



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2017 – 07:10 PM EST

PDB ID : 5UQY  
Title : Crystal structure of Marburg virus GP in complex with the human survivor antibody MR78  
Authors : Hashiguchi, T.; Fusco, M.L.; Hastie, K.M.; Bomholdt, Z.A.; Lee, J.E.; Flyak, A.I.; Matsuoka, R.; Kohda, D.; Yanagi, Y.; Hammel, M.; Crowe, J.E.; Saphire, E.O.  
Deposited on : 2017-02-08  
Resolution : 3.60 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-20028442
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-20028442

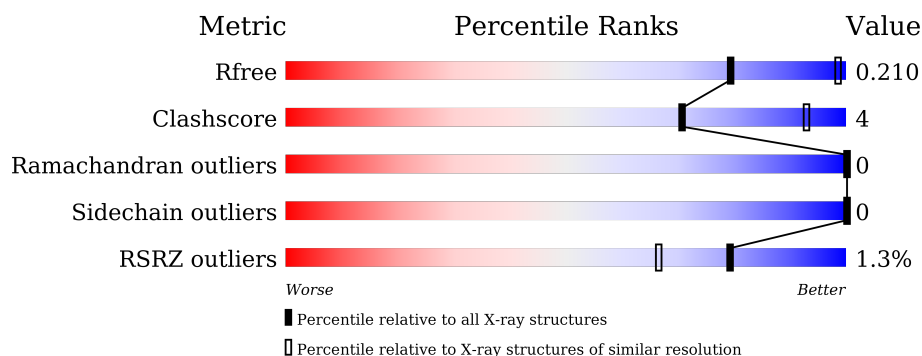
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	250	<div> <div>51%</div> <div>7%</div> <div>42%</div> </div>
1	E	250	<div>2%</div> <div>52%</div> <div>6%</div> <div>42%</div>

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Mol	Chain	Length	Quality of chain
2	J	237	
2	N	237	
3	C	211	
3	G	211	
3	K	211	
3	O	211	
4	D	226	
4	H	226	
4	L	226	
4	P	226	

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
5	NAG	N	701	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21208 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 GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1131	717	198	209	7			
1	E	144	Total	C	N	O	S	0	0	0
			1122	712	197	207	6			
1	I	142	Total	C	N	O	S	0	0	0
			1112	706	195	205	6			
1	M	142	Total	C	N	O	S	0	0	0
			1112	706	195	205	6			

