	1,6	14,14,15	0.30	0	15,19,21	0.34	0
6	NAG	G	652	7,6	14,14,15	0.26	0	15,19,21	0.43	0
7	BMA	G	653	8,6	11,11,12	0.70	0	15,15,17	1.22	1 (6%)
8	MAN	G	654	8,7	11,11,12	0.85	1 (9%)	15,15,17	1.09	2 (13%)
8	MAN	G	655	8	11,11,12	0.70	0	15,15,17	1.04	1 (6%)
8	MAN	G	656	8	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
8	MAN	G	657	8,7	11,11,12	0.65	0	15,15,17	1.30	3 (20%)
8	MAN	G	658	8	11,11,12	0.70	1 (9%)	15,15,17	0.89	1 (6%)
8	MAN	G	659	8	11,11,12	0.53	0	15,15,17	1.24	2 (13%)
8	MAN	G	660	8	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
6	NAG	G	661	1	14,14,15	0.20	0	15,19,21	0.31	0
6	NAG	G	662	1	14,14,15	0.34	0	15,19,21	0.39	0
6	NAG	G	663	1,6	14,14,15	0.23	0	15,19,21	0.59	0
6	NAG	G	664	6	14,14,15	0.23	0	15,19,21	0.30	0
6	NAG	G	665	1,6	14,14,15	0.23	0	15,19,21	0.31	0
6	NAG	G	666	6	14,14,15	0.43	0	15,19,21	0.40	0
6	NAG	G	667	1,6	14,14,15	0.16	0	15,19,21	0.46	0
6	NAG	G	668	6	14,14,15	0.26	0	15,19,21	0.25	0
6	NAG	G	669	1,6	14,14,15	0.81	1 (7%)	15,19,21	0.61	0
6	NAG	G	670	6	14,14,15	0.23	0	15,19,21	0.36	0
6	NAG	J	601	1,6	14,14,15	0.33	0	15,19,21	0.40	0
6	NAG	J	602	7,6	14,14,15	0.54	0	15,19,21	1.30	1 (6%)
7	BMA	J	603	8,6	11,11,12	0.58	0	15,15,17	0.59	0
8	MAN	J	604	7	11,11,12	0.85	0	15,15,17	1.25	2 (13%)
8	MAN	J	605	7	11,11,12	0.91	1 (9%)	15,15,17	0.95	1 (6%)
6	NAG	J	606	1	14,14,15	0.21	0	15,19,21	0.33	0
6	NAG	J	607	1,6	14,14,15	0.46	0	15,19,21	0.39	0
6	NAG	J	608	7,6	14,14,15	0.27	0	15,19,21	0.23	0
7	BMA	J	609	8,6	11,11,12	0.64	0	15,15,17	0.67	0
8	MAN	J	610	7	11,11,12	0.78	1 (9%)	15,15,17	0.97	1 (6%)
6	NAG	J	611	1,6	14,14,15	0.14	0	15,19,21	0.40	0
6	NAG	J	612	7,6	14,14,15	0.19	0	15,19,21	0.30	0
7	BMA	J	613	8,6	11,11,12	0.61	0	15,15,17	0.53	0
8	MAN	J	614	7	11,11,12	0.79	0	15,15,17	1.04	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	J	615	7	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
6	NAG	J	616	1,6	14,14,15	0.25	0	15,19,21	0.43	0
6	NAG	J	617	6	14,14,15	0.52	0	15,19,21	1.26	1 (6%)
6	NAG	J	618	1,6	14,14,15	0.51	0	15,19,21	0.56	0
6	NAG	J	619	7,6	14,14,15	0.36	0	15,19,21	0.28	0
7	BMA	J	620	8,6	11,11,12	0.63	0	15,15,17	1.36	1 (6%)
8	MAN	J	621	7	11,11,12	0.66	0	15,15,17	1.27	3 (20%)
8	MAN	J	622	8,7	11,11,12	1.27	1 (9%)	15,15,17	1.26	2 (13%)
8	MAN	J	623	8	11,11,12	0.77	0	15,15,17	1.21	2 (13%)
8	MAN	J	624	8	11,11,12	0.61	0	15,15,17	1.33	3 (20%)
6	NAG	J	625	1,6	14,14,15	0.68	1 (7%)	15,19,21	0.71	0
6	NAG	J	626	7,6	14,14,15	0.39	0	15,19,21	0.26	0
7	BMA	J	627	8,6	11,11,12	0.68	0	15,15,17	1.32	2 (13%)
8	MAN	J	628	8,7	11,11,12	0.64	0	15,15,17	1.29	2 (13%)
8	MAN	J	629	8	11,11,12	0.89	0	15,15,17	1.11	1 (6%)
8	MAN	J	630	8	11,11,12	0.93	0	15,15,17	1.05	1 (6%)
8	MAN	J	631	8,7	11,11,12	1.13	2 (18%)	15,15,17	1.27	3 (20%)
8	MAN	J	632	8	11,11,12	0.89	0	15,15,17	1.21	1 (6%)
8	MAN	J	633	8	11,11,12	0.75	0	15,15,17	1.08	2 (13%)
8	MAN	J	634	8	11,11,12	0.59	0	15,15,17	1.38	2 (13%)
8	MAN	J	635	8	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
6	NAG	J	636	1,6	14,14,15	0.85	1 (7%)	15,19,21	0.62	0
6	NAG	J	637	7,6	14,14,15	0.34	0	15,19,21	0.33	0
7	BMA	J	638	8,6	11,11,12	0.64	0	15,15,17	1.06	1 (6%)
8	MAN	J	639	7	11,11,12	0.77	0	15,15,17	1.20	2 (13%)
8	MAN	J	640	7	11,11,12	0.84	0	15,15,17	1.00	1 (6%)
6	NAG	J	641	1	14,14,15	0.22	0	15,19,21	0.30	0
6	NAG	J	642	1,6	14,14,15	0.35	0	15,19,21	0.44	0
