



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2016 – 09:18 PM EDT

PDB ID : 5I8H
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer in Complex with V3 Loop-targeting Antibody PGT122 Fab and Fusion Peptide-targeting Antibody VRC34.01 Fab
Authors : Xu, K.; Zhou, T.; Kwong, P.D.
Deposited on : 2016-02-18
Resolution : 4.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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-20027674

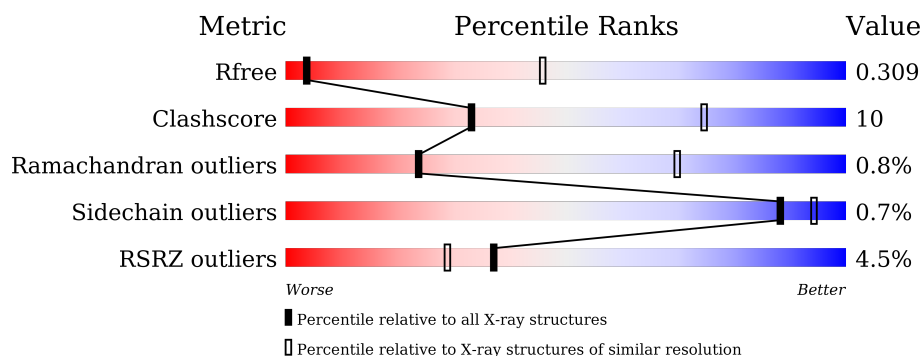
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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 ≥ 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	481	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	C	481	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• 6%</div> </div> </div>
2	B	153	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>14%</div> </div> </div>
2	D	153	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>• 14%</div> </div> </div>
3	J	210	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>•</div> </div> </div>
3	L	210	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>31%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	223	
4	G	223	
5	F	212	
5	H	212	
6	I	235	
6	K	235	

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
7	NAG	A	901	-	-	-	X
7	NAG	C	909	-	-	-	X
7	NAG	C	943	-	-	-	X
9	MAN	C	907	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23938 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 BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3576	2243	632	673	28			
1	C	450	Total	C	N	O	S	0	0	0
			3542	2223	625	666	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	GLU	conflict	UNP Q2N0S6
A	510	ARG	LYS	conflict	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			
2	D	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Fab light chain.

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

- Molecule 4 is a protein called VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			
4	G	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			

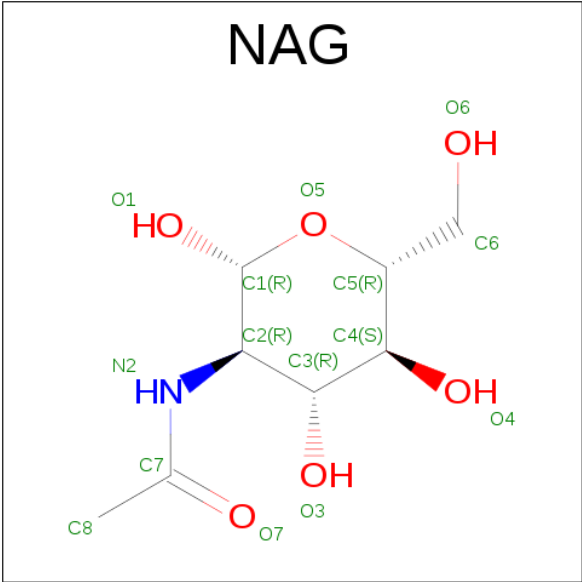
- Molecule 5 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			
5	H	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			

- Molecule 6 is a protein called PGT122 Fab heavy chain.

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

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

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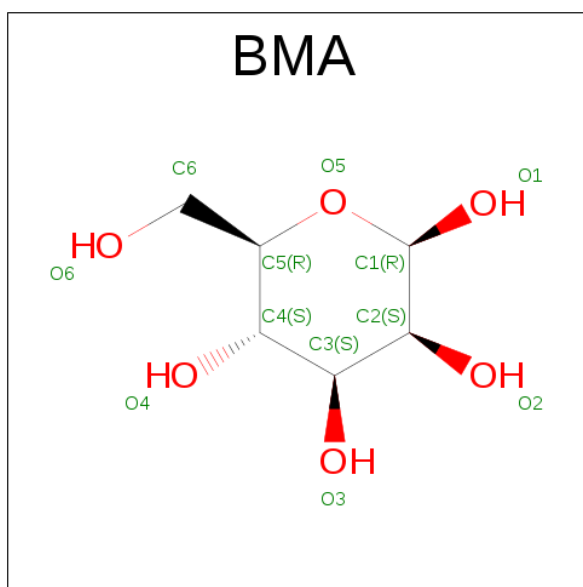
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

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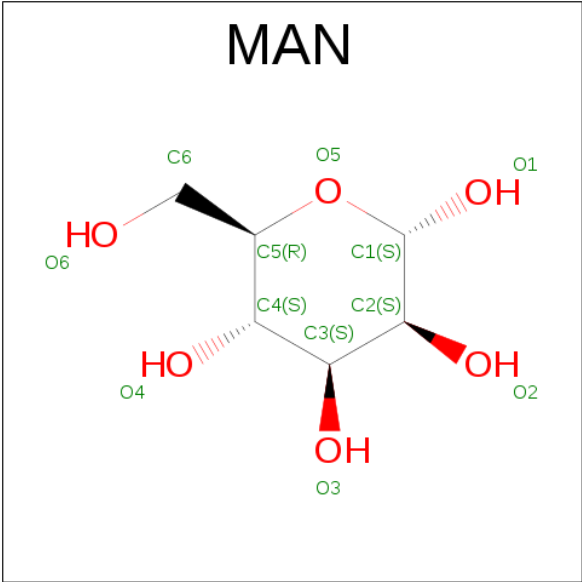
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

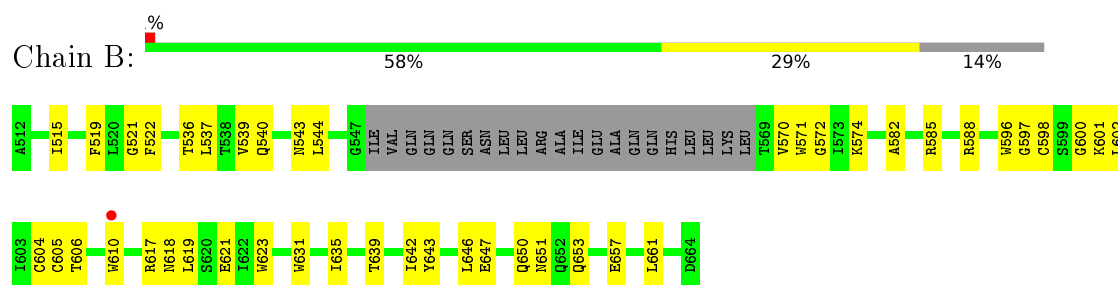


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9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

