



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2018 – 08:21 PM EST

PDB ID : 6BP2
Title : Therapeutic human monoclonal antibody MR191 bound to a marburgvirus glycoprotein
Authors : King, L.B.; Fusco, M.L.; Flyak, A.I.; Ilinykh, P.A.; Huang, K.; Gunn, B.; Kirchdoerfer, R.N.; Hastie, K.M.; Sangha, A.K.; Meiler, J.; Alter, G.; Bukreyev, A.; Crowe, J.E.J.; Saphire, E.O.
Deposited on : 2017-11-21
Resolution : 3.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

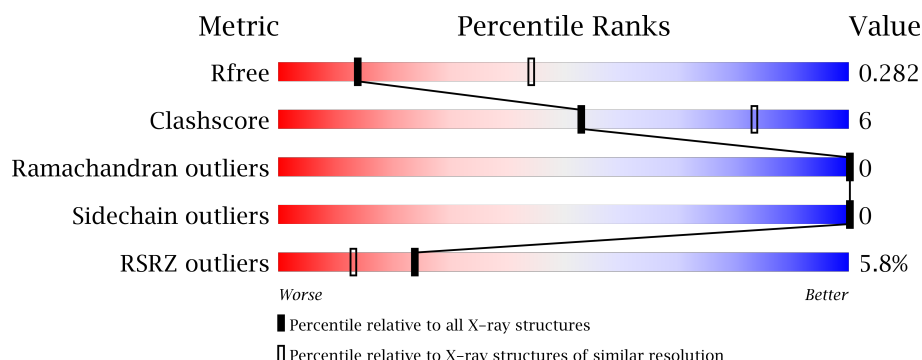
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1123 (3.20-3.16)
Clashscore	112137	1255 (3.20-3.16)
Ramachandran outliers	110173	1233 (3.20-3.16)
Sidechain outliers	110143	1232 (3.20-3.16)
RSRZ outliers	101464	1128 (3.20-3.16)

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	250	
2	B	202	
3	H	229	
4	L	217	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5684 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1152	729	201	215	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	ARG	MET	variant	UNP A0A0U2XLP5
A	258	PRO	ASN	variant	UNP A0A0U2XLP5
A	260	ILE	SER	variant	UNP A0A0U2XLP5
A	261	TYR	SER	variant	UNP A0A0U2XLP5
A	262	PHE	ASP	variant	UNP A0A0U2XLP5
A	263	ARG	ASP	variant	UNP A0A0U2XLP5
A	264	LYS	GLU	variant	UNP A0A0U2XLP5
A	265	LYS	ASP	variant	UNP A0A0U2XLP5
A	266	ARG	LEU	variant	UNP A0A0U2XLP5

- Molecule 2 is a protein called Envelope glycoprotein GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	0	0	0
			1160	728	200	227	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	438	LEU	PHE	engineered mutation	UNP A0A0U2XLP5
B	439	ALA	TRP	engineered mutation	UNP A0A0U2XLP5
B	445	GLY	PHE	engineered mutation	UNP A0A0U2XLP5
B	447	ASN	PHE	engineered mutation	UNP A0A0U2XLP5

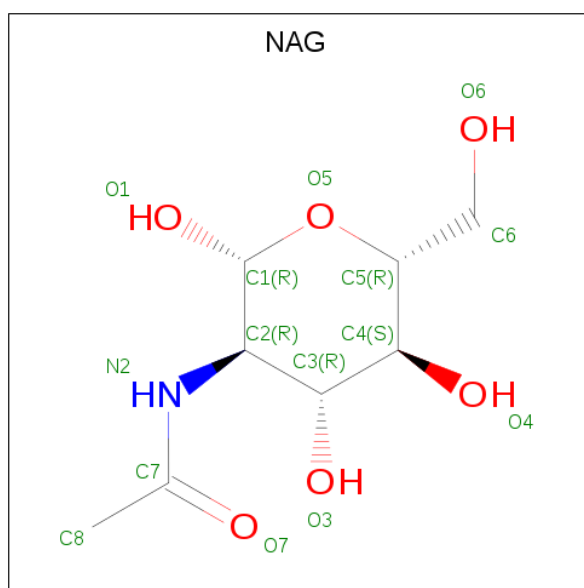
- Molecule 3 is a protein called MR191 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1653	1054	271	324	4			

- Molecule 4 is a protein called MR191 Fab Light Chain.