6	NAG	J	643	6	14,14,15	0.23	0	15,19,21	0.26	0
6	NAG	J	644	1,6	14,14,15	0.68	1 (7%)	15,19,21	0.75	1 (6%)
6	NAG	J	645	7,6	14,14,15	0.42	0	15,19,21	0.26	0
7	BMA	J	646	8,6	11,11,12	0.63	0	15,15,17	0.88	0
8	MAN	J	647	7	11,11,12	0.65	0	15,15,17	1.18	1 (6%)
8	MAN	J	648	8,7	11,11,12	1.05	1 (9%)	15,15,17	1.24	2 (13%)
8	MAN	J	649	8	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
8	MAN	J	650	8	11,11,12	0.68	0	15,15,17	1.34	3 (20%)
6	NAG	J	651	1,6	14,14,15	0.24	0	15,19,21	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	J	652	7,6	14,14,15	0.31	0	15,19,21	0.43	0
7	BMA	J	653	8,6	11,11,12	0.72	0	15,15,17	1.24	1 (6%)
8	MAN	J	654	8,7	11,11,12	0.85	1 (9%)	15,15,17	1.01	1 (6%)
8	MAN	J	655	8	11,11,12	0.75	1 (9%)	15,15,17	1.03	1 (6%)
8	MAN	J	656	8	11,11,12	0.72	0	15,15,17	0.99	1 (6%)
8	MAN	J	657	8,7	11,11,12	0.69	0	15,15,17	1.31	2 (13%)
8	MAN	J	658	8	11,11,12	0.73	1 (9%)	15,15,17	0.90	1 (6%)
8	MAN	J	659	8	11,11,12	0.55	0	15,15,17	1.20	2 (13%)
8	MAN	J	660	8	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
6	NAG	J	661	1	14,14,15	0.22	0	15,19,21	0.33	0
6	NAG	J	662	1	14,14,15	0.27	0	15,19,21	0.33	0
6	NAG	J	663	1,6	14,14,15	0.24	0	15,19,21	0.54	0
6	NAG	J	664	6	14,14,15	0.22	0	15,19,21	0.31	0
6	NAG	J	665	1,6	14,14,15	0.24	0	15,19,21	0.30	0
6	NAG	J	666	6	14,14,15	0.38	0	15,19,21	0.41	0
6	NAG	J	667	1,6	14,14,15	0.19	0	15,19,21	0.51	0
6	NAG	J	668	6	14,14,15	0.26	0	15,19,21	0.30	0
6	NAG	J	669	1,6	14,14,15	0.69	1 (7%)	15,19,21	0.60	0
6	NAG	J	670	6	14,14,15	0.22	0	15,19,21	0.38	0
6	NAG	K	701	2	14,14,15	0.23	0	15,19,21	0.41	0
6	NAG	K	702	2	14,14,15	0.19	0	15,19,21	0.35	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
6	NAG	A	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	603	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	604	7	-	0/2/19/22	0/1/1/1
8	MAN	A	605	7	-	0/2/19/22	0/1/1/1
6	NAG	A	606	1	-	0/6/23/26	0/1/1/1
6	NAG	A	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	610	7	-	0/2/19/22	0/1/1/1
6	NAG	A	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	613	8,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	A	614	7	-	0/2/19/22	0/1/1/1
8	MAN	A	615	7	-	0/2/19/22	0/1/1/1
6	NAG	A	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	617	6	-	0/6/23/26	0/1/1/1
6	NAG	A	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	621	7	-	0/2/19/22	0/1/1/1
8	MAN	A	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	623	8	-	0/2/19/22	0/1/1/1
8	MAN	A	624	8	-	0/2/19/22	0/1/1/1
6	NAG	A	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	629	8	-	0/2/19/22	0/1/1/1
8	MAN	A	630	8	-	0/2/19/22	0/1/1/1
8	MAN	A	631	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	632	8	-	0/2/19/22	0/1/1/1
8	MAN	A	633	8	-	0/2/19/22	0/1/1/1
8	MAN	A	634	8	-	0/2/19/22	0/1/1/1
8	MAN	A	635	8	-	0/2/19/22	0/1/1/1
6	NAG	A	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	637	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	639	7	-	0/2/19/22	0/1/1/1
8	MAN	A	640	7	-	0/2/19/22	0/1/1/1
6	NAG	A	641	1	-	0/6/23/26	0/1/1/1
6	NAG	A	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	643	6	-	0/6/23/26	0/1/1/1
6	NAG	A	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	645	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	647	7	-	0/2/19/22	0/1/1/1