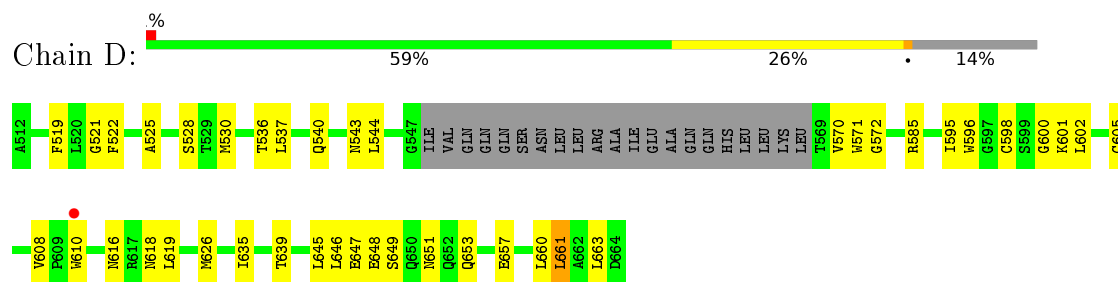
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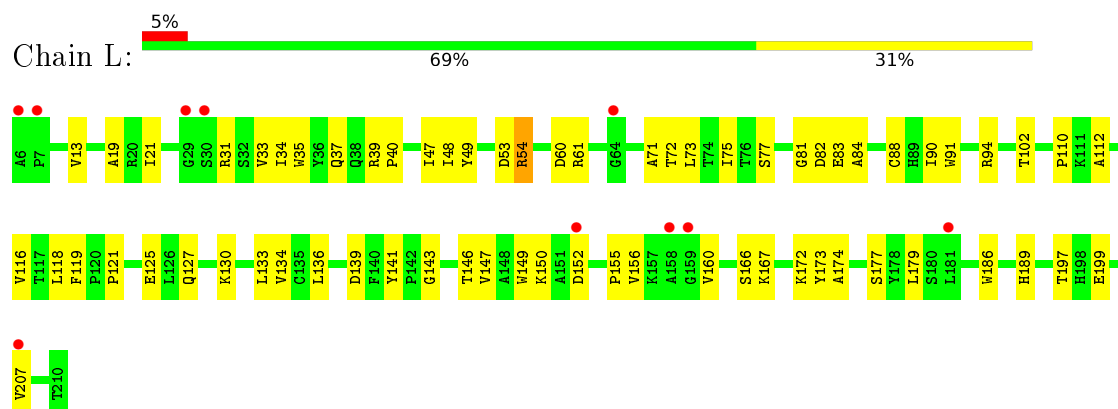
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		
9	A	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9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