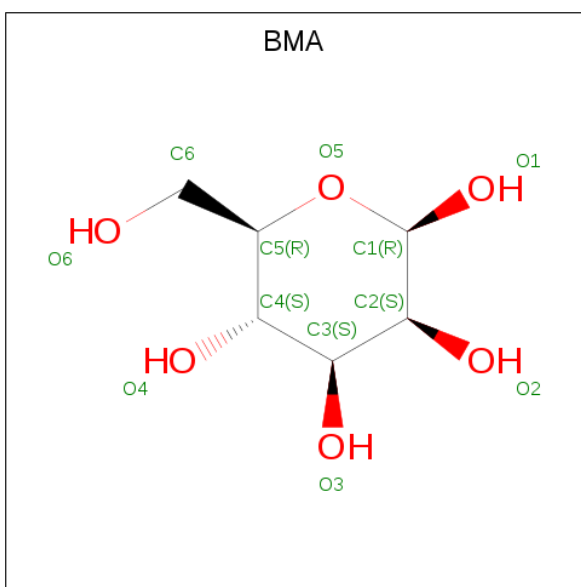
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	215	Total	C	N	O	S	0	0	0
			1591	994	265	327	5			

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



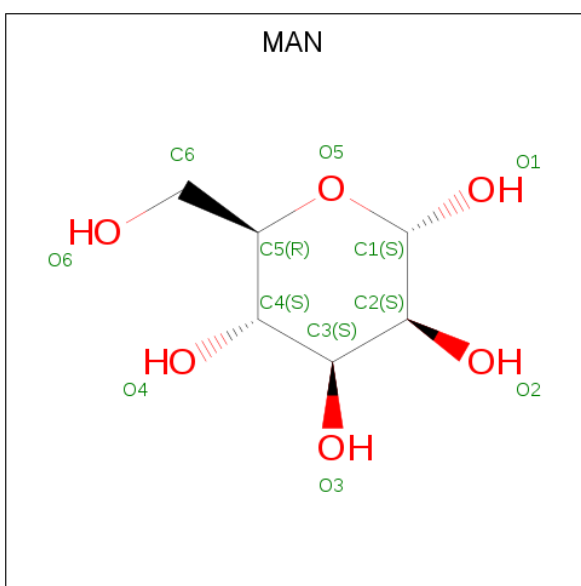
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

