



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:32 am GMT

PDB ID : 1ZLU  
Title : FAB 2G12 + Man5  
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Deposited on : 2005-05-09  
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

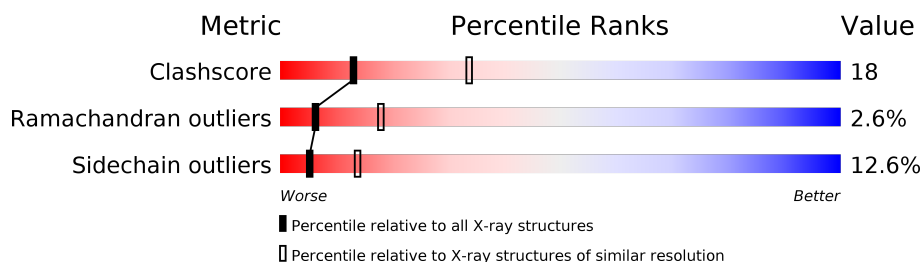
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)

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	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6546 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	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	K	209	Total	C	N	O	S	0	0	0
			1601	1008	269	319	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1649	1039	281	322	7			
2	M	212	Total	C	N	O	S	0	0	0
			1599	1010	271	311	7			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	2	Total	C	O	0	0
			23	12	11		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

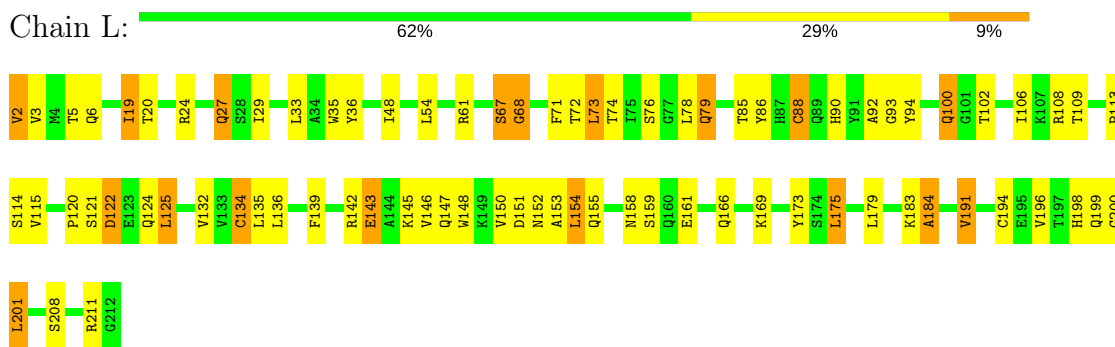
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	5	Total	C	O	0	0
			56	30	26		

### 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 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.

Note EDS was not executed.

- Molecule 1: FAB 2G12, light chain





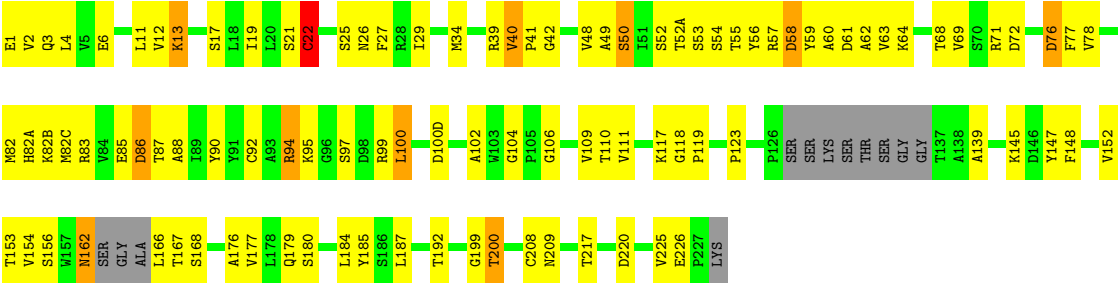
● Molecule 2: FAB 2G12, heavy chain

Chain M: 

50%

40%

5%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.89Å 131.79Å 170.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75	Depositor
% Data completeness (in resolution range)	90.9 (50.00-2.75)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.222 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