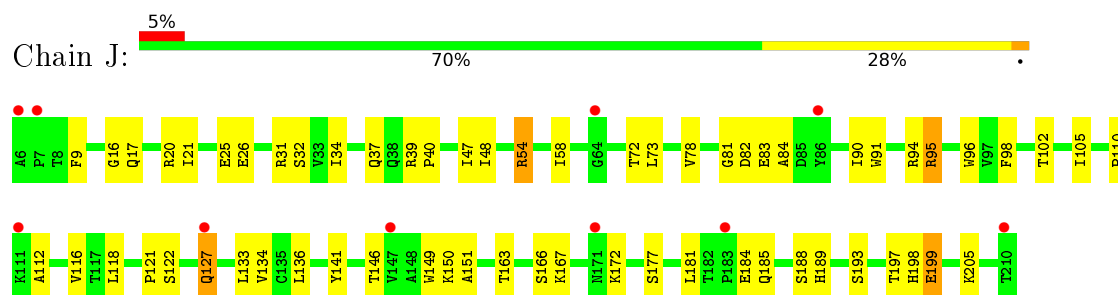
• Molecule 2: BG505 SOSIP.664 gp41



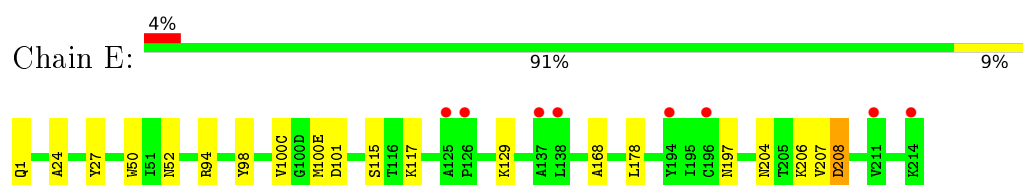
• Molecule 3: PGT122 Fab light chain



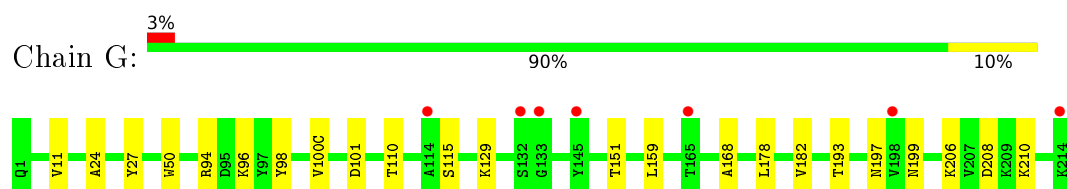
• Molecule 3: PGT122 Fab light chain



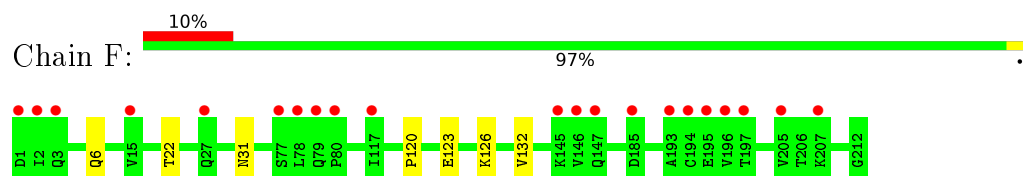
• Molecule 4: VRC34.01 Fab heavy chain



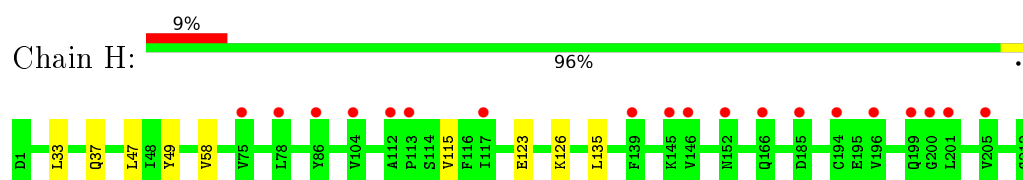
- Molecule 4: VRC34.01 Fab heavy chain



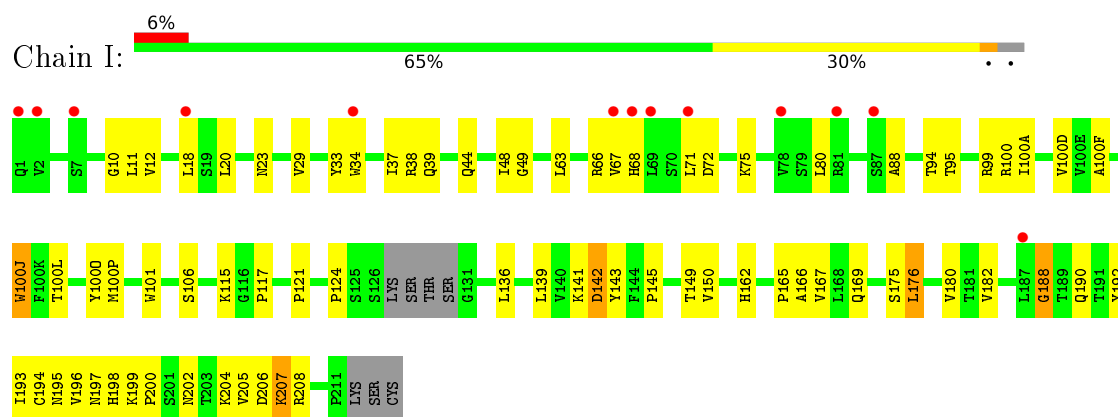
- Molecule 5: VRC34.01 Fab light chain



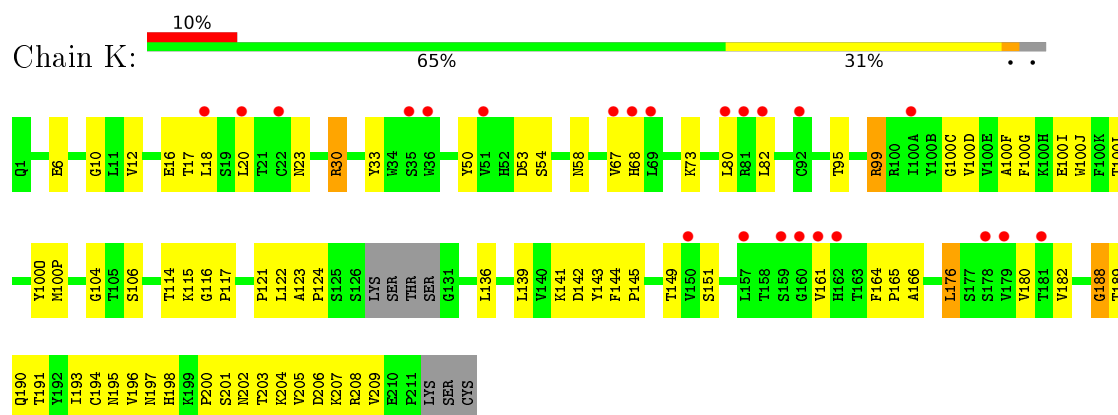
- Molecule 5: VRC34.01 Fab light chain



- Molecule 6: PGT122 Fab heavy chain



- Molecule 6: PGT122 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	252.30 Å 252.30 Å 561.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 4.30 48.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	54.9 (48.34-4.30) 55.1 (48.34-4.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 4.29 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.281 , 0.309 0.279 , 0.309	Depositor DCC
R_{free} test set	1315 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	127.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å ²)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.34	0/3650	0.66	3/4956 (0.1%)
1	C	0.34	0/3616	0.63	2/4911 (0.0%)
2	B	0.33	0/1052	0.59	0/1427
2	D	0.31	0/1052	0.61	1/1427 (0.1%)
3	J	0.36	0/1632	0.64	1/2236 (0.0%)
3	L	0.57	4/1632 (0.2%)	0.62	1/2236 (0.0%)
4	E	0.31	0/1715	0.56	0/2337
4	G	0.28	0/1715	0.50	0/2337
5	F	0.28	0/1665	0.52	0/2262
5	H	0.26	0/1665	0.50	0/2262
6	I	0.32	0/1789	0.65	3/2443 (0.1%)
6	K	0.33	0/1789	0.66	4/2443 (0.2%)
All	All	0.34	4/22972 (0.0%)	0.61	15/31277 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	54	ARG	CZ-NH1	-11.18	1.18	1.33
3	L	54	ARG	NE-CZ	-9.07	1.21	1.33
3	L	54	ARG	CZ-NH2	-7.11	1.23	1.33
3	L	54	ARG	CD-NE	-7.05	1.34	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	176	LEU	CA-CB-CG	9.21	136.48	115.30
1	A	138	ILE	CG1-CB-CG2	-9.11	91.35	111.40
6	K	176	LEU	CA-CB-CG	8.41	134.65	115.30
1	C	138	ILE	CG1-CB-CG2	-8.06	93.68	111.40
1	A	490	LYS	CA-CB-CG	6.53	127.77	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	208	ASP	Mainchain

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	3576	0	3509	88	0
1	C	3542	0	3471	92	0
2	B	1034	0	1011	42	0
2	D	1034	0	1012	31	0
3	J	1589	0	1530	55	0
3	L	1589	0	1529	54	0
4	E	1674	0	1638	25	0
4	G	1674	0	1638	20	0
5	F	1628	0	1588	12	0
5	H	1628	0	1588	8	0
6	I	1742	0	1713	59	0
6	K	1742	0	1715	67	0
7	A	420	0	371	9	0
7	B	42	0	39	0	0
7	C	434	0	384	8	0
7	D	28	0	26	0	0
7	I	42	0	37	0	0
7	K	14	0	13	0	0
8	A	66	0	52	0	0
8	C	66	0	52	0	0
8	I	11	0	9	0	0
9	A	176	0	151	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	176	0	152	1	0
9	I	11	0	9	0	0
All	All	23938	0	23237	485	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 10.