- Molecule 2 is a protein called ENVELOPE GLYCOPROTEIN GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	0
			962	608	167	182	5			
2	F	94	Total	C	N	O	S	0	0	0
			740	470	131	137	2			
2	J	97	Total	C	N	O	S	0	0	0
			752	477	133	140	2			
2	N	92	Total	C	N	O	S	0	0	0
			722	460	128	132	2			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	438	LEU	PHE	engineered mutation	UNP Q1PDC7
B	439	ALA	TRP	engineered mutation	UNP Q1PDC7
B	445	GLY	PHE	engineered mutation	UNP Q1PDC7
B	447	ASN	PHE	engineered mutation	UNP Q1PDC7
B	638	ASP	-	expression tag	UNP Q1PDC7
B	639	ASP	-	expression tag	UNP Q1PDC7
B	640	ASP	-	expression tag	UNP Q1PDC7
B	641	ASP	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	642	LYS	-	expression tag	UNP Q1PDC7
B	643	ALA	-	expression tag	UNP Q1PDC7
B	644	GLY	-	expression tag	UNP Q1PDC7
B	645	TRP	-	expression tag	UNP Q1PDC7
B	646	SER	-	expression tag	UNP Q1PDC7
B	647	HIS	-	expression tag	UNP Q1PDC7
B	648	PRO	-	expression tag	UNP Q1PDC7
B	649	GLN	-	expression tag	UNP Q1PDC7
B	650	PHE	-	expression tag	UNP Q1PDC7
B	651	GLU	-	expression tag	UNP Q1PDC7
B	652	LYS	-	expression tag	UNP Q1PDC7
B	653	GLY	-	expression tag	UNP Q1PDC7
B	654	GLY	-	expression tag	UNP Q1PDC7
B	655	GLY	-	expression tag	UNP Q1PDC7
B	656	SER	-	expression tag	UNP Q1PDC7
B	657	GLY	-	expression tag	UNP Q1PDC7
B	658	GLY	-	expression tag	UNP Q1PDC7
B	659	GLY	-	expression tag	UNP Q1PDC7
B	660	SER	-	expression tag	UNP Q1PDC7
B	661	GLY	-	expression tag	UNP Q1PDC7
B	662	GLY	-	expression tag	UNP Q1PDC7
B	663	GLY	-	expression tag	UNP Q1PDC7
B	664	SER	-	expression tag	UNP Q1PDC7
B	665	TRP	-	expression tag	UNP Q1PDC7
B	666	SER	-	expression tag	UNP Q1PDC7
B	667	HIS	-	expression tag	UNP Q1PDC7
B	668	PRO	-	expression tag	UNP Q1PDC7
B	669	GLN	-	expression tag	UNP Q1PDC7
B	670	PHE	-	expression tag	UNP Q1PDC7
B	671	GLU	-	expression tag	UNP Q1PDC7
B	672	LYS	-	expression tag	UNP Q1PDC7
F	438	LEU	PHE	engineered mutation	UNP Q1PDC7
F	439	ALA	TRP	engineered mutation	UNP Q1PDC7
F	445	GLY	PHE	engineered mutation	UNP Q1PDC7
F	447	ASN	PHE	engineered mutation	UNP Q1PDC7
F	638	ASP	-	expression tag	UNP Q1PDC7
F	639	ASP	-	expression tag	UNP Q1PDC7
F	640	ASP	-	expression tag	UNP Q1PDC7
F	641	ASP	-	expression tag	UNP Q1PDC7
F	642	LYS	-	expression tag	UNP Q1PDC7
F	643	ALA	-	expression tag	UNP Q1PDC7
F	644	GLY	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	645	TRP	-	expression tag	UNP Q1PDC7
F	646	SER	-	expression tag	UNP Q1PDC7
F	647	HIS	-	expression tag	UNP Q1PDC7
F	648	PRO	-	expression tag	UNP Q1PDC7
F	649	GLN	-	expression tag	UNP Q1PDC7
F	650	PHE	-	expression tag	UNP Q1PDC7
F	651	GLU	-	expression tag	UNP Q1PDC7
F	652	LYS	-	expression tag	UNP Q1PDC7
F	653	GLY	-	expression tag	UNP Q1PDC7
F	654	GLY	-	expression tag	UNP Q1PDC7
F	655	GLY	-	expression tag	UNP Q1PDC7
F	656	SER	-	expression tag	UNP Q1PDC7
F	657	GLY	-	expression tag	UNP Q1PDC7
F	658	GLY	-	expression tag	UNP Q1PDC7
F	659	GLY	-	expression tag	UNP Q1PDC7
F	660	SER	-	expression tag	UNP Q1PDC7
F	661	GLY	-	expression tag	UNP Q1PDC7
F	662	GLY	-	expression tag	UNP Q1PDC7
F	663	GLY	-	expression tag	UNP Q1PDC7
F	664	SER	-	expression tag	UNP Q1PDC7
F	665	TRP	-	expression tag	UNP Q1PDC7
F	666	SER	-	expression tag	UNP Q1PDC7
F	667	HIS	-	expression tag	UNP Q1PDC7
F	668	PRO	-	expression tag	UNP Q1PDC7