8	MAN	A	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	649	8	-	0/2/19/22	0/1/1/1
8	MAN	A	650	8	-	0/2/19/22	0/1/1/1
6	NAG	A	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	655	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	A	656	8	-	0/2/19/22	0/1/1/1
8	MAN	A	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	658	8	-	0/2/19/22	0/1/1/1
8	MAN	A	659	8	-	0/2/19/22	0/1/1/1
8	MAN	A	660	8	-	0/2/19/22	1/1/1/1
6	NAG	A	661	1	-	0/6/23/26	0/1/1/1
6	NAG	A	662	1	-	0/6/23/26	0/1/1/1
6	NAG	A	663	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	664	6	-	0/6/23/26	0/1/1/1
6	NAG	A	665	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	666	6	-	0/6/23/26	0/1/1/1
6	NAG	A	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	668	6	-	0/6/23/26	0/1/1/1
6	NAG	A	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	670	6	-	0/6/23/26	0/1/1/1
6	NAG	B	701	2	-	0/6/23/26	0/1/1/1
6	NAG	B	702	2	-	0/6/23/26	0/1/1/1
6	NAG	C	701	2	-	0/6/23/26	0/1/1/1
6	NAG	C	702	2	-	0/6/23/26	0/1/1/1
6	NAG	G	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	603	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	604	7	-	0/2/19/22	0/1/1/1
8	MAN	G	605	7	-	0/2/19/22	0/1/1/1
6	NAG	G	606	1	-	0/6/23/26	0/1/1/1
6	NAG	G	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	610	7	-	0/2/19/22	0/1/1/1
6	NAG	G	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	613	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	614	7	-	0/2/19/22	0/1/1/1
8	MAN	G	615	7	-	0/2/19/22	0/1/1/1
6	NAG	G	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	617	6	-	0/6/23/26	0/1/1/1
6	NAG	G	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	621	7	-	0/2/19/22	0/1/1/1
8	MAN	G	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	623	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	G	624	8	-	0/2/19/22	0/1/1/1
6	NAG	G	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	629	8	-	0/2/19/22	0/1/1/1
8	MAN	G	630	8	-	0/2/19/22	0/1/1/1
8	MAN	G	631	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	632	8	-	0/2/19/22	0/1/1/1
8	MAN	G	633	8	-	0/2/19/22	0/1/1/1
8	MAN	G	634	8	-	0/2/19/22	0/1/1/1
8	MAN	G	635	8	-	0/2/19/22	0/1/1/1
6	NAG	G	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	637	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	639	7	-	0/2/19/22	0/1/1/1
8	MAN	G	640	7	-	0/2/19/22	0/1/1/1
6	NAG	G	641	1	-	0/6/23/26	0/1/1/1
6	NAG	G	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	643	6	-	0/6/23/26	0/1/1/1
6	NAG	G	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	645	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	647	7	-	0/2/19/22	0/1/1/1
8	MAN	G	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	649	8	-	0/2/19/22	0/1/1/1
8	MAN	G	650	8	-	0/2/19/22	0/1/1/1
6	NAG	G	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	655	8	-	0/2/19/22	0/1/1/1
8	MAN	G	656	8	-	0/2/19/22	0/1/1/1
8	MAN	G	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	658	8	-	0/2/19/22	0/1/1/1
8	MAN	G	659	8	-	0/2/19/22	0/1/1/1
8	MAN	G	660	8	-	0/2/19/22	1/1/1/1
6	NAG	G	661	1	-	0/6/23/26	0/1/1/1
6	NAG	G	662	1	-	0/6/23/26	0/1/1/1
6	NAG	G	663	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	664	6	-	0/6/23/26	0/1/1/1
6	NAG	G	665	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	666	6	-	0/6/23/26	0/1/1/1