The worst 5 of 485 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:L:39:ARG:HD3	3:L:84:ALA:HB2	1.35	1.09
1:C:138:ILE:HG22	1:C:139:THR:HA	1.40	1.04
1:A:490:LYS:HG2	2:B:585:ARG:HH12	1.25	0.95
1:A:138:ILE:HG22	1:A:139:THR:HA	1.48	0.94
1:A:350:ARG:NH2	1:A:396:ILE:O	2.04	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/481 (93%)	405 (90%)	38 (8%)	6 (1%)	15	60
1	C	444/481 (92%)	402 (90%)	37 (8%)	5 (1%)	17	64
2	B	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	12	57
2	D	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	12	57
3	J	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	19	65
3	L	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	19	65
4	E	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
4	G	221/223 (99%)	218 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
5	H	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
6	I	224/235 (95%)	213 (95%)	9 (4%)	2 (1%)	21	67
6	K	224/235 (95%)	212 (95%)	10 (4%)	2 (1%)	21	67
All	All	2875/3028 (95%)	2691 (94%)	161 (6%)	23 (1%)	24	70

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	C	138	ILE
3	L	110	PRO
3	J	110	PRO
1	A	71	THR

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	405/428 (95%)	401 (99%)	4 (1%)	82	91
1	C	401/428 (94%)	399 (100%)	2 (0%)	92	96
2	B	110/129 (85%)	108 (98%)	2 (2%)	66	87
2	D	110/129 (85%)	109 (99%)	1 (1%)	84	92
3	J	178/178 (100%)	176 (99%)	2 (1%)	80	90
3	L	178/178 (100%)	178 (100%)	0	100	100
4	E	187/187 (100%)	186 (100%)	1 (0%)	92	96
4	G	187/187 (100%)	186 (100%)	1 (0%)	92	96
5	F	185/185 (100%)	185 (100%)	0	100	100
5	H	185/185 (100%)	184 (100%)	1 (0%)	92	96
6	I	198/205 (97%)	195 (98%)	3 (2%)	72	89
6	K	198/205 (97%)	197 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2522/2624 (96%)	2504 (99%)	18 (1%)	88	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	50	TRP
4	G	50	TRP
6	I	207	LYS
1	C	47	ASP
1	C	72	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	650	GLN
2	B	651	ASN
1	C	195	ASN
6	I	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