F	669	GLN	-	expression tag	UNP Q1PDC7
F	670	PHE	-	expression tag	UNP Q1PDC7
F	671	GLU	-	expression tag	UNP Q1PDC7
F	672	LYS	-	expression tag	UNP Q1PDC7
J	438	LEU	PHE	engineered mutation	UNP Q1PDC7
J	439	ALA	TRP	engineered mutation	UNP Q1PDC7
J	445	GLY	PHE	engineered mutation	UNP Q1PDC7
J	447	ASN	PHE	engineered mutation	UNP Q1PDC7
J	638	ASP	-	expression tag	UNP Q1PDC7
J	639	ASP	-	expression tag	UNP Q1PDC7
J	640	ASP	-	expression tag	UNP Q1PDC7
J	641	ASP	-	expression tag	UNP Q1PDC7
J	642	LYS	-	expression tag	UNP Q1PDC7
J	643	ALA	-	expression tag	UNP Q1PDC7
J	644	GLY	-	expression tag	UNP Q1PDC7
J	645	TRP	-	expression tag	UNP Q1PDC7
J	646	SER	-	expression tag	UNP Q1PDC7
J	647	HIS	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	648	PRO	-	expression tag	UNP Q1PDC7
J	649	GLN	-	expression tag	UNP Q1PDC7
J	650	PHE	-	expression tag	UNP Q1PDC7
J	651	GLU	-	expression tag	UNP Q1PDC7
J	652	LYS	-	expression tag	UNP Q1PDC7
J	653	GLY	-	expression tag	UNP Q1PDC7
J	654	GLY	-	expression tag	UNP Q1PDC7
J	655	GLY	-	expression tag	UNP Q1PDC7
J	656	SER	-	expression tag	UNP Q1PDC7
J	657	GLY	-	expression tag	UNP Q1PDC7
J	658	GLY	-	expression tag	UNP Q1PDC7
J	659	GLY	-	expression tag	UNP Q1PDC7
J	660	SER	-	expression tag	UNP Q1PDC7
J	661	GLY	-	expression tag	UNP Q1PDC7
J	662	GLY	-	expression tag	UNP Q1PDC7
J	663	GLY	-	expression tag	UNP Q1PDC7
J	664	SER	-	expression tag	UNP Q1PDC7
J	665	TRP	-	expression tag	UNP Q1PDC7
J	666	SER	-	expression tag	UNP Q1PDC7
J	667	HIS	-	expression tag	UNP Q1PDC7
J	668	PRO	-	expression tag	UNP Q1PDC7
J	669	GLN	-	expression tag	UNP Q1PDC7
J	670	PHE	-	expression tag	UNP Q1PDC7
J	671	GLU	-	expression tag	UNP Q1PDC7
J	672	LYS	-	expression tag	UNP Q1PDC7
N	438	LEU	PHE	engineered mutation	UNP Q1PDC7
N	439	ALA	TRP	engineered mutation	UNP Q1PDC7
N	445	GLY	PHE	engineered mutation	UNP Q1PDC7
N	447	ASN	PHE	engineered mutation	UNP Q1PDC7
N	638	ASP	-	expression tag	UNP Q1PDC7
N	639	ASP	-	expression tag	UNP Q1PDC7
N	640	ASP	-	expression tag	UNP Q1PDC7
N	641	ASP	-	expression tag	UNP Q1PDC7
N	642	LYS	-	expression tag	UNP Q1PDC7
N	643	ALA	-	expression tag	UNP Q1PDC7
N	644	GLY	-	expression tag	UNP Q1PDC7
N	645	TRP	-	expression tag	UNP Q1PDC7
N	646	SER	-	expression tag	UNP Q1PDC7
N	647	HIS	-	expression tag	UNP Q1PDC7
N	648	PRO	-	expression tag	UNP Q1PDC7
N	649	GLN	-	expression tag	UNP Q1PDC7
N	650	PHE	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	651	GLU	-	expression tag	UNP Q1PDC7
N	652	LYS	-	expression tag	UNP Q1PDC7
N	653	GLY	-	expression tag	UNP Q1PDC7
N	654	GLY	-	expression tag	UNP Q1PDC7
N	655	GLY	-	expression tag	UNP Q1PDC7
N	656	SER	-	expression tag	UNP Q1PDC7
N	657	GLY	-	expression tag	UNP Q1PDC7
N	658	GLY	-	expression tag	UNP Q1PDC7
N	659	GLY	-	expression tag	UNP Q1PDC7
N	660	SER	-	expression tag	UNP Q1PDC7
N	661	GLY	-	expression tag	UNP Q1PDC7
N	662	GLY	-	expression tag	UNP Q1PDC7
N	663	GLY	-	expression tag	UNP Q1PDC7
N	664	SER	-	expression tag	UNP Q1PDC7
N	665	TRP	-	expression tag	UNP Q1PDC7
N	666	SER	-	expression tag	UNP Q1PDC7
N	667	HIS	-	expression tag	UNP Q1PDC7
N	668	PRO	-	expression tag	UNP Q1PDC7
N	669	GLN	-	expression tag	UNP Q1PDC7
N	670	PHE	-	expression tag	UNP Q1PDC7
N	671	GLU	-	expression tag	UNP Q1PDC7
N	672	LYS	-	expression tag	UNP Q1PDC7