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

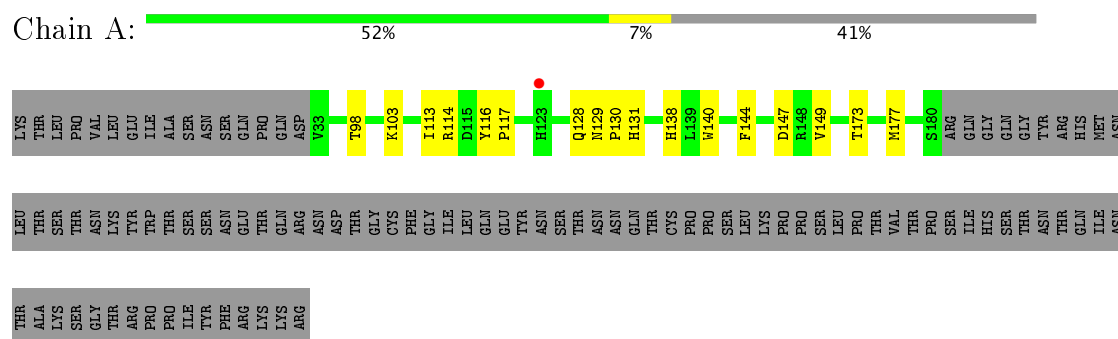


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

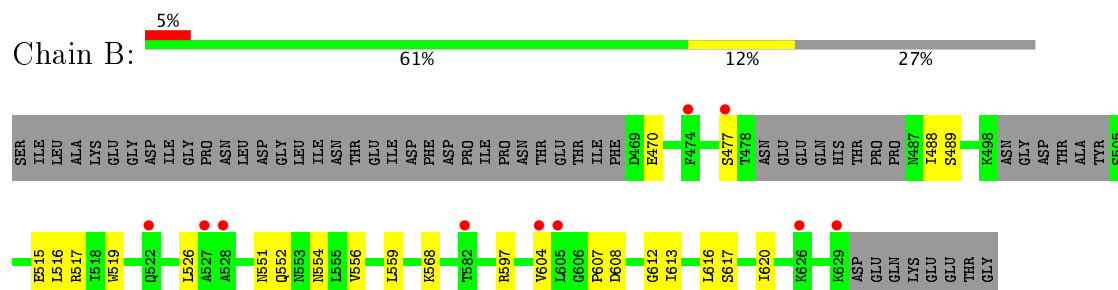
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

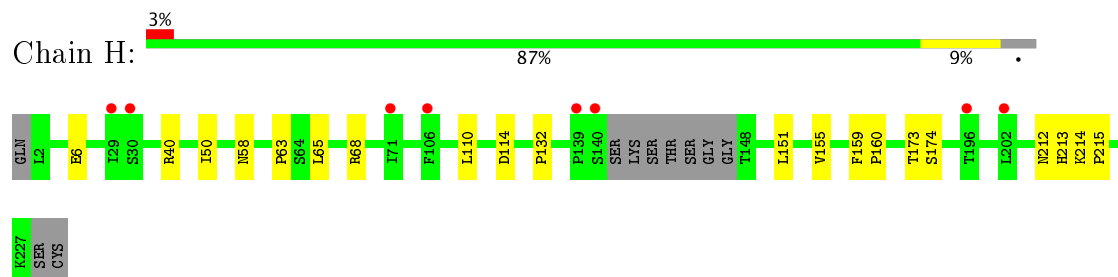
- Molecule 1: Envelope glycoprotein



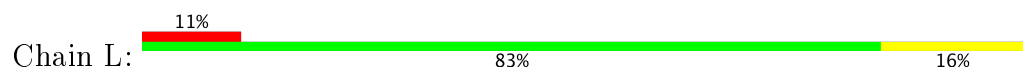
- Molecule 2: Envelope glycoprotein GP2

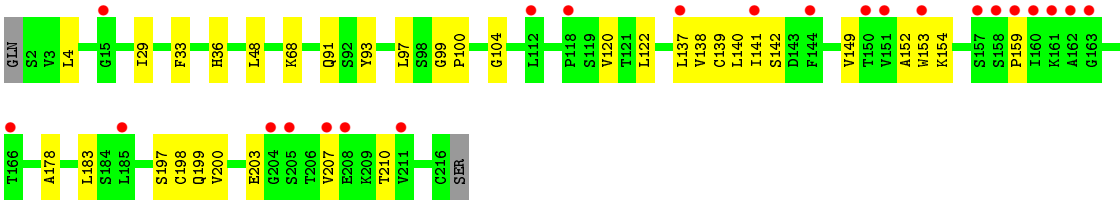


- Molecule 3: MR191 Fab Heavy Chain



- Molecule 4: MR191 Fab Light Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.80Å 133.80Å 151.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.17 – 3.17 46.17 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.17-3.17) 99.3 (46.17-3.17)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.284 0.254 , 0.282	Depositor DCC
R_{free} test set	1360 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	94.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5684	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.66	0/1180	0.77	0/1600
2	B	0.66	0/1178	0.74	0/1591
3	H	0.65	0/1696	0.78	0/2317
4	L	0.67	0/1630	0.79	0/2229
All	All	0.66	0/5684	0.77	0/7737

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	1152	0	1132	12	0
2	B	1160	0	1136	14	2
3	H	1653	0	1632	14	0
4	L	1591	0	1538	34	0
5	A	56	0	49	0	0
5	B	28	0	24	2	0
6	A	11	0	10	0	0
6	B	11	0	8	2	0
7	B	22	0	20	0	0
All	All	5684	0	5549	70	2

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 6.