116 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	901	1,7	14,14,15	0.32	0	15,19,21	0.34	0
7	NAG	A	902	8,7	14,14,15	0.49	0	15,19,21	1.34	1 (6%)
8	BMA	A	903	9,7	11,11,12	0.64	0	15,15,17	0.89	1 (6%)
9	MAN	A	904	8	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
9	MAN	A	905	9,8	11,11,12	0.83	0	15,15,17	1.37	2 (13%)
9	MAN	A	906	9	11,11,12	4.08	8 (72%)	15,15,17	2.89	7 (46%)
9	MAN	A	907	9	11,11,12	1.24	1 (9%)	15,15,17	1.12	2 (13%)
7	NAG	A	908	1	14,14,15	0.19	0	15,19,21	0.34	0
7	NAG	A	909	1,7	14,14,15	0.19	0	15,19,21	0.32	0
7	NAG	A	910	8,7	14,14,15	0.23	0	15,19,21	0.28	0
8	BMA	A	911	9,7	11,11,12	0.67	0	15,15,17	0.77	0
9	MAN	A	912	8	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
9	MAN	A	913	8	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
7	NAG	A	914	1,7	14,14,15	0.23	0	15,19,21	0.40	0
7	NAG	A	915	7	14,14,15	0.45	0	15,19,21	1.28	1 (6%)
7	NAG	A	916	1,7	14,14,15	0.19	0	15,19,21	0.32	0
7	NAG	A	917	7	14,14,15	0.29	0	15,19,21	0.31	0
7	NAG	A	918	1,7	14,14,15	0.21	0	15,19,21	0.34	0
7	NAG	A	919	7	14,14,15	0.27	0	15,19,21	0.28	0
7	NAG	A	920	7	14,14,15	0.19	0	15,19,21	0.53	0
7	NAG	A	921	8,7	14,14,15	0.27	0	15,19,21	0.45	0
8	BMA	A	922	9,7	11,11,12	0.56	0	15,15,17	0.68	0
9	MAN	A	923	8	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
9	MAN	A	924	9,8	11,11,12	0.50	0	15,15,17	1.01	2 (13%)
9	MAN	A	925	9	11,11,12	0.80	0	15,15,17	1.17	2 (13%)
7	NAG	A	926	1	14,14,15	0.43	0	15,19,21	1.26	1 (6%)
7	NAG	A	927	1,7	14,14,15	0.42	0	15,19,21	0.48	0
7	NAG	A	928	8,7	14,14,15	0.42	0	15,19,21	0.59	0
8	BMA	A	929	7	11,11,12	1.19	0	15,15,17	1.10	2 (13%)
7	NAG	A	930	1,7	14,14,15	0.24	0	15,19,21	0.26	0
7	NAG	A	931	7	14,14,15	0.28	0	15,19,21	0.33	0
7	NAG	A	932	1,7	14,14,15	0.17	0	15,19,21	0.34	0
7	NAG	A	933	8,7	14,14,15	0.21	0	15,19,21	0.43	0
8	BMA	A	934	9,7	11,11,12	0.79	0	15,15,17	1.30	3 (20%)
9	MAN	A	935	9,8	11,11,12	0.57	0	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	A	936	9	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
9	MAN	A	937	9	11,11,12	0.70	0	15,15,17	0.97	2 (13%)
9	MAN	A	938	9,8	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
9	MAN	A	939	9	11,11,12	0.73	0	15,15,17	0.94	1 (6%)
9	MAN	A	940	9	11,11,12	0.73	1 (9%)	15,15,17	1.31	2 (13%)
9	MAN	A	941	9	11,11,12	0.83	0	15,15,17	1.12	2 (13%)
7	NAG	A	942	1	14,14,15	0.18	0	15,19,21	0.24	0
7	NAG	A	943	7	14,14,15	0.30	0	15,19,21	0.30	0
7	NAG	A	944	7	14,14,15	0.22	0	15,19,21	0.33	0
7	NAG	A	945	1,7	14,14,15	0.24	0	15,19,21	0.57	0
7	NAG	A	946	7	14,14,15	0.27	0	15,19,21	0.33	0
7	NAG	A	947	1,7	14,14,15	0.20	0	15,19,21	0.35	0
7	NAG	A	948	7	14,14,15	0.24	0	15,19,21	0.35	0
7	NAG	A	949	1,7	14,14,15	0.73	1 (7%)	15,19,21	0.51	0
7	NAG	A	950	8,7	14,14,15	0.25	0	15,19,21	0.31	0
8	BMA	A	951	7	11,11,12	0.60	0	15,15,17	0.77	0
7	NAG	A	952	1	14,14,15	0.69	1 (7%)	15,19,21	0.35	0
7	NAG	B	901	2	14,14,15	0.30	0	15,19,21	0.51	0
7	NAG	B	902	2	14,14,15	0.16	0	15,19,21	0.39	0
7	NAG	B	903	2	14,14,15	0.34	0	15,19,21	0.30	0
7	NAG	C	901	1,7	14,14,15	0.39	0	15,19,21	0.45	0
7	NAG	C	902	8,7	14,14,15	0.61	0	15,19,21	1.57	2 (13%)
8	BMA	C	903	9,7	11,11,12	1.50	1 (9%)	15,15,17	1.61	2 (13%)
9	MAN	C	904	8	11,11,12	1.15	2 (18%)	15,15,17	1.33	3 (20%)
9	MAN	C	905	9,8	11,11,12	1.61	2 (18%)	15,15,17	1.14	1 (6%)
9	MAN	C	906	9	11,11,12	1.69	1 (9%)	15,15,17	1.20	1 (6%)
9	MAN	C	907	9	11,11,12	2.43	4 (36%)	15,15,17	2.87	9 (60%)
7	NAG	C	908	1	14,14,15	0.27	0	15,19,21	0.35	0
7	NAG	C	909	1	14,14,15	0.34	0	15,19,21	0.39	0
7	NAG	C	910	1,7	14,14,15	0.31	0	15,19,21	0.24	0
7	NAG	C	911	8,7	14,14,15	0.22	0	15,19,21	0.27	0
8	BMA	C	912	9,7	11,11,12	0.76	0	15,15,17	0.75	0
9	MAN	C	913	8	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
9	MAN	C	914	8	11,11,12	0.71	0	15,15,17	1.06	2 (13%)
7	NAG	C	915	1,7	14,14,15	0.25	0	15,19,21	0.37	0
7	NAG	C	916	7	14,14,15	0.53	0	15,19,21	1.28	1 (6%)
7	NAG	C	917	1,7	14,14,15	0.20	0	15,19,21	0.31	0
7	NAG	C	918	7	14,14,15	0.29	0	15,19,21	0.33	0
7	NAG	C	919	1,7	14,14,15	0.25	0	15,19,21	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	920	7	14,14,15	0.28	0	15,19,21	0.29	0
7	NAG	C	921	1,7	14,14,15	0.43	0	15,19,21	0.44	0
7	NAG	C	922	8,7	14,14,15	0.24	0	15,19,21	0.37	0
8	BMA	C	923	9,7	11,11,12	0.66	0	15,15,17	0.77	0
9	MAN	C	924	8	11,11,12	0.57	0	15,15,17	1.04	2 (13%)
9	MAN	C	925	9,8	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
9	MAN	C	926	9	11,11,12	0.75	0	15,15,17	1.13	2 (13%)
7	NAG	C	927	1	14,14,15	0.44	0	15,19,21	1.27	1 (6%)
7	NAG	C	928	1,7	14,14,15	0.50	0	15,19,21	0.46	0
7	NAG	C	929	7	14,14,15	0.31	0	15,19,21	0.27	0
7	NAG	C	930	1,7	14,14,15	0.21	0	15,19,21	0.26	0
7	NAG	C	931	7	14,14,15	0.27	0	15,19,21	0.36	0
7	NAG	C	932	1,7	14,14,15	0.21	0	15,19,21	0.36	0
7	NAG	C	933	8,7	14,14,15	0.21	0	15,19,21	0.43	0
8	BMA	C	934	9,7	11,11,12	0.65	0	15,15,17	1.26	2 (13%)
9	MAN	C	935	9,8	11,11,12	0.64	0	15,15,17	0.92	1 (6%)
9	MAN	C	936	9	11,11,12	0.69	0	15,15,17	1.01	2 (13%)
9	MAN	C	937	9	11,11,12	0.67	0	15,15,17	0.94	1 (6%)
9	MAN	C	938	9,8	11,11,12	0.76	0	15,15,17	1.03	2 (13%)
9	MAN	C	939	9	11,11,12	0.84	0	15,15,17	1.00	1 (6%)
9	MAN	C	940	9	11,11,12	0.84	1 (9%)	15,15,17	1.29	1 (6%)
9	MAN	C	941	9	11,11,12	0.81	0	15,15,17	1.21	2 (13%)
7	NAG	C	942	1	14,14,15	0.27	0	15,19,21	0.73	0
7	NAG	C	943	1,7	14,14,15	0.37	0	15,19,21	0.30	0
7	NAG	C	944	7	14,14,15	0.25	0	15,19,21	0.35	0
7	NAG	C	945	1,7	14,14,15	0.41	0	15,19,21	0.57	0
7	NAG	C	946	7	14,14,15	0.32	0	15,19,21	0.31	0
7	NAG	C	947	1,7	14,14,15	0.41	0	15,19,21	0.50	0
7	NAG	C	948	8,7	14,14,15	0.36	0	15,19,21	0.68	0
8	BMA	C	949	7	11,11,12	0.72	0	15,15,17	0.87	0
7	NAG	C	950	1,7	14,14,15	0.33	0	15,19,21	0.57	0
7	NAG	C	951	8,7	14,14,15	0.28	0	15,19,21	0.22	0
8	BMA	C	952	7	11,11,12	0.54	0	15,15,17	0.80	0
7	NAG	C	953	1	14,14,15	0.28	0	15,19,21	0.37	0
7	NAG	D	901	2	14,14,15	0.38	0	15,19,21	0.52	0
7	NAG	D	902	2	14,14,15	0.35	0	15,19,21	0.28	0