- Molecule 3 is a protein called MR78 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	G	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	K	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	O	210	Total	C	N	O	S	0	0	0
			1626	1021	270	330	5			

- Molecule 4 is a protein called MR78 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1635	1045	259	326	5			
4	H	220	Total	C	N	O	S	0	0	0
			1640	1047	260	328	5			

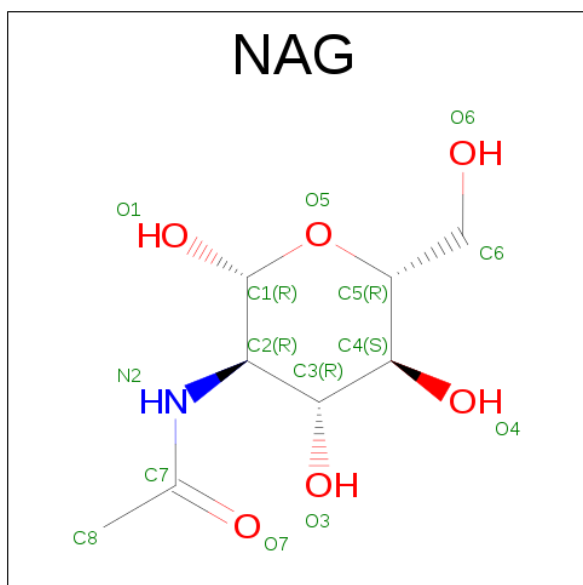
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	222	Total	C	N	O	S	0	0	0
			1655	1055	263	332	5			
4	P	211	Total	C	N	O	S	0	0	0
			1594	1019	252	318	5			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



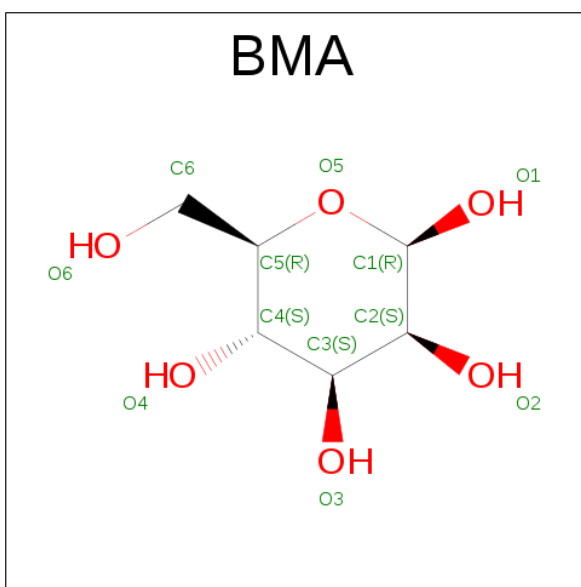
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1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

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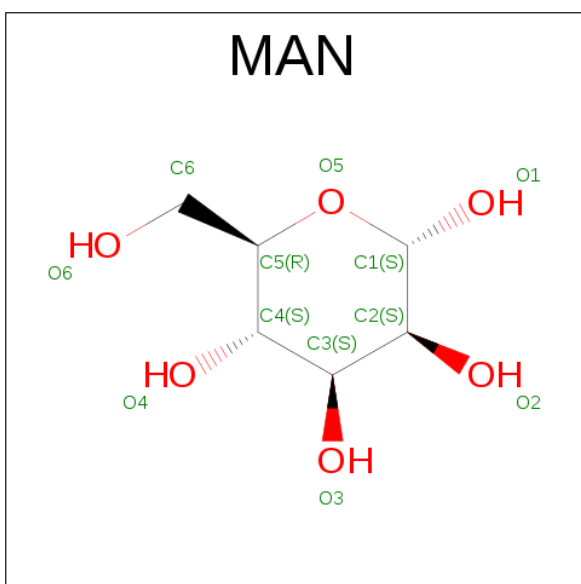
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



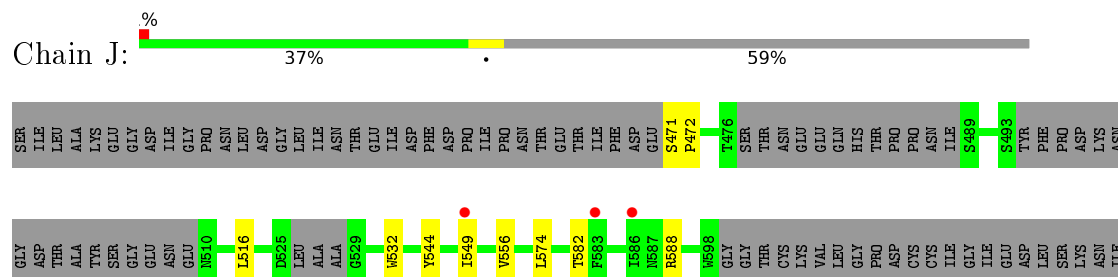
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	F	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		
6	J	1	Total	C	O	0	0
			11	6	5		
6	N	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

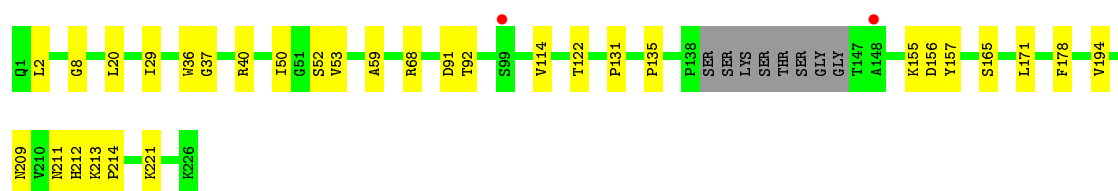


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	N	1	Total	C	O	0	0
			11	6	5		
7	N	1	Total	C	O	0	0
			11	6	5		