6	NAG	G	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	668	6	-	0/6/23/26	0/1/1/1
6	NAG	G	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	670	6	-	0/6/23/26	0/1/1/1
6	NAG	J	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	603	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	604	7	-	0/2/19/22	0/1/1/1
8	MAN	J	605	7	-	0/2/19/22	0/1/1/1
6	NAG	J	606	1	-	0/6/23/26	0/1/1/1
6	NAG	J	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	610	7	-	0/2/19/22	0/1/1/1
6	NAG	J	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	613	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	614	7	-	0/2/19/22	0/1/1/1
8	MAN	J	615	7	-	0/2/19/22	0/1/1/1
6	NAG	J	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	617	6	-	0/6/23/26	0/1/1/1
6	NAG	J	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	621	7	-	0/2/19/22	0/1/1/1
8	MAN	J	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	623	8	-	0/2/19/22	0/1/1/1
8	MAN	J	624	8	-	0/2/19/22	0/1/1/1
6	NAG	J	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	629	8	-	0/2/19/22	0/1/1/1
8	MAN	J	630	8	-	0/2/19/22	0/1/1/1
8	MAN	J	631	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	632	8	-	0/2/19/22	0/1/1/1
8	MAN	J	633	8	-	0/2/19/22	0/1/1/1
8	MAN	J	634	8	-	0/2/19/22	0/1/1/1
8	MAN	J	635	8	-	0/2/19/22	0/1/1/1
6	NAG	J	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	637	7,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	J	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	639	7	-	0/2/19/22	0/1/1/1
8	MAN	J	640	7	-	0/2/19/22	0/1/1/1
6	NAG	J	641	1	-	0/6/23/26	0/1/1/1
6	NAG	J	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	643	6	-	0/6/23/26	0/1/1/1
6	NAG	J	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	645	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	647	7	-	0/2/19/22	0/1/1/1
8	MAN	J	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	649	8	-	0/2/19/22	0/1/1/1
8	MAN	J	650	8	-	0/2/19/22	0/1/1/1
6	NAG	J	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	655	8	-	0/2/19/22	0/1/1/1
8	MAN	J	656	8	-	0/2/19/22	0/1/1/1
8	MAN	J	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	658	8	-	0/2/19/22	0/1/1/1
8	MAN	J	659	8	-	0/2/19/22	0/1/1/1
8	MAN	J	660	8	-	0/2/19/22	1/1/1/1
6	NAG	J	661	1	-	0/6/23/26	0/1/1/1
6	NAG	J	662	1	-	0/6/23/26	0/1/1/1
6	NAG	J	663	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	664	6	-	0/6/23/26	0/1/1/1
6	NAG	J	665	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	666	6	-	0/6/23/26	0/1/1/1
6	NAG	J	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	668	6	-	0/6/23/26	0/1/1/1
6	NAG	J	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	670	6	-	0/6/23/26	0/1/1/1
6	NAG	K	701	2	-	0/6/23/26	0/1/1/1
6	NAG	K	702	2	-	0/6/23/26	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	636	NAG	O5-C1	-2.98	1.38	1.43
6	G	669	NAG	O5-C1	-2.87	1.39	1.43
6	G	636	NAG	O5-C1	-2.74	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	625	NAG	O5-C1	-2.65	1.39	1.43
8	A	658	MAN	O5-C1	-2.57	1.39	1.43

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	657	MAN	O2-C2-C3	-3.21	103.71	110.19
8	A	624	MAN	O2-C2-C3	-2.98	104.18	110.19
8	J	657	MAN	O2-C2-C3	-2.90	104.33	110.19
8	J	628	MAN	O2-C2-C3	-2.88	104.38	110.19
8	G	628	MAN	O2-C2-C3	-2.84	104.47	110.19