7	NAG	I	301	1,7	14,14,15	0.44	0	15,19,21	0.45	0
7	NAG	I	302	8,7	14,14,15	0.36	0	15,19,21	0.23	0
8	BMA	I	303	9,7	11,11,12	0.56	0	15,15,17	0.74	0
9	MAN	I	304	8,6	11,11,12	0.91	1 (9%)	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	305	6	14,14,15	2.11	2 (14%)	15,19,21	0.81	0
7	NAG	K	301	6	14,14,15	2.03	2 (14%)	15,19,21	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	902	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	903	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	904	8	-	0/2/19/22	0/1/1/1
9	MAN	A	905	9,8	-	0/2/19/22	1/1/1/1
9	MAN	A	906	9	-	0/2/19/22	1/1/1/1
9	MAN	A	907	9	-	0/2/19/22	0/1/1/1
7	NAG	A	908	1	-	0/6/23/26	0/1/1/1
7	NAG	A	909	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	910	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	911	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	912	8	-	0/2/19/22	0/1/1/1
9	MAN	A	913	8	-	0/2/19/22	0/1/1/1
7	NAG	A	914	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	915	7	-	0/6/23/26	0/1/1/1
7	NAG	A	916	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	917	7	-	0/6/23/26	0/1/1/1
7	NAG	A	918	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	919	7	-	0/6/23/26	0/1/1/1
7	NAG	A	920	7	-	0/6/23/26	0/1/1/1
7	NAG	A	921	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	922	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	923	8	-	0/2/19/22	0/1/1/1
9	MAN	A	924	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	925	9	-	0/2/19/22	1/1/1/1
7	NAG	A	926	1	-	0/6/23/26	0/1/1/1
7	NAG	A	927	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	928	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	929	7	-	0/2/19/22	0/1/1/1
7	NAG	A	930	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	931	7	-	0/6/23/26	0/1/1/1
7	NAG	A	932	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	933	8,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	A	934	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	935	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	936	9	-	0/2/19/22	0/1/1/1
9	MAN	A	937	9	-	0/2/19/22	0/1/1/1
9	MAN	A	938	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	939	9	-	0/2/19/22	0/1/1/1
9	MAN	A	940	9	-	0/2/19/22	0/1/1/1
9	MAN	A	941	9	-	0/2/19/22	1/1/1/1
7	NAG	A	942	1	-	0/6/23/26	0/1/1/1
7	NAG	A	943	7	-	0/6/23/26	0/1/1/1
7	NAG	A	944	7	-	0/6/23/26	0/1/1/1
7	NAG	A	945	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	946	7	-	0/6/23/26	0/1/1/1
7	NAG	A	947	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	948	7	-	0/6/23/26	0/1/1/1
7	NAG	A	949	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	950	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	951	7	-	0/2/19/22	0/1/1/1
7	NAG	A	952	1	-	0/6/23/26	0/1/1/1
7	NAG	B	901	2	-	0/6/23/26	0/1/1/1
7	NAG	B	902	2	-	0/6/23/26	0/1/1/1
7	NAG	B	903	2	-	0/6/23/26	0/1/1/1
7	NAG	C	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	902	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	903	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	904	8	-	0/2/19/22	0/1/1/1
9	MAN	C	905	9,8	-	0/2/19/22	1/1/1/1
9	MAN	C	906	9	-	0/2/19/22	0/1/1/1
9	MAN	C	907	9	-	0/2/19/22	1/1/1/1
7	NAG	C	908	1	-	0/6/23/26	0/1/1/1
7	NAG	C	909	1	-	0/6/23/26	0/1/1/1
7	NAG	C	910	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	911	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	912	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	913	8	-	0/2/19/22	0/1/1/1
9	MAN	C	914	8	-	0/2/19/22	0/1/1/1
7	NAG	C	915	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	916	7	-	0/6/23/26	0/1/1/1
7	NAG	C	917	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	918	7	-	0/6/23/26	0/1/1/1
7	NAG	C	919	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	920	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	921	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	922	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	923	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	924	8	-	0/2/19/22	0/1/1/1
9	MAN	C	925	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	926	9	-	0/2/19/22	1/1/1/1
7	NAG	C	927	1	-	0/6/23/26	0/1/1/1
7	NAG	C	928	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	929	7	-	0/6/23/26	0/1/1/1
7	NAG	C	930	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	931	7	-	0/6/23/26	0/1/1/1
7	NAG	C	932	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	933	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	934	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	935	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	936	9	-	0/2/19/22	0/1/1/1
9	MAN	C	937	9	-	0/2/19/22	0/1/1/1
9	MAN	C	938	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	939	9	-	0/2/19/22	0/1/1/1
9	MAN	C	940	9	-	0/2/19/22	0/1/1/1
9	MAN	C	941	9	-	0/2/19/22	1/1/1/1
7	NAG	C	942	1	-	0/6/23/26	0/1/1/1
7	NAG	C	943	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	944	7	-	0/6/23/26	0/1/1/1
7	NAG	C	945	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	946	7	-	0/6/23/26	0/1/1/1
7	NAG	C	947	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	948	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	949	7	-	0/2/19/22	0/1/1/1
7	NAG	C	950	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	951	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	952	7	-	0/2/19/22	0/1/1/1
7	NAG	C	953	1	-	0/6/23/26	0/1/1/1
7	NAG	D	901	2	-	0/6/23/26	0/1/1/1
7	NAG	D	902	2	-	0/6/23/26	0/1/1/1
7	NAG	I	301	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	302	8,7	-	0/6/23/26	0/1/1/1
8	BMA	I	303	9,7	-	0/2/19/22	0/1/1/1
9	MAN	I	304	8,6	-	0/2/19/22	0/1/1/1
7	NAG	I	305	6	-	0/6/23/26	0/1/1/1
7	NAG	K	301	6	-	0/6/23/26	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	903	BMA	O5-C1	-4.28	1.36	1.43
9	A	906	MAN	O4-C4	-3.73	1.34	1.43
9	A	907	MAN	O5-C1	-3.37	1.38	1.43
7	I	305	NAG	C1-C2	-2.74	1.48	1.52
9	A	906	MAN	O5-C1	-2.72	1.39	1.43