## 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: 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	0.85	1/1637 (0.1%)	0.90	1/2224 (0.0%)
1	L	0.96	4/1654 (0.2%)	0.96	4/2246 (0.2%)
2	H	0.93	2/1687 (0.1%)	1.01	6/2300 (0.3%)
2	M	0.87	2/1636 (0.1%)	0.89	0/2230
All	All	0.91	9/6614 (0.1%)	0.94	11/9000 (0.1%)

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
1	K	0	2
2	H	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	161	GLU	CG-CD	9.20	1.65	1.51
1	L	88	CYS	CB-SG	-8.46	1.67	1.82
2	M	22	CYS	CB-SG	-6.17	1.71	1.82
2	H	142	CYS	CB-SG	-5.95	1.72	1.81
2	M	1	GLU	CG-CD	5.89	1.60	1.51
2	H	22	CYS	CB-SG	-5.61	1.72	1.81
1	L	134	CYS	CB-SG	-5.51	1.72	1.81
1	L	161	GLU	CB-CG	5.10	1.61	1.52
1	K	117	ILE	CA-CB	5.02	1.66	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2	VAL	CB-CA-C	-7.60	96.95	111.40
2	H	99	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	L	134	CYS	CA-CB-SG	-6.60	102.11	114.00
2	H	57	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	L	194	CYS	CA-CB-SG	-5.77	103.62	114.00
2	H	57	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	H	99	ARG	CD-NE-CZ	5.46	131.24	123.60
1	L	154	LEU	CA-CB-CG	5.31	127.51	115.30
2	H	99	ARG	CG-CD-NE	5.16	122.63	111.80
1	K	186	TYR	N-CA-C	5.12	124.84	111.00
2	H	142	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	150	GLU	Peptide
1	K	183	LYS	Peptide
1	K	7	SER	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	1601	0	1560	56	0
1	L	1618	0	1580	53	0
2	H	1649	0	1603	64	0
2	M	1599	0	1563	65	0
3	H	23	0	21	1	0
4	M	56	0	48	4	0
All	All	6546	0	6375	236	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 18.