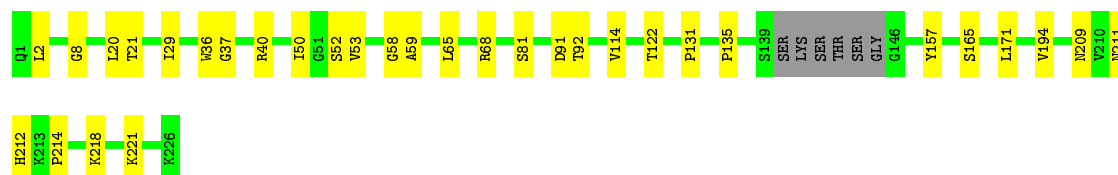






- Molecule 4: MR78 Fab heavy chain

Chain H: 83% 14% .



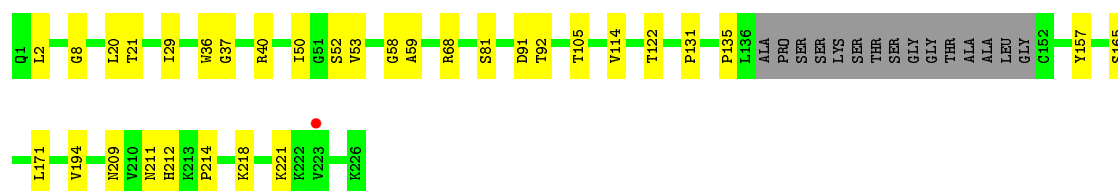
- Molecule 4: MR78 Fab heavy chain

Chain L: 87% 12% .



- Molecule 4: MR78 Fab heavy chain

Chain P: 79% 14% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.65Å 204.65Å 192.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.74 – 3.60 130.53 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.74-3.60) 99.4 (130.53-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.221 , 0.262 0.184 , 0.210	Depositor DCC
$R_{free}$ test set	2676 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.0	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 75.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.178 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.25	0/1159	0.43	0/1571
1	E	0.25	0/1150	0.43	0/1559
1	I	0.25	0/1140	0.43	0/1545
1	M	0.24	0/1140	0.43	0/1545
2	B	0.24	0/976	0.42	0/1324
2	F	0.24	0/751	0.39	0/1017
2	J	0.24	0/763	0.40	0/1034
2	N	0.23	0/733	0.40	0/992
3	C	0.25	0/1667	0.45	0/2263
3	G	0.24	0/1667	0.45	0/2263
3	K	0.24	0/1667	0.45	0/2263
3	O	0.24	0/1661	0.45	0/2256
4	D	0.25	0/1680	0.45	0/2294
4	H	0.25	0/1685	0.45	0/2303
4	L	0.25	0/1700	0.45	0/2320
4	P	0.24	0/1638	0.44	0/2235
All	All	0.24	0/21177	0.44	0/28784

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	1131	0	1115	11	0
1	E	1122	0	1101	10	0
1	I	1112	0	1097	14	0
1	M	1112	0	1097	13	0
2	B	962	0	918	10	0
2	F	740	0	726	12	0
2	J	752	0	729	9	0
2	N	722	0	715	9	0
3	C	1632	0	1590	15	0
3	G	1632	0	1590	17	0
3	K	1632	0	1590	12	0
3	O	1626	0	1579	12	0
4	D	1635	0	1591	16	0
4	H	1640	0	1588	17	0
4	L	1655	0	1607	14	0
4	P	1594	0	1548	18	0
5	A	56	0	50	0	0
5	B	28	0	24	0	0
5	E	42	0	38	0	0
5	F	28	0	24	1	0
5	I	56	0	49	0	0
5	J	28	0	24	1	0
5	M	56	0	50	0	0
5	N	28	0	24	1	0
6	B	11	0	8	0	0
6	F	11	0	8	0	0
6	I	11	0	9	0	0
6	J	11	0	9	0	0
6	N	11	0	9	0	0
7	B	33	0	29	1	0
7	F	33	0	29	0	0
7	I	22	0	20	0	0
7	J	11	0	10	0	0
7	M	11	0	10	0	0
7	N	22	0	19	0	0
All	All	21208	0	20624	185	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 4.