All (70) 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)
6:B:701:BMA:C1	5:B:705:NAG:O4	1.64	1.44
6:B:701:BMA:C1	5:B:705:NAG:C4	2.61	0.78
4:L:141:ILE:HG21	4:L:200:VAL:HG21	1.76	0.68
4:L:120:VAL:CG1	4:L:207:VAL:HG11	2.26	0.66
2:B:613:ILE:HG22	2:B:613:ILE:O	1.94	0.65
2:B:470:GLU:OE1	2:B:597:ARG:NH1	2.30	0.64
2:B:477:SER:HB3	2:B:489:SER:HB3	1.78	0.64
4:L:122:LEU:HD12	4:L:138:VAL:O	1.98	0.63
4:L:197:SER:HB2	4:L:210:THR:HG22	1.80	0.63
3:H:40:ARG:HB3	3:H:50:ILE:HD11	1.82	0.62
2:B:607:PRO:O	2:B:608:ASP:HB2	1.99	0.61
4:L:120:VAL:HB	4:L:141:ILE:HG22	1.83	0.61
4:L:141:ILE:HD11	4:L:149:VAL:HG21	1.83	0.60
2:B:488:ILE:HG22	2:B:488:ILE:O	2.01	0.60
4:L:203:GLU:OE1	4:L:203:GLU:HA	2.03	0.59
4:L:137:LEU:HD12	4:L:137:LEU:N	2.19	0.58
3:H:63:PRO:HG2	4:L:97:LEU:O	2.04	0.57
3:H:65:LEU:HD22	3:H:68:ARG:HH21	1.71	0.56
4:L:142:SER:HA	4:L:178:ALA:HA	1.89	0.55
1:A:173:THR:O	1:A:177:MET:HG3	2.06	0.54
3:H:114:ASP:HA	4:L:48:LEU:HD22	1.90	0.53
1:A:114:ARG:HB2	1:A:147:ASP:HB3	1.91	0.53
3:H:159:PHE:CD2	3:H:160:PRO:HD3	2.44	0.53
1:A:129:ASN:OD1	1:A:130:PRO:HD2	2.10	0.52
4:L:36:HIS:HB2	4:L:91:GLN:HB3	1.91	0.52
4:L:139:CYS:HB2	4:L:153:TRP:CH2	2.46	0.51
4:L:141:ILE:HG13	4:L:141:ILE:O	2.10	0.51
4:L:120:VAL:HG12	4:L:207:VAL:HG11	1.93	0.50
2:B:613:ILE:CG2	2:B:613:ILE:O	2.60	0.50
4:L:197:SER:CB	4:L:210:THR:HG22	2.40	0.50
1:A:128:GLN:OE1	3:H:58:ASN:ND2	2.45	0.50
2:B:613:ILE:HD12	2:B:616:LEU:HD23	1.93	0.50
3:H:132:PRO:HB2	3:H:155:VAL:HG13	1.95	0.49
4:L:154:LYS:O	4:L:154:LYS:HG3	2.12	0.49
4:L:137:LEU:HD22	4:L:183:LEU:HD23	1.94	0.49
4:L:120:VAL:HG11	4:L:207:VAL:CG1	2.42	0.49
1:A:138:HIS:CE1	1:A:140:TRP:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:GLU:OE2	2:B:517:ARG:NE	2.34	0.48
4:L:154:LYS:HA	4:L:159:PRO:HA	1.94	0.48
2:B:489:SER:HA	2:B:552:GLN:HE22	1.79	0.48
4:L:120:VAL:CG1	4:L:207:VAL:CG1	2.91	0.47
3:H:212:ASN:OD1	3:H:213:HIS:N	2.48	0.47
3:H:6:GLU:OE1	3:H:6:GLU:N	2.47	0.47
2:B:551:ASN:ND2	2:B:554:ASN:HA	2.30	0.47
4:L:152:ALA:HB3	4:L:199:GLN:CG	2.43	0.47
4:L:29:ILE:HG23	4:L:68:LYS:HE2	1.96	0.46
1:A:138:HIS:HB2	1:A:144:PHE:CE2	2.51	0.46
3:H:151:LEU:HD12	3:H:151:LEU:C	2.35	0.46
1:A:117:PRO:HD3	1:A:147:ASP:HA	1.98	0.45
1:A:131:HIS:ND1	1:A:131:HIS:O	2.50	0.45
1:A:116:TYR:HA	1:A:117:PRO:HD3	1.78	0.44
4:L:137:LEU:N	4:L:137:LEU:CD1	2.80	0.44
4:L:122:LEU:HD22	4:L:198:CYS:CB	2.47	0.44
1:A:117:PRO:HG2	2:B:519:TRP:CZ2	2.53	0.44
3:H:110:LEU:HD12	4:L:100:PRO:HB2	2.01	0.43
2:B:617:SER:HA	2:B:620:ILE:HD12	2.00	0.43
3:H:214:LYS:N	3:H:215:PRO:CD	2.81	0.43
4:L:122:LEU:HD22	4:L:198:CYS:HB3	1.99	0.43
3:H:63:PRO:HD2	4:L:99:GLY:N	2.34	0.43
2:B:516:LEU:HD22	2:B:556:VAL:HG13	2.01	0.42
1:A:98:THR:HB	1:A:103:LYS:O	2.19	0.42
4:L:120:VAL:CB	4:L:141:ILE:HG22	2.48	0.42
4:L:33:PHE:CD1	4:L:93:TYR:HB3	2.55	0.41
4:L:4:LEU:HB2	4:L:104:GLY:HA2	2.02	0.41
4:L:138:VAL:HG12	4:L:140:LEU:HG	2.02	0.41
4:L:29:ILE:CG2	4:L:68:LYS:HE2	2.51	0.41
3:H:173:THR:OG1	3:H:174:SER:N	2.53	0.41
1:A:113:ILE:CD1	1:A:149:VAL:HG11	2.50	0.41
2:B:556:VAL:O	2:B:559:LEU:HB2	2.21	0.40
4:L:36:HIS:O	4:L:91:GLN:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:LEU:CG	2:B:568:LYS:NZ[2_745]	2.13	0.07
2:B:604:VAL:CG2	2:B:612:GLY:O[3_875]	2.15	0.05