All (236) 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)
2:M:12:VAL:HG11	2:M:82(C):MET:HE3	1.39	1.01
2:H:4:LEU:HD23	2:H:24:VAL:HG12	1.42	0.99
2:M:12:VAL:HG11	2:M:82(C):MET:CE	1.98	0.94
1:K:2:VAL:HG22	1:K:27:GLN:HE21	1.38	0.89
2:H:132:SER:O	2:H:137:THR:N	2.06	0.89
1:K:197:THR:HG22	1:K:204:PRO:HB3	1.56	0.87
1:L:132:VAL:CG2	1:L:179:LEU:HB3	2.06	0.85
1:K:48:ILE:HD13	1:K:64:GLY:H	1.48	0.79
4:M:231:MAN:O2	4:M:233:MAN:H3	1.83	0.77
2:M:199:GLY:O	2:M:200:THR:HG23	1.85	0.77
2:H:5:VAL:O	2:H:5:VAL:HG13	1.84	0.76
2:M:3:GLN:C	2:M:4:LEU:HD12	2.08	0.74
2:M:123:PRO:HB3	2:M:225:VAL:HG22	1.71	0.73
2:H:13:LYS:HD3	2:H:148:PHE:CE1	2.24	0.72
2:M:12:VAL:HG21	2:M:82(C):MET:HE1	1.72	0.71
2:H:19:ILE:HD12	2:H:19:ILE:H	1.57	0.70
1:K:2:VAL:HG22	1:K:27:GLN:NE2	2.06	0.70
2:M:11:LEU:HD12	2:M:110:THR:HB	1.72	0.70
2:M:94:ARG:HD3	2:M:102:ALA:HB3	1.74	0.70
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.75	0.68
2:M:87:THR:OG1	2:M:111:VAL:HG23	1.94	0.68
2:M:83:ARG:O	2:M:86:ASP:HB2	1.94	0.68
1:L:33:LEU:HD13	1:L:71:PHE:CG	2.29	0.67
1:L:151:ASP:HA	1:L:191:VAL:HG13	1.76	0.67
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.44	0.66
2:H:19:ILE:N	2:H:19:ILE:HD12	2.10	0.66
2:H:207:ILE:HA	2:H:221:LYS:O	1.95	0.65
2:H:94:ARG:O	2:H:100(F):PHE:HA	1.97	0.64
2:H:184:LEU:N	2:H:184:LEU:CD1	2.61	0.64
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.79	0.64
2:M:85:GLU:N	2:M:85:GLU:OE1	2.31	0.64
2:H:179:GLN:HB2	2:H:184:LEU:O	1.98	0.63
2:H:184:LEU:N	2:H:184:LEU:HD13	2.13	0.63
2:M:53:SER:HB2	2:M:55:THR:HG23	1.81	0.62
2:H:52:SER:OG	2:H:56:TYR:N	2.28	0.62
2:M:90:TYR:CD1	2:M:109:VAL:HG23	2.35	0.62
2:H:18:LEU:N	2:H:82(C):MET:HE2	2.15	0.62
1:K:33:LEU:HD12	1:K:89:GLN:O	2.01	0.61
1:K:159:SER:HA	1:K:178:THR:O	2.00	0.61
2:M:52(A):THR:OG1	4:M:231:MAN:O4	2.18	0.61
2:M:145:LYS:HE3	2:M:179:GLN:HE22	1.66	0.61
1:K:167:ASP:OD2	1:K:169:LYS:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:HD12	2:H:110:THR:HG23	1.83	0.60
2:H:157:TRP:CZ3	2:H:208:CYS:HB3	2.36	0.60
1:K:11:LEU:HD23	1:K:11:LEU:C	2.23	0.60
1:L:198:HIS:CD2	1:L:200:GLY:H	2.21	0.59
1:L:2:VAL:HA	1:L:27:GLN:NE2	2.18	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.83	0.59
2:H:212:HIS:HD2	2:H:215:SER:OG	1.85	0.59
2:H:18:LEU:HB2	2:H:82(C):MET:HE1	1.84	0.59
1:L:19:ILE:HD11	1:L:78:LEU:HD21	1.85	0.58
1:K:136:LEU:HD21	1:K:146:VAL:HG22	1.86	0.58
2:M:6:GLU:OE1	2:M:104:GLY:HA3	2.03	0.58
1:K:209:PHE:C	1:K:210:ASN:HD22	2.08	0.57
2:H:146:ASP:HB3	2:H:184:LEU:HD23	1.86	0.57
2:H:146:ASP:HA	2:H:184:LEU:HB3	1.87	0.57
2:H:16:GLY:O	2:H:82(C):MET:HG3	2.05	0.56
2:H:171:VAL:HG22	2:H:191:VAL:HG21	1.87	0.56
1:K:33:LEU:HD22	1:K:71:PHE:CG	2.40	0.56
2:H:171:VAL:HG22	2:H:191:VAL:CG2	2.35	0.56