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	660	MAN	C1-C2-C3-C4-C5-O5
8	G	660	MAN	C1-C2-C3-C4-C5-O5
8	J	660	MAN	C1-C2-C3-C4-C5-O5

29 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	NAG	1	0
6	A	608	NAG	1	0
6	A	616	NAG	1	0
6	A	617	NAG	2	0
6	A	636	NAG	1	0
6	A	652	NAG	1	0
6	A	663	NAG	1	0
6	A	664	NAG	1	0
6	G	601	NAG	1	0
6	G	602	NAG	1	0
6	G	607	NAG	1	0
6	G	608	NAG	1	0
8	G	610	MAN	1	0
6	G	617	NAG	1	0
8	G	621	MAN	1	0
8	G	624	MAN	1	0
6	G	641	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	663	NAG	1	0
6	G	664	NAG	1	0
6	G	667	NAG	1	0
6	J	602	NAG	1	0
6	J	608	NAG	1	0
8	J	610	MAN	1	0
6	J	617	NAG	1	0
8	J	621	MAN	1	0
6	J	636	NAG	1	0
6	J	641	NAG	1	0
6	J	663	NAG	1	0
6	J	664	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	448/472 (94%)	0.02	5 (1%) 82 76	138, 198, 269, 365	0
1	G	448/472 (94%)	-0.05	13 (2%) 55 44	133, 193, 262, 390	0
1	J	448/472 (94%)	-0.04	11 (2%) 61 50	113, 193, 270, 367	0
2	B	121/152 (79%)	-0.05	5 (4%) 41 32	140, 200, 245, 279	0
2	C	121/152 (79%)	-0.10	0 100 100	132, 199, 244, 290	0
2	K	121/152 (79%)	-0.06	4 (3%) 50 39	128, 205, 240, 274	0
3	E	208/211 (98%)	0.13	7 (3%) 49 39	159, 212, 241, 269	0
3	L	208/211 (98%)	0.40	14 (6%) 21 15	179, 234, 277, 291	0
3	M	208/211 (98%)	0.17	11 (5%) 30 23	148, 199, 250, 269	0
4	F	227/235 (96%)	0.02	9 (3%) 42 33	135, 192, 242, 301	0
4	H	227/235 (96%)	0.08	12 (5%) 30 23	167, 211, 278, 383	0
4	N	227/235 (96%)	-0.16	4 (1%) 71 62	138, 188, 248, 275	0
5	D	221/241 (91%)	0.26	6 (2%) 58 48	178, 227, 270, 317	0
5	I	221/241 (91%)	0.48	13 (5%) 26 19	200, 267, 312, 339	0
5	O	221/241 (91%)	0.54	20 (9%) 12 9	210, 267, 301, 322	0
All	All	3675/3933 (93%)	0.10	134 (3%) 46 37	113, 208, 284, 390	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	8	GLY	8.6
4	H	187	LEU	5.3
4	H	188	GLY	5.3
3	L	204	GLU	5.2
5	D	7	SER	5.0

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

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
5	PCA	I	1	8/9	0.53	0.97	-	267,277,289,294	0
5	PCA	O	1	8/9	0.64	0.80	-	222,231,268,273	0
5	PCA	D	1	8/9	0.83	0.57	-	184,193,214,219	0

## 6.3 Carbohydrates ⓘ

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
6	NAG	G	641	14/15	0.73	0.42	3.95	261,261,261,261	0
6	NAG	J	667	14/15	0.84	0.38	3.33	259,277,289,292	0
6	NAG	G	616	14/15	0.77	0.54	3.01	252,275,284,297	0
6	NAG	G	662	14/15	0.60	0.54	2.45	267,275,300,318	0
6	NAG	G	625	14/15	0.79	0.30	2.18	261,261,261,261	0
6	NAG	G	601	14/15	0.85	0.34	1.52	221,229,242,243	0
6	NAG	G	669	14/15	0.69	0.39	1.37	261,261,261,261	0
6	NAG	A	662	14/15	0.61	0.52	1.35	267,275,300,318	0
6	NAG	J	669	14/15	0.71	0.50	1.31	261,261,261,261	0
6	NAG	A	616	14/15	0.79	0.49	1.08	252,275,284,297	0
6	NAG	J	641	14/15	0.71	0.46	1.08	261,261,261,261	0
6	NAG	J	662	14/15	0.61	0.54	1.02	267,275,300,318	0
6	NAG	A	651	14/15	0.84	0.38	0.98	237,248,265,270	0
6	NAG	G	618	14/15	0.71	0.34	0.69	261,261,261,261	0
6	NAG	A	669	14/15	0.72	0.38	0.55	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	618	14/15	0.71	0.33	0.54	261,261,261,261	0
6	NAG	J	636	14/15	0.92	0.27	0.51	261,261,261,261	0
6	NAG	G	651	14/15	0.91	0.31	0.41	237,248,265,270	0
6	NAG	A	625	14/15	0.83	0.26	0.34	261,261,261,261	0
6	NAG	J	651	14/15	0.90	0.35	0.31	237,248,265,270	0
6	NAG	J	616	14/15	0.84	0.37	0.16	252,275,284,297	0
6	NAG	J	611	14/15	0.91	0.26	0.12	213,259,277,280	0
