



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:05 AM GMT

PDB ID : 1ZLW  
Title : Fab 2G12 + Man8  
Authors : Calarese, D.A.; Lee, H.-K.; Best, M.D.; Astronomo, R.D.; Stanfield, R.L.;  
Burton, D.R.; Wong, C.H.; Wilson, I.A.  
Deposited on : 2005-05-09  
Resolution : 2.85 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

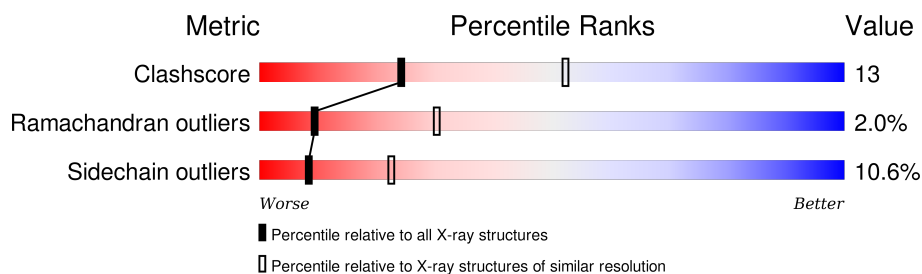
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	K	211	
1	L	211	
2	H	224	
2	M	224	

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
3	BMA	M	235	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6535 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 FAB 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	209	Total	C	N	O	S	0	0	0
			1599	1007	266	321	5			
1	K	209	Total	C	N	O	S	0	0	0
			1602	1008	269	320	5			

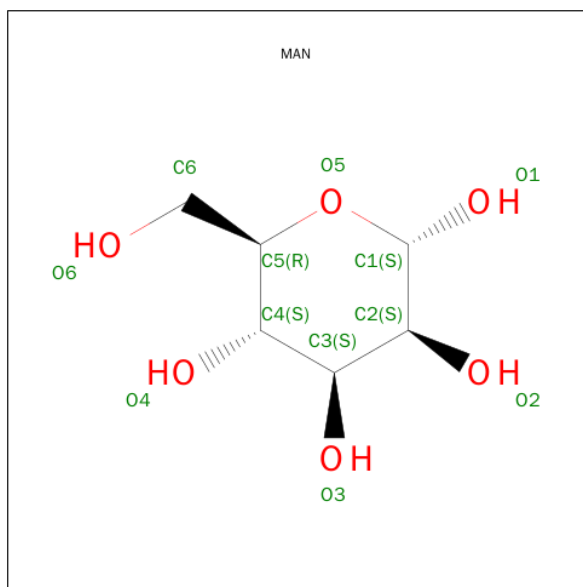
- Molecule 2 is a protein called FAB 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1671	1050	285	329	7			
2	M	209	Total	C	N	O	S	0	0	0
			1575	994	269	305	7			

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	7	Total	C	O	0	0
			77	42	35		

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



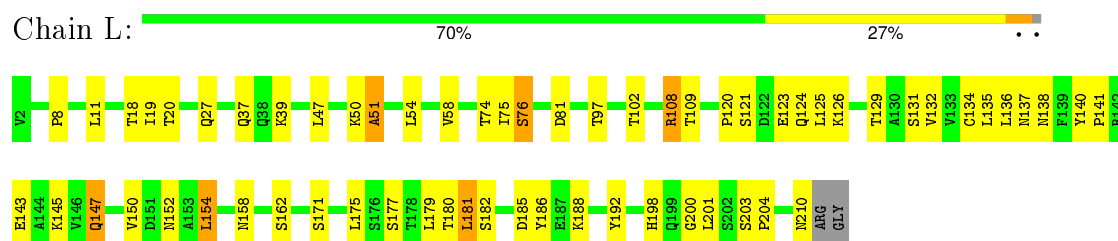
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			11	6	5		