2:H:18:LEU:HB2	2:H:82(C):MET:CE	2.36	0.56
1:L:20:THR:HG22	1:L:74:THR:HG23	1.87	0.56
1:L:198:HIS:HB3	1:L:201:LEU:HD22	1.88	0.55
1:K:6:GLN:HE22	1:K:101:GLY:C	2.10	0.55
1:L:122:ASP:N	1:L:122:ASP:OD1	2.37	0.55
2:M:99:ARG:O	2:M:100:LEU:HB2	2.06	0.55
2:H:4:LEU:HD23	2:H:24:VAL:CG1	2.28	0.55
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.88	0.55
2:M:12:VAL:HG11	2:M:82(C):MET:HE1	1.86	0.55
2:M:26:ASN:O	2:M:27:PHE:HB3	2.07	0.54
2:H:5:VAL:O	2:H:5:VAL:CG1	2.54	0.54
2:M:60:ALA:O	2:M:63:VAL:HG22	2.08	0.54
1:K:189:HIS:O	1:K:211:ARG:HD3	2.07	0.54
1:L:143:GLU:CD	1:L:143:GLU:H	2.10	0.54
1:L:135:LEU:HD12	1:L:136:LEU:N	2.23	0.54
1:K:181:LEU:CD1	1:K:186:TYR:HB2	2.37	0.54
2:M:39:ARG:O	2:M:88:ALA:HB1	2.08	0.54
2:M:4:LEU:HD12	2:M:4:LEU:N	2.23	0.54
1:L:154:LEU:HD12	1:L:155:GLN:H	1.72	0.53
1:K:6:GLN:HB2	1:K:100:GLN:OE1	2.06	0.53
1:K:135:LEU:HD22	1:K:136:LEU:N	2.24	0.53
1:K:181:LEU:HD13	1:K:186:TYR:HB2	1.91	0.53
1:L:115:VAL:HA	1:L:135:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:PHE:HA	2:H:81:GLN:O	2.10	0.52
2:H:1:GLU:O	2:H:26:ASN:ND2	2.37	0.52
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.44	0.52
1:L:33:LEU:HD13	1:L:71:PHE:CD2	2.44	0.52
2:H:166:LEU:HD21	2:H:191:VAL:HG11	1.91	0.52
2:H:213:LYS:N	2:H:214:PRO:CD	2.73	0.52
2:M:59:TYR:OH	2:M:69:VAL:HG12	2.10	0.52
2:M:82(A):HIS:O	2:M:82(B):LYS:C	2.49	0.51
1:K:150:VAL:O	1:K:151:ASP:C	2.48	0.51
2:M:90:TYR:CD1	2:M:109:VAL:CG2	2.93	0.51
2:M:119:PRO:HD2	2:M:217:THR:HG21	1.93	0.51
2:M:22:CYS:O	2:M:22:CYS:SG	2.68	0.51
2:H:4:LEU:HD11	2:H:102:ALA:HB1	1.93	0.51
1:L:136:LEU:HD22	1:L:175:LEU:HD22	1.93	0.51
1:K:6:GLN:NE2	1:K:101:GLY:C	2.64	0.51
1:K:2:VAL:HG12	1:K:3:VAL:N	2.26	0.51
1:L:121:SER:O	1:L:124:GLN:N	2.43	0.50
2:H:100:LEU:HD13	3:H:229:MAN:H2	1.91	0.50
1:K:90:HIS:HB3	1:K:97:THR:HG22	1.93	0.50
1:L:35:TRP:CG	1:L:73:LEU:HD13	2.47	0.50
2:M:95:LYS:HG3	2:M:100(D):ASP:O	2.12	0.50
2:M:52:SER:O	2:M:71:ARG:NH1	2.44	0.50
1:K:181:LEU:C	1:K:182:SER:O	2.48	0.49
1:L:132:VAL:HG23	1:L:179:LEU:HB3	1.88	0.49
2:H:12:VAL:HG11	2:H:82(C):MET:HE3	1.94	0.49
1:K:64:GLY:HA2	1:K:72:THR:O	2.12	0.49
2:M:166:LEU:HD12	2:M:167:THR:N	2.28	0.49
2:M:34:MET:HG3	2:M:78:VAL:HG21	1.93	0.49
2:H:12:VAL:HG21	2:H:82(C):MET:HE1	1.94	0.49
1:K:6:GLN:NE2	1:K:102:THR:OG1	2.43	0.49
1:K:54:LEU:HD11	1:K:58:VAL:CG1	2.42	0.49
2:H:47:TRP:HZ2	2:H:50:SER:HB3	1.78	0.49
1:K:48:ILE:HD13	1:K:64:GLY:N	2.23	0.49
2:H:21:SER:HB3	2:M:19:ILE:HG12	1.94	0.49
2:H:157:TRP:CH2	2:H:208:CYS:HB3	2.47	0.49
2:M:90:TYR:O	2:M:106:GLY:HA2	2.14	0.48
2:H:157:TRP:HB3	2:H:166:LEU:HD23	1.94	0.48
2:M:145:LYS:CE	2:M:179:GLN:HE22	2.27	0.48
2:M:52:SER:OG	2:M:56:TYR:N	2.47	0.48
2:H:107:THR:HG23	2:H:107:THR:O	2.13	0.48