The worst 5 of 185 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:L:68:ARG:NH2	4:L:91:ASP:OD2	2.19	0.75
1:I:147:ASP:OD2	2:J:544:TYR:OH	2.07	0.71
1:A:147:ASP:OD2	2:B:544:TYR:OH	2.06	0.71
4:H:68:ARG:NH2	4:H:91:ASP:OD2	2.23	0.69
4:D:68:ARG:NH2	4:D:91:ASP:OD2	2.25	0.69

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	143/250 (57%)	139 (97%)	4 (3%)	0	100	100
1	E	142/250 (57%)	138 (97%)	4 (3%)	0	100	100
1	I	140/250 (56%)	137 (98%)	3 (2%)	0	100	100
1	M	140/250 (56%)	136 (97%)	4 (3%)	0	100	100
2	B	117/237 (49%)	110 (94%)	7 (6%)	0	100	100
2	F	86/237 (36%)	81 (94%)	5 (6%)	0	100	100
2	J	89/237 (38%)	84 (94%)	5 (6%)	0	100	100
2	N	84/237 (35%)	80 (95%)	4 (5%)	0	100	100
3	C	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
3	G	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
3	K	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
3	O	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
4	D	214/226 (95%)	202 (94%)	12 (6%)	0	100	100
4	H	216/226 (96%)	204 (94%)	12 (6%)	0	100	100
4	L	218/226 (96%)	205 (94%)	13 (6%)	0	100	100
4	P	207/226 (92%)	196 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2628/3696 (71%)	2523 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	124/222 (56%)	124 (100%)	0	100	100
1	E	121/222 (54%)	121 (100%)	0	100	100
1	I	121/222 (54%)	121 (100%)	0	100	100
1	M	121/222 (54%)	121 (100%)	0	100	100
2	B	103/202 (51%)	103 (100%)	0	100	100
2	F	80/202 (40%)	80 (100%)	0	100	100
2	J	80/202 (40%)	80 (100%)	0	100	100
2	N	78/202 (39%)	78 (100%)	0	100	100
3	C	188/189 (100%)	188 (100%)	0	100	100
3	G	188/189 (100%)	188 (100%)	0	100	100
3	K	188/189 (100%)	188 (100%)	0	100	100
3	O	187/189 (99%)	187 (100%)	0	100	100
4	D	186/192 (97%)	186 (100%)	0	100	100
4	H	186/192 (97%)	186 (100%)	0	100	100
4	L	188/192 (98%)	188 (100%)	0	100	100
4	P	183/192 (95%)	183 (100%)	0	100	100
All	All	2322/3220 (72%)	2322 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

40 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	$\# Z  > 2$
5	NAG	A	301	1,5	14,14,15	0.29	0	15,19,21	0.30	0
5	NAG	A	302	5	14,14,15	0.23	0	15,19,21	0.39	0
5	NAG	A	303	1,5	14,14,15	0.46	0	15,19,21	0.38	0
5	NAG	A	304	5	14,14,15	0.34	0	15,19,21	0.32	0
5	NAG	B	701	2,5	14,14,15	0.20	0	15,19,21	0.40	0
5	NAG	B	702	5,6	14,14,15	0.26	0	15,19,21	0.47	0
6	BMA	B	703	5,7	11,11,12	0.64	0	15,15,17	0.82	0
7	MAN	B	704	7,6	11,11,12	0.72	0	15,15,17	0.94	0
7	MAN	B	705	7	11,11,12	0.78	0	15,15,17	0.91	1 (6%)
7	MAN	B	706	6	11,11,12	0.87	1 (9%)	15,15,17	1.16	3 (20%)
5	NAG	E	301	1,5	14,14,15	0.32	0	15,19,21	0.25	0
5	NAG	E	302	5	14,14,15	0.23	0	15,19,21	0.41	0
5	NAG	E	303	1	14,14,15	0.35	0	15,19,21	0.32	0
5	NAG	F	701	2,5	14,14,15	0.22	0	15,19,21	0.40	0
5	NAG	F	702	5,6	14,14,15	0.26	0	15,19,21	0.38	0
6	BMA	F	703	5,7	11,11,12	0.58	0	15,15,17	0.75	0
7	MAN	F	704	7,6	11,11,12	1.09	1 (9%)	15,15,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	F	705	7	11,11,12	0.95	0	15,15,17	1.19	2 (13%)
7	MAN	F	706	6	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
5	NAG	I	301	1,5	14,14,15	0.42	0	15,19,21	0.30	0
5	NAG	I	302	5,6	14,14,15	0.26	0	15,19,21	0.35	0
6	BMA	I	303	5,7	11,11,12	0.50	0	15,15,17	0.67	0
7	MAN	I	304	6	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
7	MAN	I	305	-	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
5	NAG	I	306	1,5	14,14,15	0.32	0	15,19,21	0.21	0
5	NAG	I	307	5	14,14,15	0.30	0	15,19,21	0.41	0
5	NAG	J	701	2,5	14,14,15	0.18	0	15,19,21	0.40	0
5	NAG	J	702	5,6	14,14,15	0.22	0	15,19,21	0.38	0
6	BMA	J	703	5,7	11,11,12	0.71	0	15,15,17	0.79	0
7	MAN	J	704	6	11,11,12	0.75	0	15,15,17	0.94	1 (6%)
5	NAG	M	301	1,5	14,14,15	0.29	0	15,19,21	0.30	0
5	NAG	M	302	5	14,14,15	0.24	0	15,19,21	0.40	0
5	NAG	M	303	1,5	14,14,15	0.33	0	15,19,21	0.38	0
5	NAG	M	304	5	14,14,15	0.37	0	15,19,21	0.51	0
7	MAN	M	305	-	11,11,12	0.94	1 (9%)	15,15,17	1.24	2 (13%)
5	NAG	N	701	2,5	14,14,15	0.24	0	15,19,21	0.43	0
5	NAG	N	702	5,6	14,14,15	0.25	0	15,19,21	0.36	0
6	BMA	N	703	5,7	11,11,12	0.86	0	15,15,17	1.16	1 (6%)
7	MAN	N	704	7,6	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
7	MAN	N	705	7	11,11,12	0.64	0	15,15,17	0.96	2 (13%)