6	NAG	A	607	14/15	0.89	0.40	0.07	258,284,302,304	0
6	NAG	A	641	14/15	0.79	0.35	0.03	261,261,261,261	0
6	NAG	A	606	14/15	0.72	0.40	-0.03	290,305,316,319	0
6	NAG	G	606	14/15	0.69	0.39	-0.18	290,305,316,319	0
6	NAG	G	611	14/15	0.91	0.26	-0.19	213,259,277,280	0
6	NAG	J	606	14/15	0.78	0.29	-0.20	290,305,316,319	0
6	NAG	J	625	14/15	0.86	0.20	-0.21	261,261,261,261	0
6	NAG	J	607	14/15	0.91	0.33	-0.25	258,284,302,304	0
6	NAG	J	618	14/15	0.83	0.25	-0.33	261,261,261,261	0
6	NAG	G	642	14/15	0.92	0.22	-0.40	245,261,286,296	0
6	NAG	A	611	14/15	0.93	0.23	-0.45	213,259,277,280	0
6	NAG	G	652	14/15	0.85	0.36	-0.48	257,273,294,300	0
6	NAG	G	637	14/15	0.91	0.23	-0.54	261,261,261,261	0
6	NAG	G	607	14/15	0.85	0.31	-0.58	258,284,302,304	0
6	NAG	G	667	14/15	0.84	0.28	-0.69	259,277,289,292	0
8	MAN	A	658	11/12	0.94	0.24	-0.79	262,265,279,286	0
8	MAN	G	657	11/12	0.97	0.28	-0.79	235,240,258,278	0
6	NAG	A	667	14/15	0.87	0.26	-0.81	259,277,289,292	0
6	NAG	G	636	14/15	0.96	0.20	-0.88	261,261,261,261	0
6	NAG	J	642	14/15	0.86	0.19	-0.95	245,261,286,296	0
8	MAN	J	658	11/12	0.88	0.20	-1.00	262,265,279,286	0
8	MAN	G	658	11/12	0.85	0.18	-1.09	262,265,279,286	0
6	NAG	A	636	14/15	0.93	0.26	-1.12	261,261,261,261	0
8	MAN	J	657	11/12	0.96	0.18	-1.16	235,240,258,278	0
8	MAN	A	657	11/12	0.98	0.19	-1.30	235,240,258,278	0
6	NAG	A	642	14/15	0.88	0.17	-1.33	245,261,286,296	0
6	NAG	A	652	14/15	0.86	0.27	-1.38	257,273,294,300	0
6	NAG	J	652	14/15	0.90	0.19	-2.07	257,273,294,300	0
8	MAN	G	655	11/12	0.84	0.23	-	280,295,301,303	0
6	NAG	G	666	14/15	0.61	0.32	-	307,328,330,330	0
6	NAG	A	601	14/15	0.78	0.36	-	221,229,242,243	0
8	MAN	G	648	11/12	0.80	0.49	-	261,261,261,261	0
6	NAG	J	644	14/15	0.80	0.34	-	261,261,261,261	0
8	MAN	J	605	11/12	0.67	0.36	-	293,300,308,309	0
6	NAG	A	602	14/15	0.91	0.48	-	230,242,258,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	643	14/15	0.82	0.33	-	303,317,328,336	0
8	MAN	J	630	11/12	0.65	0.74	-	261,261,261,261	0
7	BMA	G	613	11/12	0.64	0.19	-	312,321,331,341	0
6	NAG	G	608	14/15	0.85	0.26	-	295,304,312,313	0
8	MAN	A	655	11/12	0.50	0.40	-	280,295,301,303	0
8	MAN	A	610	11/12	0.82	0.37	-	325,342,352,353	0
8	MAN	A	631	11/12	0.59	0.34	-	261,261,261,261	0
7	BMA	G	609	11/12	0.77	0.35	-	309,319,327,335	0
6	NAG	G	643	14/15	0.85	0.33	-	303,317,328,336	0
8	MAN	J	647	11/12	0.78	0.35	-	261,261,261,261	0
6	NAG	J	619	14/15	0.88	0.23	-	261,261,261,261	0
8	MAN	J	655	11/12	0.71	0.35	-	280,295,301,303	0
6	NAG	B	702	14/15	0.73	0.86	-	285,303,316,317	0
6	NAG	J	663	14/15	0.88	0.23	-	260,297,316,323	0
8	MAN	J	633	11/12	0.67	0.94	-	261,261,261,261	0
6	NAG	A	645	14/15	0.87	0.25	-	261,261,261,261	0
8	MAN	G	654	11/12	0.81	0.23	-	286,303,309,318	0
6	NAG	G	645	14/15	0.88	0.28	-	261,261,261,261	0
8	MAN	J	649	11/12	0.71	0.44	-	261,261,261,261	0
7	BMA	A	613	11/12	0.74	0.33	-	312,321,331,341	0
6	NAG	J	602	14/15	0.85	0.62	-	230,242,258,262	0
7	BMA	J	638	11/12	0.87	0.30	-	261,261,261,261	0
7	BMA	A	646	11/12	0.71	0.25	-	261,261,261,261	0
6	NAG	J	601	14/15	0.88	0.51	-	221,229,242,243	0
6	NAG	G	612	14/15	0.87	0.23	-	277,291,302,313	0
8	MAN	G	650	11/12	0.65	1.00	-	261,261,261,261	0
7	BMA	J	646	11/12	0.74	0.23	-	261,261,261,261	0
6	NAG	G	617	14/15	0.77	0.32	-	279,293,304,311	0
8	MAN	A	647	11/12	0.74	0.39	-	261,261,261,261	0