1:K:35:TRP:CZ3	1:K:88:CYS:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:HG12	1:L:54:LEU:HD12	1.95	0.48
2:M:162:ASN:OD1	2:M:162:ASN:N	2.47	0.48
2:H:167:THR:C	2:H:171:VAL:HG23	2.35	0.47
2:M:123:PRO:CB	2:M:225:VAL:HG22	2.41	0.47
1:K:210:ASN:O	1:K:211:ARG:C	2.51	0.47
1:K:126:LYS:HB3	1:K:126:LYS:NZ	2.29	0.47
1:K:70:GLU:C	1:K:71:PHE:CD1	2.88	0.47
1:L:147:GLN:HG2	1:L:154:LEU:CD1	2.44	0.47
1:L:92:ALA:O	1:L:93:GLY:C	2.53	0.47
2:H:25:SER:O	2:H:26:ASN:HB2	2.14	0.47
2:M:110:THR:C	2:M:111:VAL:CG2	2.81	0.47
2:H:22:CYS:O	2:H:77:PHE:HA	2.15	0.47
1:L:2:VAL:HG22	1:L:27:GLN:HE22	1.79	0.47
1:L:94:TYR:N	1:L:94:TYR:CD1	2.83	0.47
2:M:208:CYS:O	2:M:220:ASP:HA	2.15	0.47
1:L:36:TYR:O	1:L:86:TYR:HA	2.15	0.47
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.49	0.47
1:L:196:VAL:HG12	1:L:201:LEU:HD21	1.96	0.46
2:H:171:VAL:HA	2:H:191:VAL:HG23	1.96	0.46
1:L:85:THR:HA	1:L:102:THR:O	2.16	0.46
2:H:4:LEU:CD1	2:H:102:ALA:HB1	2.45	0.46
2:M:154:VAL:HA	2:M:209:ASN:O	2.15	0.46
2:M:69:VAL:O	2:M:69:VAL:HG13	2.15	0.46
2:H:60:ALA:O	2:H:61:ASP:C	2.51	0.46
2:M:17:SER:HA	2:M:82:MET:O	2.15	0.46
2:M:119:PRO:HB3	2:M:147:TYR:HB3	1.97	0.46
1:K:80:PHE:CD2	1:K:81:ASP:N	2.84	0.46
1:L:150:VAL:O	1:L:153:ALA:HB3	2.16	0.46
1:K:33:LEU:CD2	1:K:71:PHE:CG	2.98	0.45
2:M:68:THR:HG22	2:M:69:VAL:N	2.30	0.45
1:L:136:LEU:N	1:L:136:LEU:HD12	2.31	0.45
4:M:231:MAN:O2	4:M:232:MAN:H2	2.17	0.45
2:H:193:VAL:HG23	2:H:194:PRO:O	2.17	0.45
1:L:125:LEU:HD12	1:L:125:LEU:HA	1.75	0.45
2:M:118:GLY:HA2	2:M:119:PRO:HD3	1.81	0.45
2:M:41:PRO:O	2:M:42:GLY:C	2.55	0.45
2:M:6:GLU:OE2	2:M:106:GLY:N	2.41	0.44
1:L:19:ILE:HG12	1:L:78:LEU:HD11	1.98	0.44
2:M:29:ILE:HG12	2:M:76:ASP:HA	1.99	0.44
2:H:149:PRO:O	2:H:212:HIS:HE1	2.00	0.44
1:L:6:GLN:HB2	1:L:100:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:LEU:HD11	2:H:102:ALA:CB	2.47	0.44
1:L:147:GLN:HG2	1:L:154:LEU:HD13	1.99	0.44
1:L:20:THR:HB	1:L:72:THR:CG2	2.48	0.44
2:H:72:ASP:O	2:H:76:ASP:N	2.50	0.44
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.99	0.44
2:M:177:VAL:O	2:M:185:TYR:HA	2.18	0.44
1:K:118:PHE:HA	1:K:119:PRO:HD2	1.76	0.44
1:K:190:LYS:HD3	1:K:210:ASN:HB3	1.99	0.44
1:K:61:ARG:NH1	1:K:79:GLN:HE21	2.14	0.44
1:L:29:ILE:HB	1:L:90:HIS:CD2	2.52	0.44
4:M:231:MAN:O2	4:M:232:MAN:C1	2.66	0.44
1:L:6:GLN:N	1:L:100:GLN:NE2	2.65	0.44
2:M:40:VAL:O	2:M:41:PRO:C	2.56	0.43
1:K:58:VAL:O	1:K:59:PRO:C	2.56	0.43
2:H:68:THR:HG21	2:M:77:PHE:CE1	2.54	0.43
1:L:142:ARG:HD2	1:L:173:TYR:CE2	2.53	0.43
1:L:136:LEU:N	1:L:136:LEU:CD1	2.82	0.43
2:H:18:LEU:CB	2:H:82(C):MET:HE2	2.49	0.43
1:K:94:TYR:HB3	2:M:50:SER:OG	2.19	0.43
2:M:154:VAL:HG12	2:M:156:SER:N	2.33	0.43
1:K:108:ARG:NH1	1:K:111:ALA:HB2	2.34	0.43
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.83	0.43