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	NAG	A	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	302	5	-	0/6/23/26	0/1/1/1
5	NAG	A	303	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	304	5	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	704	7,6	-	0/2/19/22	0/1/1/1
7	MAN	B	705	7	-	0/2/19/22	0/1/1/1
7	MAN	B	706	6	-	0/2/19/22	0/1/1/1
5	NAG	E	301	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	302	5	-	0/6/23/26	0/1/1/1
5	NAG	E	303	1	-	0/6/23/26	0/1/1/1
5	NAG	F	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	704	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	705	7	-	0/2/19/22	0/1/1/1
7	MAN	F	706	6	-	0/2/19/22	0/1/1/1
5	NAG	I	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	302	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	303	5,7	-	0/2/19/22	0/1/1/1
7	MAN	I	304	6	-	0/2/19/22	0/1/1/1
7	MAN	I	305	-	-	0/2/19/22	0/1/1/1
5	NAG	I	306	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	307	5	-	0/6/23/26	0/1/1/1
5	NAG	J	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	J	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	J	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	J	704	6	-	0/2/19/22	0/1/1/1
5	NAG	M	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	302	5	-	0/6/23/26	0/1/1/1
5	NAG	M	303	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	304	5	-	0/6/23/26	0/1/1/1
7	MAN	M	305	-	-	0/2/19/22	0/1/1/1
5	NAG	N	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	N	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	N	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	N	704	7,6	-	0/2/19/22	0/1/1/1
7	MAN	N	705	7	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	305	MAN	O5-C1	-2.06	1.40	1.43
7	F	704	MAN	C2-C3	2.17	1.55	1.52
7	B	706	MAN	C1-C2	2.36	1.58	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	703	BMA	O6-C6-C5	-2.50	102.97	111.30
7	B	706	MAN	O2-C2-C3	-2.29	105.56	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	704	MAN	O2-C2-C3	-2.27	105.60	110.19
7	F	706	MAN	O2-C2-C3	-2.27	105.61	110.19
7	B	705	MAN	O2-C2-C3	-2.23	105.70	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	704	MAN	1	0
7	B	705	MAN	1	0
5	F	701	NAG	1	0
5	J	701	NAG	1	0
5	N	701	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	145/250 (58%)	0.14	0 100 100	55, 86, 119, 147	0
1	E	144/250 (57%)	0.48	4 (2%) 56 42	70, 94, 132, 148	0
1	I	142/250 (56%)	0.60	5 (3%) 48 34	70, 99, 133, 149	0
1	M	142/250 (56%)	0.49	2 (1%) 78 65	94, 116, 139, 155	0
2	B	127/237 (53%)	0.11	1 (0%) 87 78	73, 110, 158, 174	0
2	F	94/237 (39%)	0.49	5 (5%) 30 21	79, 120, 149, 158	0
2	J	97/237 (40%)	0.51	3 (3%) 52 38	80, 120, 149, 176	0
2	N	92/237 (38%)	0.35	1 (1%) 82 70	93, 124, 150, 173	0
3	C	210/211 (99%)	0.36	5 (2%) 62 47	72, 116, 136, 149	0
3	G	210/211 (99%)	0.43	3 (1%) 78 65	68, 99, 128, 161	0
3	K	210/211 (99%)	0.35	1 (0%) 91 86	61, 95, 124, 141	0
3	O	210/211 (99%)	0.17	3 (1%) 78 65	110, 138, 158, 168	0
4	D	218/226 (96%)	0.30	2 (0%) 85 75	59, 86, 127, 155	0
4	H	220/226 (97%)	0.35	0 100 100	59, 82, 111, 128	0
4	L	222/226 (98%)	0.26	0 100 100	57, 80, 124, 151	0
4	P	211/226 (93%)	0.12	1 (0%) 91 86	99, 126, 148, 174	0
All	All	2694/3696 (72%)	0.33	36 (1%) 79 66	55, 105, 145, 176	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	476	THR	4.0
2	J	583	PHE	3.6
3	G	30	SER	3.3
3	C	105	ASP	3.0
1	E	50	MET	2.9