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	906	MAN	C3-C4-C5	-5.15	101.05	110.23
8	C	903	BMA	O6-C6-C5	-4.52	96.22	111.30
7	C	902	NAG	O4-C4-C5	-3.16	100.89	109.23
9	C	904	MAN	O2-C2-C3	-2.84	104.47	110.19
9	A	907	MAN	O2-C2-C3	-2.55	105.04	110.19

There are no chirality outliers.

There are no torsion outliers.

5 of 8 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	905	MAN	C1-C2-C3-C4-C5-O5
9	C	907	MAN	C1-C2-C3-C4-C5-O5
9	C	905	MAN	C1-C2-C3-C4-C5-O5
9	A	941	MAN	C1-C2-C3-C4-C5-O5
9	C	941	MAN	C1-C2-C3-C4-C5-O5

20 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	902	NAG	1	0
9	A	905	MAN	2	0
7	A	908	NAG	2	0
7	A	914	NAG	3	0
7	A	915	NAG	2	0
9	A	924	MAN	2	0
7	A	926	NAG	1	0
9	A	937	MAN	1	0
9	A	941	MAN	1	0
7	A	949	NAG	1	0
7	C	901	NAG	1	0
7	C	902	NAG	1	0
7	C	915	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	916	NAG	2	0
9	C	925	MAN	1	0
7	C	927	NAG	1	0
7	C	933	NAG	1	0
7	C	943	NAG	1	0
7	C	945	NAG	1	0
7	C	946	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/481 (94%)	-0.06	7 (1%) 76 67	118, 169, 241, 272	0
1	C	450/481 (93%)	-0.02	10 (2%) 65 56	125, 167, 239, 284	0
2	B	132/153 (86%)	-0.22	1 (0%) 87 82	115, 171, 238, 256	0
2	D	132/153 (86%)	-0.14	1 (0%) 87 82	122, 177, 233, 246	0
3	J	210/210 (100%)	0.14	10 (4%) 34 26	190, 267, 327, 375	0
3	L	210/210 (100%)	0.13	10 (4%) 34 26	188, 278, 318, 331	0
4	E	223/223 (100%)	0.08	8 (3%) 46 37	136, 205, 293, 332	0
4	G	223/223 (100%)	0.08	7 (3%) 52 41	141, 192, 284, 320	0
5	F	212/212 (100%)	0.30	21 (9%) 9 8	171, 266, 317, 340	0
5	H	212/212 (100%)	0.46	19 (8%) 12 9	157, 244, 296, 314	0
6	I	228/235 (97%)	0.18	13 (5%) 27 20	187, 251, 285, 313	0
6	K	228/235 (97%)	0.33	23 (10%) 9 8	188, 249, 281, 302	0
All	All	2915/3028 (96%)	0.10	130 (4%) 37 29	115, 214, 301, 375	0

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	126	PRO	7.2
5	F	194	CYS	6.3
5	H	113	PRO	5.7
3	J	6	ALA	5.3
5	F	78	LEU	5.1