1:K:33:LEU:HD12	1:K:89:GLN:C	2.39	0.43
1:K:132:VAL:HG12	1:K:148:TRP:CH2	2.54	0.42
1:K:182:SER:OG	1:K:183:LYS:N	2.50	0.42
2:H:66:ARG:O	2:H:82(A):HIS:HB2	2.18	0.42
2:M:117:LYS:HG2	2:M:118:GLY:O	2.19	0.42
2:H:12:VAL:HG11	2:H:82(C):MET:CE	2.49	0.42
1:K:190:LYS:HD2	1:K:191:VAL:HG23	2.01	0.42
1:L:2:VAL:O	1:L:2:VAL:HG12	2.20	0.42
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.55	0.42
2:M:56:TYR:CD2	2:M:56:TYR:C	2.92	0.42
1:K:29:ILE:O	1:K:29:ILE:CG1	2.67	0.42
1:K:33:LEU:HA	1:K:89:GLN:O	2.20	0.42
1:L:148:TRP:O	1:L:154:LEU:HA	2.19	0.42
2:H:122:PHE:HA	2:H:123:PRO:HD3	1.88	0.42
1:K:189:HIS:HB2	1:K:192:TYR:OH	2.20	0.42
1:L:106:ILE:HD12	1:L:166:GLN:OE1	2.20	0.42
2:H:52(A):THR:O	2:H:54:SER:N	2.52	0.42
2:H:68:THR:O	2:H:80:LEU:HD12	2.20	0.42
1:L:61:ARG:CZ	1:L:79:GLN:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:4:LEU:HD23	2:M:92:CYS:SG	2.60	0.42
1:K:80:PHE:CD2	1:K:80:PHE:C	2.93	0.41
1:L:183:LYS:O	1:L:184:ALA:C	2.58	0.41
2:M:176:ALA:HA	2:M:187:LEU:HB3	2.01	0.41
1:K:28:SER:O	1:K:29:ILE:HG22	2.21	0.41
2:M:29:ILE:HD11	2:M:72:ASP:O	2.20	0.41
1:K:62:PHE:O	1:K:63:SER:HB3	2.20	0.41
1:L:113:PRO:HB3	1:L:139:PHE:CD1	2.55	0.41
2:H:171:VAL:CA	2:H:191:VAL:HG23	2.51	0.41
1:K:106:ILE:N	1:K:166:GLN:OE1	2.50	0.41
1:L:113:PRO:HB3	1:L:139:PHE:HD1	1.85	0.41
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.56	0.41
2:M:48:VAL:HG12	2:M:49:ALA:N	2.35	0.41
1:K:29:ILE:O	1:K:29:ILE:HG13	2.21	0.41
1:L:146:VAL:HG12	1:L:147:GLN:N	2.36	0.41
2:M:60:ALA:O	2:M:62:ALA:N	2.54	0.41
2:H:212:HIS:CD2	2:H:215:SER:OG	2.70	0.41
2:H:18:LEU:CB	2:H:82(C):MET:CE	2.99	0.41
1:K:108:ARG:HD3	1:K:109:THR:O	2.20	0.41
1:L:67:SER:O	1:L:68:GLY:C	2.59	0.41
2:H:122:PHE:HE1	1:K:123:GLU:HG2	1.86	0.40
2:H:208:CYS:O	2:H:220:ASP:HA	2.21	0.40
2:M:56:TYR:CD2	2:M:57:ARG:N	2.89	0.40
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.56	0.40
2:H:97:SER:HA	2:H:101:ASP:OD2	2.22	0.40
2:H:177:VAL:HG13	1:K:160:GLN:NE2	2.37	0.40
2:M:13:LYS:HG3	2:M:148:PHE:CE1	2.56	0.40
2:M:139:ALA:HB2	2:M:192:THR:HG22	2.01	0.40
1:K:132:VAL:O	1:K:178:THR:HG23	2.21	0.40
2:M:56:TYR:HE2	2:M:58:ASP:CG	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	207/211 (98%)	179 (86%)	22 (11%)	6 (3%)	5	15
1	L	209/211 (99%)	184 (88%)	22 (10%)	3 (1%)	13	35
2	H	217/224 (97%)	184 (85%)	26 (12%)	7 (3%)	5	13
2	M	206/224 (92%)	176 (85%)	24 (12%)	6 (3%)	5	15
All	All	839/870 (96%)	723 (86%)	94 (11%)	22 (3%)	6	18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	26	ASN
2	H	53	SER
2	H	130	SER
2	H	216	ASN
1	K	63	SER
1	K	186	TYR
1	L	68	GLY
1	L	199	GLN
1	K	93	GLY
2	M	64	LYS
2	M	76	ASP
2	M	100	LEU
2	M	200	THR
2	H	127	SER
2	H	131	THR
1	K	182	SER
2	M	54	SER
2	M	86	ASP
1	L	184	ALA
1	K	26	SER
1	K	59	PRO
2	H	9	GLY