### 3 Residue-property plots

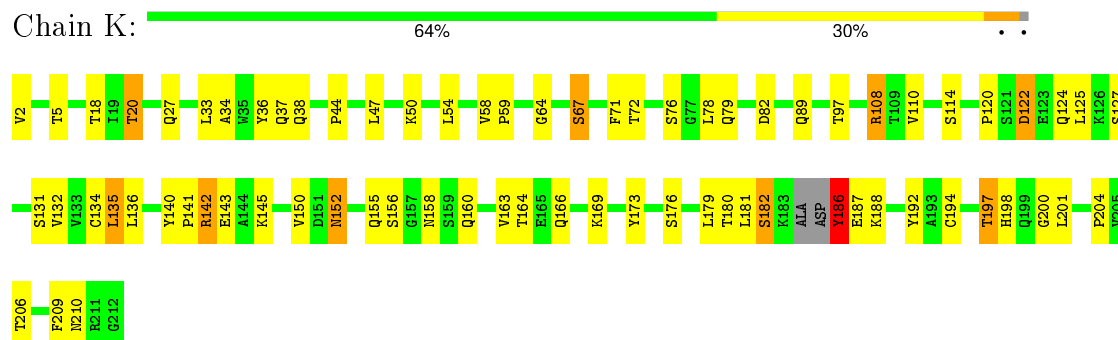
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

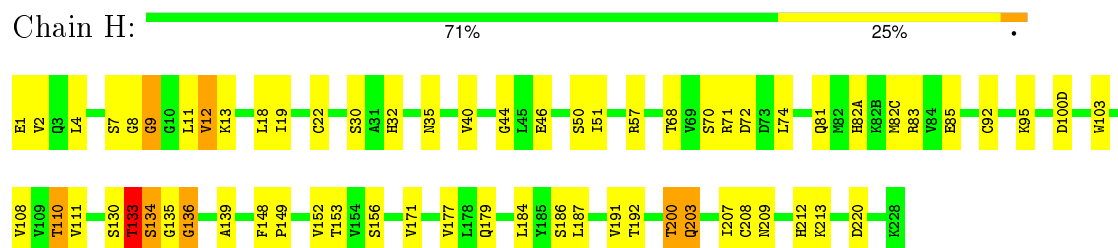
- Molecule 1: FAB 2G12, light chain



- Molecule 1: FAB 2G12, light chain

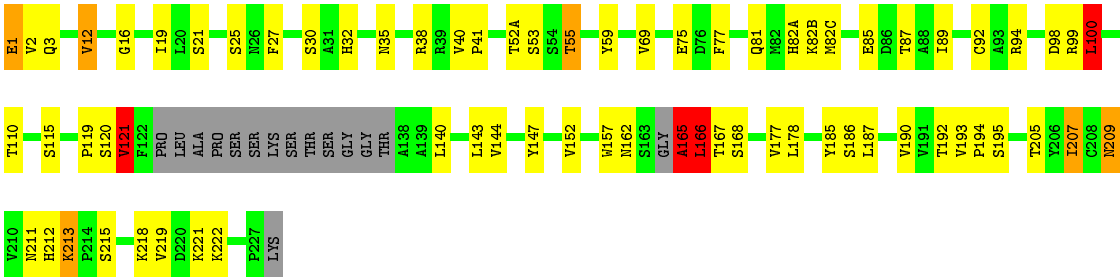


- Molecule 2: FAB 2G12, heavy chain



- Molecule 2: FAB 2G12, heavy chain





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.21Å 165.71Å 169.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85	Depositor
% Data completeness (in resolution range)	99.5 (50.00-2.85)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	K	0.87	0/1638	0.89	2/2224 (0.1%)
1	L	0.80	1/1635 (0.1%)	0.81	0/2223
2	H	0.89	1/1710 (0.1%)	0.92	0/2330
2	M	0.85	0/1611	0.89	1/2194 (0.0%)
All	All	0.85	2/6594 (0.0%)	0.88	3/8971 (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
2	H	0	1
2	M	0	1
3	M	1	0
All	All	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	210	ASN	C-O	9.23	1.40	1.23
2	H	46	GLU	CG-CD	5.32	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	166	LEU	N-CA-C	-5.31	96.67	111.00
1	K	186	TYR	CB-CG-CD2	5.12	124.08	121.00
1	K	2	VAL	CB-CA-C	-5.01	101.88	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	235	BMA	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	133	THR	Peptide
2	M	165	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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	K	1602	0	1560	45	0
1	L	1599	0	1553	42	0
2	H	1671	0	1637	40	0
2	M	1575	0	1541	48	0
3	M	77	0	64	2	0
4	M	11	0	10	2	0
All	All	6535	0	6365	167	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 13.