8	MAN	A	604	11/12	0.77	0.74	-	253,260,277,291	0
8	MAN	J	610	11/12	0.69	0.56	-	325,342,352,353	0
7	BMA	G	638	11/12	0.89	0.16	-	261,261,261,261	0
8	MAN	A	635	11/12	0.65	0.58	-	261,261,261,261	0
8	MAN	G	640	11/12	0.61	0.32	-	261,261,261,261	0
8	MAN	G	615	11/12	0.70	0.62	-	339,341,344,346	0
8	MAN	G	622	11/12	0.47	0.61	-	261,261,261,261	0
8	MAN	A	654	11/12	0.85	0.44	-	286,303,309,318	0
8	MAN	G	631	11/12	0.55	0.28	-	261,261,261,261	0
8	MAN	G	604	11/12	0.84	0.53	-	253,260,277,291	0
6	NAG	G	668	14/15	0.80	0.27	-	288,310,336,363	0
7	BMA	J	620	11/12	0.87	0.15	-	261,261,261,261	0
8	MAN	J	632	11/12	0.86	0.95	-	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BMA	G	627	11/12	0.78	0.16	-	261,261,261,261	0
8	MAN	J	654	11/12	0.71	0.22	-	286,303,309,318	0
6	NAG	G	665	14/15	0.87	0.38	-	296,306,323,326	0
8	MAN	G	647	11/12	0.75	0.38	-	261,261,261,261	0
6	NAG	J	608	14/15	0.82	0.31	-	295,304,312,313	0
6	NAG	A	617	14/15	0.72	0.30	-	279,293,304,311	0
6	NAG	A	665	14/15	0.88	0.68	-	296,306,323,326	0
6	NAG	J	664	14/15	0.72	0.37	-	317,335,342,344	0
8	MAN	A	633	11/12	0.67	1.06	-	261,261,261,261	0
8	MAN	J	623	11/12	0.67	1.21	-	261,261,261,261	0
6	NAG	A	668	14/15	0.76	0.28	-	288,310,336,363	0
8	MAN	G	630	11/12	0.66	0.74	-	261,261,261,261	0
8	MAN	A	615	11/12	0.76	0.56	-	339,341,344,346	0
8	MAN	A	628	11/12	0.90	0.27	-	261,261,261,261	0
6	NAG	G	663	14/15	0.88	0.26	-	260,297,316,323	0
7	BMA	J	627	11/12	0.60	0.19	-	261,261,261,261	0
6	NAG	B	701	14/15	0.77	0.25	-	296,313,326,330	0
8	MAN	G	624	11/12	0.56	0.65	-	261,261,261,261	0
8	MAN	J	621	11/12	0.80	0.27	-	261,261,261,261	0
8	MAN	G	632	11/12	0.82	0.90	-	261,261,261,261	0
6	NAG	A	644	14/15	0.84	0.32	-	261,261,261,261	0
8	MAN	J	631	11/12	0.63	0.43	-	261,261,261,261	0
7	BMA	A	609	11/12	0.76	0.41	-	309,319,327,335	0
8	MAN	A	632	11/12	0.72	0.80	-	261,261,261,261	0
6	NAG	G	644	14/15	0.75	0.30	-	261,261,261,261	0
6	NAG	A	663	14/15	0.90	0.25	-	260,297,316,323	0
6	NAG	J	661	14/15	0.77	0.44	-	293,311,318,323	0
6	NAG	A	612	14/15	0.87	0.26	-	277,291,302,313	0
8	MAN	G	659	11/12	0.78	0.39	-	301,306,311,311	0
8	MAN	A	623	11/12	0.72	1.37	-	261,261,261,261	0
6	NAG	J	666	14/15	0.83	0.44	-	307,328,330,330	0
8	MAN	G	635	11/12	0.58	0.67	-	261,261,261,261	0
6	NAG	J	668	14/15	0.82	0.24	-	288,310,336,363	0
6	NAG	J	645	14/15	0.82	0.31	-	261,261,261,261	0
7	BMA	A	627	11/12	0.58	0.25	-	261,261,261,261	0
8	MAN	G	656	11/12	0.78	0.60	-	321,323,332,338	0
6	NAG	A	661	14/15	0.75	0.49	-	293,311,318,323	0
6	NAG	G	619	14/15	0.91	0.30	-	261,261,261,261	0
8	MAN	G	660	11/12	0.82	0.45	-	327,335,339,340	0
8	MAN	A	656	11/12	0.86	0.60	-	321,323,332,338	0
8	MAN	G	633	11/12	0.68	0.93	-	261,261,261,261	0
7	BMA	A	603	11/12	0.81	0.39	-	252,263,287,290	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	J	640	11/12	0.67	0.36	-	261,261,261,261	0
8	MAN	A	659	11/12	0.85	0.27	-	301,306,311,311	0
7	BMA	J	613	11/12	0.86	0.27	-	312,321,331,341	0
7	BMA	G	603	11/12	0.80	0.30	-	252,263,287,290	0
6	NAG	K	701	14/15	0.76	0.23	-	296,313,326,330	0
8	MAN	G	634	11/12	0.86	0.35	-	261,261,261,261	0
6	NAG	G	670	14/15	0.62	0.64	-	261,261,261,261	0
8	MAN	J	628	11/12	0.87	0.27	-	261,261,261,261	0
6	NAG	J	626	14/15	0.84	0.21	-	261,261,261,261	0
6	NAG	J	617	14/15	0.72	0.36	-	279,293,304,311	0