### 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	K	180/182 (99%)	158 (88%)	22 (12%)	6	15
1	L	182/182 (100%)	157 (86%)	25 (14%)	4	11
2	H	183/189 (97%)	156 (85%)	27 (15%)	3	9
2	M	180/189 (95%)	163 (91%)	17 (9%)	10	26
All	All	725/742 (98%)	634 (87%)	91 (13%)	5	14

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	5	THR
1	L	19	ILE
1	L	24	ARG
1	L	27	GLN
1	L	67	SER
1	L	73	LEU
1	L	76	SER
1	L	79	GLN
1	L	100	GLN
1	L	108	ARG
1	L	109	THR
1	L	114	SER
1	L	122	ASP
1	L	125	LEU
1	L	143	GLU
1	L	145	LYS
1	L	152	ASN
1	L	159	SER
1	L	169	LYS
1	L	175	LEU
1	L	191	VAL
1	L	201	LEU
1	L	208	SER
1	L	211	ARG
2	H	3	GLN
2	H	7	SER
2	H	11	LEU
2	H	21	SER
2	H	22	CYS
2	H	30	SER

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Mol	Chain	Res	Type
2	H	50	SER
2	H	64	LYS
2	H	71	ARG
2	H	74	LEU
2	H	99	ARG
2	H	110	THR
2	H	112	SER
2	H	140	LEU
2	H	142	CYS
2	H	145	LYS
2	H	153	THR
2	H	173	THR
2	H	179	GLN
2	H	184	LEU
2	H	187	LEU
2	H	189	SER
2	H	192	THR
2	H	193	VAL
2	H	200	THR
2	H	225	VAL
2	H	226	GLU
1	K	11	LEU
1	K	29	ILE
1	K	42	LYS
1	K	47	LEU
1	K	72	THR
1	K	74	THR
1	K	76	SER
1	K	80	PHE
1	K	89	GLN
1	K	94	TYR
1	K	108	ARG
1	K	126	LYS
1	K	135	LEU
1	K	156	SER
1	K	163	VAL
1	K	169	LYS
1	K	174	SER
1	K	177	SER
1	K	181	LEU
1	K	186	TYR
1	K	190	LYS