All (167) 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)
1:L:147:GLN:NE2	1:L:154:LEU:HD11	1.64	1.11
1:L:147:GLN:HE22	1:L:154:LEU:HD11	1.19	1.07
3:M:234:MAN:O2	4:M:236:MAN:C1	2.08	1.01
1:L:158:ASN:ND2	1:L:179:LEU:HD11	1.87	0.90
1:L:18:THR:HG23	1:L:76:SER:HA	1.54	0.88
2:H:12:VAL:HG11	2:H:82(C):MET:CE	2.05	0.86
1:L:147:GLN:HE22	1:L:154:LEU:CD1	1.89	0.84
2:H:12:VAL:HG11	2:H:82(C):MET:HE3	1.60	0.84
1:L:147:GLN:NE2	1:L:154:LEU:CD1	2.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:THR:HG22	2:H:203:GLN:HB2	1.60	0.82
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.65	0.78
1:L:137:ASN:ND2	2:M:192:THR:HG21	1.99	0.78
2:M:81:GLN:HE21	2:M:82(A):HIS:HE1	1.32	0.74
2:H:13:LYS:HD3	2:H:148:PHE:CE2	2.22	0.74
2:M:12:VAL:HG21	2:M:82(C):MET:CE	2.21	0.70
1:L:135:LEU:C	1:L:136:LEU:HD12	2.14	0.68
1:L:180:THR:O	1:L:181:LEU:HD23	1.94	0.68
2:M:207:ILE:HA	2:M:221:LYS:O	1.94	0.67
1:K:182:SER:O	1:K:186:TYR:HB3	1.95	0.66
1:K:136:LEU:HD12	1:K:136:LEU:N	2.08	0.66
2:H:177:VAL:CG1	1:K:160:GLN:NE2	2.59	0.66
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.78	0.65
1:K:33:LEU:HD22	1:K:71:PHE:CG	2.34	0.63
1:L:124:GLN:HE22	1:L:131:SER:CB	2.12	0.63
2:M:12:VAL:HG21	2:M:82(C):MET:HE1	1.80	0.61
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.47	0.61
2:H:177:VAL:HG13	1:K:160:GLN:NE2	2.15	0.61
1:L:50:LYS:O	1:L:51:ALA:HB3	1.99	0.61
1:L:198:HIS:CD2	1:L:200:GLY:H	2.19	0.61
2:M:85:GLU:OE1	2:M:85:GLU:N	2.22	0.61
2:M:81:GLN:HE21	2:M:82(A):HIS:CE1	2.17	0.61
2:M:81:GLN:NE2	2:M:82(A):HIS:HE1	1.98	0.60
1:K:135:LEU:C	1:K:136:LEU:HD12	2.22	0.59
2:H:13:LYS:HD3	2:H:148:PHE:CZ	2.37	0.59
1:K:150:VAL:HB	1:K:155:GLN:NE2	2.18	0.58
2:H:139:ALA:HB2	2:H:192:THR:HG22	1.84	0.58
1:K:38:GLN:NE2	1:K:44:PRO:HD3	2.19	0.58
2:M:187:LEU:HD12	2:M:187:LEU:C	2.25	0.58
2:M:166:LEU:HD12	2:M:167:THR:N	2.19	0.58
1:L:137:ASN:HD21	2:M:192:THR:HG21	1.69	0.57
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.86	0.57
1:L:186:TYR:O	1:L:192:TYR:OH	2.22	0.57
1:K:136:LEU:N	1:K:136:LEU:CD1	2.67	0.57
1:K:18:THR:HG23	1:K:76:SER:HA	1.87	0.56
2:H:135:GLY:O	2:H:136:GLY:O	2.23	0.56
2:H:81:GLN:HE21	2:H:82(A):HIS:CE1	2.24	0.56
2:M:53:SER:HB2	2:M:55:THR:HG22	1.87	0.56
1:K:67:SER:HA	1:K:71:PHE:CE2	2.41	0.56
2:H:4:LEU:N	2:H:4:LEU:HD12	2.21	0.56
1:L:108:ARG:HD2	1:L:140:TYR:CG	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:O	1:L:136:LEU:HD12	2.07	0.55
2:M:87:THR:HG23	2:M:110:THR:HA	1.89	0.55
2:M:162:ASN:O	2:M:209:ASN:OD1	2.25	0.54