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	146/250 (58%)	139 (95%)	7 (5%)	0	100	100
2	B	141/202 (70%)	131 (93%)	10 (7%)	0	100	100
3	H	215/229 (94%)	208 (97%)	7 (3%)	0	100	100
4	L	213/217 (98%)	200 (94%)	13 (6%)	0	100	100
All	All	715/898 (80%)	678 (95%)	37 (5%)	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	127/222 (57%)	127 (100%)	0	100	100
2	B	130/178 (73%)	130 (100%)	0	100	100
3	H	191/199 (96%)	191 (100%)	0	100	100
4	L	180/182 (99%)	180 (100%)	0	100	100
All	All	628/781 (80%)	628 (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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	619	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 ⓘ

10 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	0.27	0	15,19,21	1.11	1 (6%)
5	NAG	A	302	5,6	14,14,15	0.29	0	15,19,21	1.20	2 (13%)
6	BMA	A	303	5	11,11,12	0.35	0	13,15,17	0.75	1 (7%)
5	NAG	A	304	1,5	14,14,15	0.31	0	15,19,21	0.60	0
5	NAG	A	305	5	14,14,15	0.31	0	15,19,21	0.99	2 (13%)
6	BMA	B	701	7	11,11,12	0.95	1 (9%)	13,15,17	1.63	3 (23%)
7	MAN	B	702	6	11,11,12	1.17	1 (9%)	13,15,17	0.88	1 (7%)
7	MAN	B	703	6	11,11,12	1.26	1 (9%)	13,15,17	1.00	1 (7%)
5	NAG	B	704	2,5	14,14,15	0.78	0	15,19,21	1.86	4 (26%)
5	NAG	B	705	5	14,14,15	0.28	0	15,19,21	0.58	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
5	NAG	A	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	302	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	303	5	-	0/2/19/22	0/1/1/1
5	NAG	A	304	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	305	5	-	0/6/23/26	0/1/1/1
6	BMA	B	701	7	-	0/2/19/22	0/1/1/1
7	MAN	B	702	6	-	0/2/19/22	0/1/1/1
7	MAN	B	703	6	-	0/2/19/22	0/1/1/1
5	NAG	B	704	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	705	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	702	MAN	O5-C1	2.23	1.47	1.43
6	B	701	BMA	C2-C3	2.59	1.56	1.52
7	B	703	MAN	O5-C1	2.60	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	NAG	O5-C1-C2	-4.89	104.66	111.47
5	A	301	NAG	O5-C1-C2	-3.83	106.14	111.47
5	A	302	NAG	O5-C1-C2	-3.52	106.57	111.47
6	B	701	BMA	O3-C3-C4	-3.44	102.87	110.36
5	B	704	NAG	C4-C3-C2	-3.44	105.98	111.02
5	B	704	NAG	C3-C4-C5	-2.84	105.21	110.22