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Mol	Chain	Res	Type
1	K	201	LEU
2	M	13	LYS
2	M	21	SER
2	M	22	CYS
2	M	25	SER
2	M	40	VAL
2	M	50	SER
2	M	58	ASP
2	M	61	ASP
2	M	94	ARG
2	M	97	SER
2	M	152	VAL
2	M	153	THR
2	M	162	ASN
2	M	168	SER
2	M	180	SER
2	M	184	LEU
2	M	226	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	38	GLN
1	L	87	HIS
1	L	89	GLN
1	L	90	HIS
1	L	100	GLN
1	L	152	ASN
1	L	198	HIS
2	H	3	GLN
2	H	82(A)	HIS
2	H	212	HIS
1	K	6	GLN
1	K	27	GLN
1	K	79	GLN
1	K	89	GLN
1	K	90	HIS
1	K	138	ASN
1	K	160	GLN
1	K	189	HIS
1	K	198	HIS

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Mol	Chain	Res	Type
2	M	26	ASN
2	M	32	HIS
2	M	81	GLN
2	M	82(A)	HIS
2	M	179	GLN
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	H	229	3	11,11,12	0.95	0	13,15,17	1.44	1 (7%)
3	MAN	H	230	3	12,12,12	0.56	0	17,17,17	2.18	7 (41%)
4	MAN	M	229	4	11,11,12	0.72	0	13,15,17	2.46	8 (61%)
4	MAN	M	230	4	11,11,12	1.23	2 (18%)	13,15,17	1.56	3 (23%)
4	MAN	M	231	4	12,12,12	1.11	1 (8%)	17,17,17	3.26	10 (58%)
4	MAN	M	232	4	11,11,12	0.69	0	13,15,17	2.16	4 (30%)
4	MAN	M	233	4	11,11,12	0.87	1 (9%)	13,15,17	3.22	4 (30%)

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	H	229	3	-	0/2/19/22	0/1/1/1
3	MAN	H	230	3	-	0/2/22/22	0/1/1/1
4	MAN	M	229	4	-	0/2/19/22	0/1/1/1
4	MAN	M	230	4	-	0/2/19/22	0/1/1/1
4	MAN	M	231	4	-	0/2/22/22	0/1/1/1
4	MAN	M	232	4	-	0/2/19/22	0/1/1/1
4	MAN	M	233	4	-	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)
4	M	230	MAN	O5-C1	-2.63	1.39	1.43
4	M	230	MAN	C2-C3	-2.14	1.49	1.52
4	M	231	MAN	C3-C2	2.38	1.58	1.52
4	M	233	MAN	C2-C3	2.42	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	231	MAN	O2-C2-C1	-6.01	97.27	109.75
4	M	231	MAN	C3-C4-C5	-4.60	102.12	110.22
4	M	229	MAN	O5-C1-C2	-3.93	104.63	110.79
3	H	230	MAN	C4-C3-C2	-3.85	104.04	110.84
3	H	229	MAN	O2-C2-C3	-3.73	102.84	110.17
4	M	231	MAN	O6-C6-C5	-3.64	99.10	111.34
4	M	229	MAN	O2-C2-C1	-3.25	102.58	109.18
4	M	230	MAN	O5-C1-C2	-3.10	105.93	110.79
4	M	233	MAN	O2-C2-C1	-3.09	102.89	109.18
4	M	232	MAN	C2-C3-C4	-2.99	105.66	110.88
4	M	231	MAN	C1-O5-C5	-2.70	108.52	113.39
4	M	232	MAN	O5-C1-C2	-2.51	106.85	110.79
4	M	231	MAN	O5-C5-C4	-2.42	105.21	109.66
3	H	230	MAN	O3-C3-C2	-2.24	105.49	110.36
4	M	229	MAN	C3-C4-C5	-2.21	106.32	110.22
4	M	229	MAN	C1-C2-C3	-2.17	106.90	109.65
3	H	230	MAN	O2-C2-C3	-2.17	105.64	110.36
4	M	230	MAN	O3-C3-C2	-2.13	106.15	110.02
4	M	229	MAN	C2-C3-C4	-2.11	107.20	110.88
4	M	230	MAN	C1-O5-C5	-2.07	109.31	112.17
3	H	230	MAN	O4-C4-C5	2.00	114.33	109.28
3	H	230	MAN	O1-C1-C2	2.23	115.73	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	232	MAN	C1-C2-C3	2.36	112.64	109.65
4	M	231	MAN	O2-C2-C3	2.40	115.57	110.36
4	M	231	MAN	O5-C5-C6	2.71	112.90	106.41
3	H	230	MAN	O4-C4-C3	2.96	116.80	110.36
4	M	229	MAN	O2-C2-C3	3.17	116.41	110.17
4	M	229	MAN	C1-O5-C5	3.35	116.78	112.17
4	M	229	MAN	O3-C3-C2	3.57	116.51	110.02
4	M	233	MAN	C2-C3-C4	3.90	117.68	110.88
4	M	231	MAN	C6-C5-C4	4.20	122.82	113.00
4	M	231	MAN	O3-C3-C2	4.70	120.58	110.36
3	H	230	MAN	C1-O5-C5	5.48	123.28	113.39
4	M	232	MAN	C1-O5-C5	5.49	119.73	112.17
4	M	233	MAN	C1-C2-C3	5.58	116.72	109.65
4	M	231	MAN	C1-C2-C3	5.71	120.96	110.65
4	M	233	MAN	C1-O5-C5	8.21	123.48	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	MAN	1	0
4	M	231	MAN	4	0
4	M	232	MAN	2	0
4	M	233	MAN	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.