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.42	0.54
2:H:108:VAL:HG12	2:H:110:THR:HG22	1.89	0.53
1:K:180:THR:O	1:K:181:LEU:HD23	2.08	0.53
1:L:11:LEU:HD22	1:L:19:ILE:HD12	1.91	0.53
2:M:100:LEU:C	2:M:100:LEU:HD13	2.28	0.53
1:K:124:GLN:HE22	1:K:131:SER:HB2	1.74	0.52
1:K:124:GLN:O	1:K:127:SER:OG	2.18	0.52
2:M:178:LEU:HD13	2:M:185:TYR:CE1	2.44	0.52
2:M:121:VAL:HG21	2:M:219:VAL:HG11	1.91	0.51
1:K:58:VAL:HG13	1:K:59:PRO:HD2	1.93	0.51
1:L:135:LEU:HD22	2:M:190:VAL:HG21	1.93	0.51
1:K:186:TYR:CE1	1:K:192:TYR:CZ	2.99	0.51
3:M:234:MAN:O2	4:M:236:MAN:C2	2.58	0.50
2:H:12:VAL:HG21	2:H:82(C):MET:HE1	1.91	0.50
1:K:150:VAL:HG22	1:K:192:TYR:CD2	2.48	0.49
1:K:158:ASN:HD22	1:K:181:LEU:HD21	1.77	0.49
2:H:12:VAL:HG11	2:H:82(C):MET:HE1	1.89	0.49
1:K:142:ARG:O	1:K:142:ARG:HG3	2.13	0.49
1:L:150:VAL:HG22	1:L:192:TYR:CD2	2.48	0.49
2:M:1:GLU:HG2	2:M:2:VAL:N	2.27	0.49
2:H:72:ASP:C	2:H:72:ASP:OD1	2.50	0.48
2:M:100:LEU:CD1	2:M:100:LEU:C	2.82	0.48
1:K:110:VAL:HG22	1:K:141:PRO:HD3	1.94	0.48
2:H:81:GLN:NE2	2:H:82(A):HIS:HE1	2.11	0.48
1:L:150:VAL:HG22	1:L:192:TYR:HD2	1.78	0.48
2:M:207:ILE:HG22	2:M:222:LYS:HA	1.95	0.47
1:K:197:THR:HG23	1:K:204:PRO:HB3	1.94	0.47
1:L:18:THR:HA	1:L:75:ILE:O	2.15	0.47
1:K:150:VAL:HG22	1:K:192:TYR:CE2	2.50	0.47
2:M:193:VAL:HB	2:M:194:PRO:HD2	1.97	0.47
1:K:122:ASP:N	1:K:122:ASP:OD1	2.39	0.47
2:H:51:ILE:HG21	2:H:71:ARG:HB3	1.96	0.47
1:K:198:HIS:CD2	1:K:200:GLY:H	2.32	0.47
1:L:20:THR:HG22	1:L:74:THR:OG1	2.15	0.47
2:M:59:TYR:CE2	2:M:69:VAL:HG12	2.50	0.47
1:L:136:LEU:N	1:L:136:LEU:HD12	2.30	0.46
2:H:209:ASN:ND2	2:H:220:ASP:OD2	2.48	0.46
2:H:40:VAL:HG22	2:H:44:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:CD2	2:M:190:VAL:HG21	2.45	0.46
2:M:40:VAL:HB	2:M:41:PRO:HD2	1.98	0.46
2:M:30:SER:O	2:M:52(A):THR:HG22	2.14	0.46
2:H:57:ARG:NH2	2:M:75:GLU:HG3	2.31	0.46
2:M:209:ASN:ND2	2:M:209:ASN:N	2.62	0.46
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.80	0.46
1:L:108:ARG:HD3	1:L:109:THR:O	2.15	0.46
2:M:38:ARG:HA	2:M:89:ILE:O	2.16	0.46
1:K:108:ARG:HD2	1:K:140:TYR:CB	2.46	0.46
1:K:145:LYS:HB3	1:K:197:THR:OG1	2.16	0.46
2:H:95:LYS:HE3	2:H:100(D):ASP:O	2.15	0.46
2:M:3:GLN:HB2	2:M:25:SER:HB2	1.98	0.46
2:M:35:ASN:O	2:M:92:CYS:HA	2.16	0.45
1:K:158:ASN:ND2	1:K:179:LEU:HD11	2.32	0.45
1:K:54:LEU:HD11	1:K:58:VAL:HG12	1.97	0.45
1:L:8:PRO:O	1:L:102:THR:HG23	2.16	0.45
1:K:163:VAL:HG12	1:K:164:THR:N	2.32	0.45
2:H:68:THR:HG21	2:M:77:PHE:CE1	2.51	0.45