5	A	305	NAG	O5-C1-C2	-2.66	107.77	111.47
5	B	704	NAG	C2-N2-C7	-2.28	119.62	122.94
7	B	702	MAN	C1-O5-C5	2.03	114.96	112.17
5	A	305	NAG	C1-O5-C5	2.07	115.03	112.17
5	A	302	NAG	C1-O5-C5	2.15	115.13	112.17
6	A	303	BMA	C1-O5-C5	2.16	115.15	112.17
6	B	701	BMA	C1-O5-C5	2.16	115.15	112.17
6	B	701	BMA	C2-C3-C4	2.48	115.20	110.88
7	B	703	MAN	C1-O5-C5	2.56	115.70	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	701	BMA	2	0
5	B	705	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	148/250 (59%)	-0.03	1 (0%) 87 79	60, 78, 100, 127	0
2	B	147/202 (72%)	0.47	10 (6%) 18 10	58, 94, 147, 172	0
3	H	219/229 (95%)	0.02	8 (3%) 42 27	74, 104, 133, 145	0
4	L	215/217 (99%)	0.53	23 (10%) 7 4	78, 116, 171, 181	0
All	All	729/898 (81%)	0.25	42 (5%) 24 13	58, 98, 157, 181	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	153	TRP	4.3
4	L	162	ALA	3.9
2	B	626	LYS	3.8
4	L	118	PRO	3.8
4	L	160	ILE	3.8
4	L	151	VAL	3.7
4	L	158	SER	3.5
4	L	157	SER	3.3
4	L	141	ILE	3.2
3	H	202	LEU	3.1
3	H	106	PHE	3.0
4	L	208	GLU	3.0
4	L	161	LYS	2.9
4	L	159	PRO	2.9
2	B	605	LEU	2.9
3	H	29	ILE	2.8
4	L	204	GLY	2.8
4	L	211	VAL	2.8
3	H	140	SER	2.7
4	L	166	THR	2.7
4	L	185	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	30	SER	2.6
4	L	137	LEU	2.6
2	B	474	PHE	2.6
2	B	527	ALA	2.6
2	B	522	GLN	2.6
2	B	528	ALA	2.5
4	L	15	GLY	2.5
2	B	604	VAL	2.4
3	H	139	PRO	2.4
4	L	150	THR	2.4
4	L	112	LEU	2.3
2	B	477	SER	2.3
4	L	205	SER	2.3
4	L	163	GLY	2.2
2	B	582	THR	2.2
1	A	123	HIS	2.1
4	L	144	PHE	2.1
3	H	196	THR	2.1
4	L	207	VAL	2.0
2	B	629	LYS	2.0
3	H	71	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	NAG	A	301	14/15	0.94	0.17	-0.40	77,89,98,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	304	14/15	0.91	0.18	-0.78	111,125,138,147	0
5	NAG	B	704	14/15	0.94	0.19	-1.50	83,93,95,99	0
6	BMA	B	701	11/12	0.73	0.18	-	116,129,138,139	0
5	NAG	A	302	14/15	0.90	0.21	-	109,117,135,138	0
6	BMA	A	303	11/12	0.75	0.31	-	125,144,154,159	0
5	NAG	B	705	14/15	0.94	0.15	-	90,101,110,114	0
5	NAG	A	305	14/15	0.78	0.35	-	145,147,157,158	0
7	MAN	B	703	11/12	0.63	0.27	-	137,138,144,144	0
7	MAN	B	702	11/12	0.86	0.15	-	126,138,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.