8	MAN	J	639	11/12	0.87	0.34	-	261,261,261,261	0
6	NAG	C	702	14/15	0.86	0.61	-	285,303,316,317	0
6	NAG	C	701	14/15	0.82	0.21	-	296,313,326,330	0
8	MAN	J	650	11/12	0.82	0.64	-	261,261,261,261	0
8	MAN	G	623	11/12	0.66	1.33	-	261,261,261,261	0
8	MAN	A	640	11/12	0.63	0.28	-	261,261,261,261	0
7	BMA	A	653	11/12	0.87	0.33	-	251,268,283,285	0
8	MAN	A	630	11/12	0.60	0.98	-	261,261,261,261	0
8	MAN	J	656	11/12	0.79	0.50	-	321,323,332,338	0
8	MAN	A	622	11/12	0.68	0.71	-	261,261,261,261	0
6	NAG	A	608	14/15	0.80	0.32	-	295,304,312,313	0
6	NAG	J	665	14/15	0.88	0.37	-	296,306,323,326	0
7	BMA	G	646	11/12	0.73	0.29	-	261,261,261,261	0
6	NAG	K	702	14/15	0.81	0.57	-	285,303,316,317	0
6	NAG	G	661	14/15	0.92	0.46	-	293,311,318,323	0
8	MAN	G	621	11/12	0.68	0.27	-	261,261,261,261	0
8	MAN	J	622	11/12	0.72	0.49	-	261,261,261,261	0
6	NAG	J	637	14/15	0.90	0.28	-	261,261,261,261	0
8	MAN	J	660	11/12	0.81	0.44	-	327,335,339,340	0
7	BMA	J	603	11/12	0.74	0.42	-	252,263,287,290	0
8	MAN	J	635	11/12	0.78	0.46	-	261,261,261,261	0
8	MAN	G	649	11/12	0.74	0.48	-	261,261,261,261	0
8	MAN	J	648	11/12	0.92	0.40	-	261,261,261,261	0
8	MAN	J	659	11/12	0.84	0.25	-	301,306,311,311	0
8	MAN	A	649	11/12	0.74	0.69	-	261,261,261,261	0
7	BMA	A	638	11/12	0.81	0.19	-	261,261,261,261	0
8	MAN	A	639	11/12	0.85	0.36	-	261,261,261,261	0
8	MAN	A	621	11/12	0.54	0.35	-	261,261,261,261	0
7	BMA	J	653	11/12	0.90	0.21	-	251,268,283,285	0
6	NAG	A	666	14/15	0.80	0.44	-	307,328,330,330	0
8	MAN	G	610	11/12	0.61	0.54	-	325,342,352,353	0
8	MAN	A	648	11/12	0.87	0.49	-	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BMA	G	620	11/12	0.70	0.20	-	261,261,261,261	0
8	MAN	A	605	11/12	0.79	0.40	-	293,300,308,309	0
8	MAN	G	639	11/12	0.90	0.29	-	261,261,261,261	0
8	MAN	G	629	11/12	0.66	0.38	-	261,261,261,261	0
8	MAN	A	660	11/12	0.87	0.31	-	327,335,339,340	0
8	MAN	J	634	11/12	0.92	0.30	-	261,261,261,261	0
8	MAN	A	650	11/12	0.82	0.79	-	261,261,261,261	0
8	MAN	J	615	11/12	0.62	0.46	-	339,341,344,346	0
6	NAG	G	664	14/15	0.77	0.35	-	317,335,342,344	0
6	NAG	A	637	14/15	0.92	0.17	-	261,261,261,261	0
8	MAN	G	605	11/12	0.84	0.30	-	293,300,308,309	0
8	MAN	J	629	11/12	0.66	0.49	-	261,261,261,261	0
6	NAG	G	626	14/15	0.92	0.15	-	261,261,261,261	0
8	MAN	A	634	11/12	0.82	0.35	-	261,261,261,261	0
8	MAN	A	629	11/12	0.78	0.55	-	261,261,261,261	0
8	MAN	G	628	11/12	0.86	0.23	-	261,261,261,261	0
6	NAG	A	619	14/15	0.90	0.29	-	261,261,261,261	0
8	MAN	J	604	11/12	0.69	0.66	-	253,260,277,291	0
6	NAG	J	643	14/15	0.84	0.27	-	303,317,328,336	0
7	BMA	A	620	11/12	0.82	0.27	-	261,261,261,261	0
6	NAG	A	670	14/15	0.75	0.55	-	261,261,261,261	0
8	MAN	J	614	11/12	0.88	0.22	-	296,308,312,313	0
8	MAN	J	624	11/12	0.74	0.66	-	261,261,261,261	0
7	BMA	G	653	11/12	0.94	0.22	-	251,268,283,285	0
8	MAN	A	614	11/12	0.85	0.19	-	296,308,312,313	0
6	NAG	J	670	14/15	0.65	0.44	-	261,261,261,261	0
8	MAN	A	624	11/12	0.60	0.88	-	261,261,261,261	0
8	MAN	G	614	11/12	0.81	0.21	-	296,308,312,313	0
6	NAG	A	626	14/15	0.89	0.18	-	261,261,261,261	0
7	BMA	J	609	11/12	0.83	0.58	-	309,319,327,335	0
6	NAG	A	664	14/15	0.82	0.33	-	317,335,342,344	0
6	NAG	G	602	14/15	0.81	0.61	-	230,242,258,262	0
6	NAG	J	612	14/15	0.84	0.26	-	277,291,302,313	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.