2:M:12:VAL:CG2	2:M:82(C):MET:CE	2.93	0.44
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.48	0.44
2:H:171:VAL:HG22	2:H:191:VAL:HB	1.99	0.44
1:L:158:ASN:HD21	1:L:179:LEU:HD11	1.76	0.44
2:H:19:ILE:HD13	2:M:21:SER:HB3	1.99	0.44
2:M:12:VAL:CG2	2:M:82(C):MET:HE1	2.46	0.44
2:H:18:LEU:HB2	2:H:82(C):MET:HE1	1.99	0.44
1:K:54:LEU:HD11	1:K:58:VAL:CG1	2.47	0.44
1:K:64:GLY:HA2	1:K:72:THR:O	2.18	0.43
2:M:119:PRO:HB2	2:M:144:VAL:HG13	2.01	0.43
1:L:124:GLN:HE21	1:L:129:THR:HG22	1.83	0.43
2:H:179:GLN:HG3	2:H:184:LEU:O	2.18	0.43
1:L:50:LYS:O	1:L:51:ALA:CB	2.63	0.43
2:H:133:THR:HB	2:H:134:SER:O	2.18	0.43
1:L:175:LEU:HD23	1:L:175:LEU:C	2.39	0.43
1:L:54:LEU:HD11	1:L:58:VAL:HG12	2.01	0.43
2:M:19:ILE:HG12	2:M:81:GLN:HG2	2.01	0.43
1:L:203:SER:HB2	1:L:204:PRO:CD	2.49	0.43
2:H:83:ARG:C	2:H:111:VAL:HG11	2.40	0.43
2:M:16:GLY:O	2:M:82(C):MET:HG3	2.19	0.42
2:M:157:TRP:O	2:M:165:ALA:N	2.52	0.42
2:M:212:HIS:HD2	2:M:215:SER:OG	2.02	0.42
2:M:27:PHE:CE1	2:M:94:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:NE2	1:L:129:THR:HG22	2.34	0.42
2:H:85:GLU:N	2:H:85:GLU:OE1	2.45	0.42
2:H:207:ILE:HG22	2:H:209:ASN:ND2	2.34	0.42
1:K:79:GLN:O	1:K:82:ASP:HB2	2.20	0.42
2:M:12:VAL:HG21	2:M:82(C):MET:HE2	1.98	0.41
2:H:57:ARG:CZ	2:M:75:GLU:HG3	2.50	0.41
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.01	0.41
2:M:143:LEU:C	2:M:143:LEU:HD12	2.41	0.41
2:H:12:VAL:HG21	2:H:82(C):MET:CE	2.50	0.41
1:K:34:ALA:HB3	1:K:89:GLN:HE21	1.85	0.41
1:L:39:LYS:NZ	1:L:81:ASP:O	2.42	0.41
2:M:211:ASN:HD21	2:M:213:LYS:HE2	1.85	0.41
2:H:103:TRP:CD1	2:H:103:TRP:N	2.89	0.41
1:L:141:PRO:O	1:L:198:HIS:HE1	2.03	0.41
2:M:119:PRO:HB3	2:M:147:TYR:HB3	2.02	0.41
1:K:194:CYS:O	1:K:206:THR:HA	2.21	0.41
2:H:149:PRO:O	2:H:212:HIS:HE1	2.03	0.41
1:L:125:LEU:HD12	1:L:126:LYS:N	2.36	0.41
2:H:35:ASN:O	2:H:92:CYS:HA	2.20	0.41
2:H:8:GLY:O	2:H:9:GLY:O	2.38	0.41
1:K:20:THR:O	1:K:20:THR:HG22	2.21	0.41
2:H:32:HIS:HD2	2:H:95:LYS:O	2.04	0.40
2:H:200:THR:HG22	2:H:203:GLN:CB	2.40	0.40
2:H:156:SER:OG	2:H:209:ASN:HB2	2.21	0.40
2:M:82(A):HIS:O	2:M:82(B):LYS:C	2.59	0.40
1:K:158:ASN:O	1:K:179:LEU:HD12	2.20	0.40
1:K:186:TYR:CD1	1:K:192:TYR:OH	2.74	0.40
2:M:32:HIS:CD2	2:M:94:ARG:HD2	2.57	0.40
1:L:121:SER:O	1:L:125:LEU:HG	2.21	0.40
1:K:209:PHE:HD1	1:K:210:ASN:O	2.04	0.40
1:K:166:GLN:HG3	1:K:173:TYR:CE2	2.56	0.40
1:K:143:GLU:CD	1:K:143:GLU:N	2.75	0.40
1:L:150:VAL:CG1	1:L:192:TYR:CE2	3.05	0.40
1:K:36:TYR:OH	1:K:89:GLN:NE2	2.54	0.40
1:K:152:ASN:HA	1:K:152:ASN:HD22	1.66	0.40