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

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	A	901	14/15	0.82	0.39	3.88	163,173,183,185	0
7	NAG	C	943	14/15	0.79	0.79	1.53	229,247,272,295	0
7	NAG	C	909	14/15	0.57	0.44	1.53	197,225,250,254	0
9	MAN	I	304	11/12	0.82	0.35	0.69	245,269,280,281	0
7	NAG	C	921	14/15	0.96	0.27	0.65	150,168,186,195	0
7	NAG	A	916	14/15	0.81	0.36	0.62	167,198,218,233	0
7	NAG	C	908	14/15	0.79	0.28	0.59	232,249,265,272	0
7	NAG	C	915	14/15	0.81	0.25	0.55	174,198,206,219	0
7	NAG	I	301	14/15	0.79	0.28	0.52	213,241,264,267	0
9	MAN	C	907	11/12	0.73	0.47	0.37	193,214,225,236	0
9	MAN	A	939	11/12	0.90	0.31	0.05	220,225,240,246	0
7	NAG	C	910	14/15	0.88	0.33	-0.10	152,193,211,215	0
7	NAG	A	909	14/15	0.87	0.26	-0.19	154,199,216,219	0
7	NAG	A	920	14/15	0.95	0.25	-0.19	134,153,170,180	0
7	NAG	C	917	14/15	0.86	0.29	-0.33	160,193,213,228	0
7	NAG	A	908	14/15	0.82	0.25	-0.47	217,234,248,253	0
7	NAG	A	932	14/15	0.89	0.24	-0.48	171,178,197,199	0
7	NAG	C	928	14/15	0.81	0.23	-0.48	175,193,219,228	0
7	NAG	A	933	14/15	0.93	0.31	-0.63	173,191,216,220	0
7	NAG	C	933	14/15	0.92	0.26	-0.80	182,200,232,234	0
7	NAG	A	914	14/15	0.86	0.23	-0.83	180,203,213,224	0
7	NAG	A	927	14/15	0.87	0.20	-0.89	177,194,220,229	0
9	MAN	C	939	11/12	0.81	0.20	-0.92	214,223,238,241	0
9	MAN	A	938	11/12	0.94	0.18	-1.51	193,197,218,238	0
7	NAG	A	921	14/15	0.93	0.14	-1.52	182,197,208,218	0
9	MAN	C	938	11/12	0.92	0.14	-1.61	194,198,219,238	0
7	NAG	C	932	14/15	0.93	0.16	-1.69	173,180,196,200	0
7	NAG	C	920	14/15	0.74	0.68	-	262,273,276,279	0
7	NAG	B	903	14/15	0.78	0.43	-	230,262,292,295	0
8	BMA	A	911	11/12	0.64	0.27	-	256,265,276,285	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	BMA	C	934	11/12	0.93	0.11	-	178,200,214,222	0
8	BMA	C	912	11/12	0.84	0.14	-	245,253,263,273	0
7	NAG	A	919	14/15	0.85	0.72	-	241,246,251,252	0
9	MAN	C	941	11/12	0.93	0.21	-	227,237,242,243	0
8	BMA	C	903	11/12	0.91	0.27	-	192,205,231,233	0
9	MAN	A	905	11/12	0.75	0.23	-	221,227,234,235	0
7	NAG	A	946	14/15	0.73	0.32	-	226,244,249,249	0
7	NAG	A	918	14/15	0.93	0.48	-	193,211,222,236	0
7	NAG	D	901	14/15	0.78	0.37	-	265,277,303,319	0
8	BMA	C	949	11/12	0.54	0.64	-	273,279,285,287	0
9	MAN	A	913	11/12	0.61	0.24	-	288,291,294,297	0
9	MAN	A	906	11/12	0.81	0.39	-	219,226,240,243	0
9	MAN	A	925	11/12	0.94	0.31	-	226,232,234,235	0
7	NAG	C	951	14/15	0.66	0.44	-	226,247,272,300	0
7	NAG	A	910	14/15	0.90	0.47	-	219,233,244,254	0
9	MAN	A	923	11/12	0.90	0.12	-	232,250,257,258	0
9	MAN	A	904	11/12	0.93	0.76	-	207,216,231,247	0
7	NAG	A	931	14/15	0.84	0.42	-	222,235,246,253	0
7	NAG	C	947	14/15	0.74	0.27	-	233,245,258,269	0
9	MAN	C	940	11/12	0.90	0.20	-	229,236,242,244	0
7	NAG	C	919	14/15	0.78	0.61	-	216,233,245,258	0
7	NAG	C	945	14/15	0.90	0.24	-	178,218,237,249	0
8	BMA	A	922	11/12	0.88	0.13	-	225,231,246,253	0
8	BMA	I	303	11/12	0.61	0.25	-	259,268,274,282	0
7	NAG	C	948	14/15	0.61	0.43	-	241,271,282,284	0
7	NAG	C	911	14/15	0.91	0.27	-	206,220,230,238	0
8	BMA	C	952	11/12	0.65	0.68	-	268,300,328,382	0
7	NAG	A	902	14/15	0.91	0.37	-	171,183,199,203	0
7	NAG	D	902	14/15	0.60	0.24	-	225,248,271,272	0
7	NAG	A	926	14/15	0.85	0.30	-	210,217,221,223	0
7	NAG	C	918	14/15	0.63	1.06	-	224,242,261,263	0
7	NAG	C	931	14/15	0.86	0.28	-	219,230,241,248	0
9	MAN	C	905	11/12	0.81	0.25	-	199,208,215,215	0
7	NAG	C	946	14/15	0.87	0.22	-	224,246,254,254	0
8	BMA	C	923	11/12	0.88	0.12	-	238,243,259,266	0
9	MAN	A	912	11/12	0.84	0.25	-	241,253,257,259	0
9	MAN	C	913	11/12	0.84	0.20	-	229,240,246,246	0
9	MAN	C	926	11/12	0.89	0.25	-	254,262,264,266	0
7	NAG	A	943	14/15	0.84	0.34	-	219,234,259,280	0
7	NAG	A	947	14/15	0.92	0.24	-	231,245,265,272	0
9	MAN	C	937	11/12	0.96	0.12	-	236,237,242,246	0
7	NAG	A	949	14/15	0.82	0.25	-	189,207,219,223	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	C	902	14/15	0.93	0.28	-	173,188,199,202	0
7	NAG	A	945	14/15	0.86	0.26	-	184,222,240,252	0
9	MAN	A	935	11/12	0.96	0.19	-	189,208,215,222	0
7	NAG	C	927	14/15	0.87	0.67	-	218,225,232,234	0
7	NAG	C	922	14/15	0.93	0.19	-	197,210,221,229	0
7	NAG	A	952	14/15	0.89	0.16	-	233,255,262,265	0
9	MAN	C	906	11/12	0.75	0.39	-	220,225,239,240	0
7	NAG	A	928	14/15	0.81	0.28	-	212,223,235,244	0
7	NAG	B	902	14/15	0.52	1.27	-	260,274,299,300	0
7	NAG	A	950	14/15	0.76	0.28	-	199,221,246,273	0
9	MAN	C	925	11/12	0.85	0.36	-	248,257,269,274	0
7	NAG	C	929	14/15	0.89	0.22	-	204,213,227,236	0
7	NAG	A	944	14/15	0.81	0.50	-	252,267,276,276	0
9	MAN	A	940	11/12	0.93	0.18	-	233,240,243,244	0
9	MAN	A	937	11/12	0.94	0.28	-	235,238,245,250	0
7	NAG	K	301	14/15	0.43	0.87	-	255,274,293,293	0
7	NAG	A	930	14/15	0.88	0.54	-	179,194,209,223	0
7	NAG	C	916	14/15	0.63	0.64	-	224,237,247,255	0
8	BMA	A	903	11/12	0.85	0.37	-	192,202,224,227	0
9	MAN	A	941	11/12	0.77	0.39	-	237,244,248,248	0
7	NAG	C	901	14/15	0.92	0.30	-	177,185,200,200	0
7	NAG	A	948	14/15	0.84	0.30	-	243,268,273,274	0
7	NAG	A	942	14/15	0.63	0.52	-	246,259,268,272	0
7	NAG	B	901	14/15	0.89	0.33	-	239,260,288,303	0
7	NAG	A	915	14/15	0.78	0.70	-	224,236,248,255	0
8	BMA	A	951	11/12	0.76	0.23	-	209,244,274,327	0
9	MAN	A	907	11/12	0.77	0.34	-	189,208,218,228	0
7	NAG	C	950	14/15	0.83	0.25	-	196,212,229,234	0
9	MAN	C	936	11/12	0.73	0.45	-	207,223,229,232	0
9	MAN	A	924	11/12	0.88	0.46	-	235,244,255,261	0
9	MAN	C	914	11/12	0.72	0.20	-	291,294,295,297	0
7	NAG	A	917	14/15	0.65	0.67	-	235,250,266,269	0
7	NAG	I	302	14/15	0.85	0.19	-	242,251,265,266	0
8	BMA	A	929	11/12	0.72	0.43	-	238,239,241,241	0
7	NAG	C	953	14/15	0.81	0.17	-	212,234,244,246	0
9	MAN	C	924	11/12	0.89	0.20	-	246,266,272,274	0
9	MAN	C	935	11/12	0.92	0.15	-	201,219,226,237	0
7	NAG	I	305	14/15	0.04	1.67	-	262,282,291,294	0
7	NAG	C	930	14/15	0.87	0.36	-	182,197,215,223	0
7	NAG	C	942	14/15	0.83	0.32	-	230,246,255,260	0
9	MAN	A	936	11/12	0.86	0.27	-	200,214,222,222	0
8	BMA	A	934	11/12	0.96	0.21	-	178,197,213,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MAN	C	904	11/12	0.89	0.45	-	196,199,218,231	0
7	NAG	C	944	14/15	0.67	1.01	-	276,295,304,306	0

6.5 Other polymers [i](#)

There are no such residues in this entry.