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	N	701	14/15	0.92	0.46	1.07	108,126,155,155	0
5	NAG	B	701	14/15	0.95	0.32	0.28	75,87,93,99	0
5	NAG	J	701	14/15	0.95	0.32	-0.03	88,107,118,123	0
5	NAG	A	301	14/15	0.95	0.25	-0.13	82,103,124,127	0
5	NAG	E	301	14/15	0.94	0.24	-0.19	97,105,130,157	0
5	NAG	M	301	14/15	0.85	0.25	-0.28	122,137,150,152	0
5	NAG	I	301	14/15	0.92	0.25	-0.63	104,113,126,141	0
5	NAG	E	303	14/15	0.76	0.25	-0.70	119,150,167,170	0
5	NAG	F	701	14/15	0.95	0.29	-0.77	96,106,115,119	0
5	NAG	M	303	14/15	0.86	0.15	-0.93	131,149,167,169	0
5	NAG	A	303	14/15	0.88	0.16	-1.08	109,132,148,159	0
5	NAG	I	306	14/15	0.91	0.16	-1.57	146,161,166,172	0
7	MAN	B	706	11/12	0.77	0.25	-	98,121,144,159	0
6	BMA	J	703	11/12	0.86	0.17	-	89,135,147,164	0
7	MAN	I	304	11/12	0.78	0.29	-	116,160,172,172	0
5	NAG	A	304	14/15	0.83	0.17	-	119,161,166,173	0
7	MAN	I	305	11/12	0.72	0.21	-	115,144,163,168	0
5	NAG	A	302	14/15	0.85	0.25	-	94,123,152,155	0
7	MAN	F	704	11/12	0.84	0.31	-	139,150,160,161	0
6	BMA	B	703	11/12	0.87	0.21	-	129,143,167,173	0
5	NAG	N	702	14/15	0.91	0.34	-	110,122,148,152	0
7	MAN	B	705	11/12	0.88	0.22	-	116,129,139,141	0
7	MAN	F	705	11/12	0.89	0.20	-	129,138,146,157	0
6	BMA	I	303	11/12	0.74	0.20	-	143,162,184,184	0
5	NAG	I	302	14/15	0.87	0.24	-	115,138,152,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MAN	F	706	11/12	0.75	0.21	-	107,150,161,168	0
5	NAG	M	302	14/15	0.82	0.24	-	125,157,178,198	0
7	MAN	N	704	11/12	0.82	0.25	-	167,178,185,195	0
5	NAG	B	702	14/15	0.91	0.35	-	90,104,122,125	0
7	MAN	M	305	11/12	0.69	0.41	-	152,184,193,196	0
6	BMA	F	703	11/12	0.88	0.16	-	111,118,133,145	0
6	BMA	N	703	11/12	0.85	0.22	-	143,167,178,180	0
5	NAG	F	702	14/15	0.92	0.26	-	82,102,128,131	0
7	MAN	N	705	11/12	0.86	0.14	-	111,156,169,170	0
5	NAG	J	702	14/15	0.90	0.24	-	88,101,119,124	0
7	MAN	B	704	11/12	0.90	0.27	-	119,131,156,166	0
5	NAG	M	304	14/15	0.59	0.30	-	148,168,184,187	0
5	NAG	I	307	14/15	0.67	0.23	-	101,164,178,181	0
7	MAN	J	704	11/12	0.78	0.23	-	141,152,161,171	0
5	NAG	E	302	14/15	0.90	0.19	-	118,143,154,159	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.