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	K	207/211 (98%)	190 (92%)	15 (7%)	2 (1%)	19	49
1	L	207/211 (98%)	188 (91%)	15 (7%)	4 (2%)	10	32
2	H	222/224 (99%)	203 (91%)	13 (6%)	6 (3%)	6	22
2	M	205/224 (92%)	178 (87%)	22 (11%)	5 (2%)	7	25
All	All	841/870 (97%)	759 (90%)	65 (8%)	17 (2%)	9	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	133	THR
2	H	136	GLY
2	H	200	THR
1	K	188	LYS
2	M	121	VAL
2	M	165	ALA
1	L	188	LYS
2	H	130	SER
2	M	100	LEU
1	L	138	ASN
1	K	67	SER
2	M	99	ARG
2	H	9	GLY
2	H	186	SER
1	L	123	GLU
2	M	186	SER
1	L	51	ALA

### 5.3.2 Protein sidechains [i](#)

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	K	180/182 (99%)	158 (88%)	22 (12%)	6	16
1	L	180/182 (99%)	163 (91%)	17 (9%)	11	29
2	H	188/189 (100%)	169 (90%)	19 (10%)	9	25
2	M	176/189 (93%)	157 (89%)	19 (11%)	8	21
All	All	724/742 (98%)	647 (89%)	77 (11%)	8	22

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	76	SER
1	L	97	THR
1	L	108	ARG
1	L	134	CYS
1	L	143	GLU
1	L	145	LYS
1	L	147	GLN
1	L	152	ASN
1	L	154	LEU
1	L	162	SER
1	L	171	SER
1	L	177	SER
1	L	181	LEU
1	L	182	SER
1	L	185	ASP
1	L	201	LEU
2	H	1	GLU
2	H	2	VAL
2	H	7	SER
2	H	11	LEU
2	H	12	VAL
2	H	22	CYS
2	H	30	SER
2	H	50	SER
2	H	70	SER
2	H	74	LEU
2	H	110	THR

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Mol	Chain	Res	Type
2	H	133	THR
2	H	134	SER
2	H	152	VAL
2	H	153	THR
2	H	187	LEU
2	H	203	GLN
2	H	208	CYS
2	H	213	LYS
1	K	5	THR
1	K	20	THR
1	K	27	GLN
1	K	50	LYS
1	K	78	LEU
1	K	97	THR
1	K	108	ARG
1	K	114	SER
1	K	122	ASP
1	K	125	LEU
1	K	134	CYS
1	K	135	LEU
1	K	142	ARG
1	K	152	ASN
1	K	156	SER
1	K	169	LYS
1	K	176	SER
1	K	182	SER
1	K	186	TYR
1	K	187	GLU
1	K	197	THR
1	K	201	LEU
2	M	1	GLU
2	M	12	VAL
2	M	55	THR
2	M	98	ASP
2	M	100	LEU
2	M	115	SER
2	M	120	SER
2	M	121	VAL
2	M	140	LEU
2	M	152	VAL
2	M	166	LEU
2	M	168	SER

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Mol	Chain	Res	Type
2	M	177	VAL
2	M	195	SER
2	M	205	THR
2	M	207	ILE
2	M	209	ASN
2	M	213	LYS
2	M	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	124	GLN
1	L	137	ASN
1	L	147	GLN
1	L	152	ASN
1	L	198	HIS
2	H	32	HIS
2	H	81	GLN
2	H	82(A)	HIS
2	H	212	HIS
1	K	27	GLN
1	K	38	GLN
1	K	87	HIS
1	K	89	GLN
1	K	90	HIS
1	K	124	GLN
1	K	152	ASN
1	K	160	GLN
1	K	198	HIS
2	M	32	HIS
2	M	81	GLN
2	M	82(A)	HIS
2	M	209	ASN
2	M	212	HIS

### 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 ⓘ

7 carbohydrates 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$
3	MAN	M	229	3	11,11,12	1.07	1 (9%)	14,15,17	2.40	5 (35%)
3	MAN	M	230	3	11,11,12	0.65	0	14,15,17	2.13	6 (42%)
3	MAN	M	231	3	11,11,12	1.12	1 (9%)	14,15,17	1.90	6 (42%)
3	MAN	M	232	3	11,11,12	0.62	0	14,15,17	1.35	1 (7%)
3	BMA	M	233	3	11,11,12	0.86	0	14,15,17	6.31	11 (78%)
3	MAN	M	234	3	11,11,12	1.00	1 (9%)	14,15,17	2.32	5 (35%)
3	BMA	M	235	3	11,11,12	1.25	1 (9%)	14,15,17	4.21	7 (50%)

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
3	MAN	M	229	3	-	0/2/19/22	0/1/1/1
3	MAN	M	230	3	-	0/2/19/22	0/1/1/1
3	MAN	M	231	3	-	0/2/19/22	0/1/1/1
3	MAN	M	232	3	-	0/2/19/22	0/1/1/1
3	BMA	M	233	3	-	0/2/19/22	0/1/1/1
3	MAN	M	234	3	-	0/2/19/22	0/1/1/1
3	BMA	M	235	3	1/1/4/5	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	229	MAN	O5-C1	-2.44	1.39	1.43
3	M	235	BMA	O5-C1	-2.23	1.40	1.43
3	M	231	MAN	O5-C1	-2.19	1.40	1.43
3	M	234	MAN	O4-C4	-2.18	1.37	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	233	BMA	C2-C3-C4	-15.34	84.99	111.04
3	M	235	BMA	C1-O5-C5	-10.78	98.57	112.25
3	M	235	BMA	C1-C2-C3	-10.10	97.59	109.54
3	M	233	BMA	C3-C4-C5	-8.82	94.81	110.20
3	M	233	BMA	O2-C2-C1	-6.45	96.27	109.21
3	M	233	BMA	C6-C5-C4	-5.36	99.79	113.02
3	M	234	MAN	O2-C2-C3	-5.08	99.90	110.12
3	M	234	MAN	C2-C3-C4	-4.14	104.00	111.04
3	M	229	MAN	O4-C4-C3	-3.81	101.75	110.34
3	M	229	MAN	O5-C1-C2	-3.65	104.94	110.86
3	M	231	MAN	C1-O5-C5	-3.22	108.16	112.25
3	M	230	MAN	C2-C3-C4	-3.22	105.58	111.04
3	M	231	MAN	C1-C2-C3	-2.83	106.19	109.54
3	M	233	BMA	O2-C2-C3	-2.80	104.49	110.12
3	M	229	MAN	C2-C3-C4	-2.55	106.71	111.04
3	M	231	MAN	O5-C1-C2	-2.53	106.75	110.86
3	M	232	MAN	C6-C5-C4	-2.52	106.79	113.02
3	M	235	BMA	O4-C4-C3	-2.36	105.01	110.34
3	M	230	MAN	C6-C5-C4	-2.36	107.20	113.02
3	M	231	MAN	O4-C4-C3	-2.33	105.09	110.34
3	M	234	MAN	O4-C4-C3	-2.25	105.27	110.34
3	M	230	MAN	C3-C4-C5	-2.18	106.40	110.20
3	M	231	MAN	O2-C2-C3	-2.08	105.94	110.12
3	M	235	BMA	O3-C3-C4	2.01	114.87	110.34
3	M	235	BMA	C6-C5-C4	2.02	118.00	113.02
3	M	235	BMA	O5-C1-C2	2.03	114.16	110.86
3	M	233	BMA	O4-C4-C3	2.04	114.93	110.34
3	M	234	MAN	O2-C2-C1	2.05	113.32	109.21
3	M	230	MAN	O4-C4-C3	2.66	116.32	110.34
3	M	235	BMA	C3-C4-C5	2.89	115.24	110.20
3	M	234	MAN	C3-C4-C5	2.93	115.30	110.20
3	M	230	MAN	C1-O5-C5	2.94	115.98	112.25
3	M	231	MAN	C6-C5-C4	2.98	120.37	113.02
3	M	229	MAN	O2-C2-C1	3.09	115.40	109.21
3	M	230	MAN	O3-C3-C4	3.42	118.04	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	233	BMA	O5-C1-C2	3.43	116.42	110.86
3	M	233	BMA	O5-C5-C6	4.17	116.38	107.35
3	M	229	MAN	O3-C3-C2	4.43	118.00	110.00
3	M	233	BMA	O4-C4-C5	4.94	122.33	109.24
3	M	233	BMA	C1-C2-C3	5.88	116.50	109.54
3	M	233	BMA	O3-C3-C2	8.33	125.04	110.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	235	BMA	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	234	MAN	2	0

## 5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z  > 2$
4	MAN	M	236	-	11,11,12	0.97	1 (9%)	14,15,17	2.98	7 (50%)

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
4	MAN	M	236	-	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	236	MAN	O5-C5	-2.08	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	236	MAN	O5-C5-C6	-2.85	101.19	107.35
4	M	236	MAN	O3-C3-C2	-2.41	105.64	110.00
4	M	236	MAN	O2-C2-C3	-2.36	105.36	110.12
4	M	236	MAN	C6-C5-C4	-2.02	108.02	113.02
4	M	236	MAN	C1-C2-C3	3.76	113.99	109.54
4	M	236	MAN	C1-O5-C5	4.26	117.66	112.25
4	M	236	MAN	O5-C1-C2	7.82	123.55	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	236	MAN	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.