Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:05 AM GMT

PDB ID	:	1ZLV
Title	:	Fab 2G12 + Man7
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	:	2.33 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:

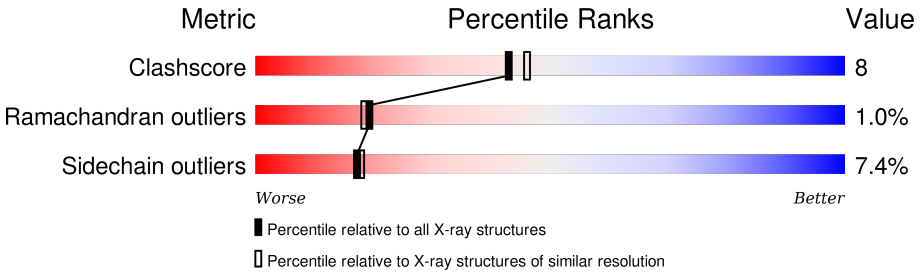
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)

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 <=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	78% 19% •
1	L	211	84% 14% •
2	H	224	78% 15% • 5%
2	M	224	74% 20% • •

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	MAN	H	230	X	-	-	-
4	MAN	H	232	X	-	-	-
4	MAN	M	232	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6598 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.

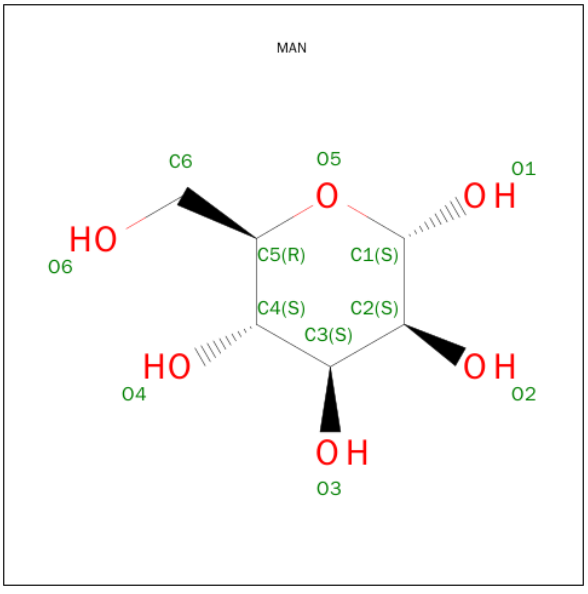
- Molecule 1 is a protein called FAB 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1611	1011	272	323	5			
1	K	211	Total	C	N	O	S	0	0	0
			1611	1011	272	323	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1585	1001	270	307	7			
2	M	217	Total	C	N	O	S	0	0	0
			1624	1022	277	318	7			

- Molecule 3 is SUGAR (4-MER) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 11 6 5	0	0
3	H	1	Total C O 11 6 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	2	Total C O 23 12 11	0	0
4	M	2	Total C O 22 12 10	0	0
4	M	2	Total C O 23 12 11	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	18	Total O 18 18	0	0
5	K	18	Total O 18 18	0	0
5	L	26	Total O 26 26	0	0
5	M	15	Total O 15 15	0	0

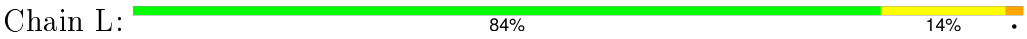
3 Residue-property plots (i)

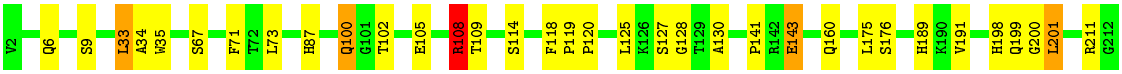
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

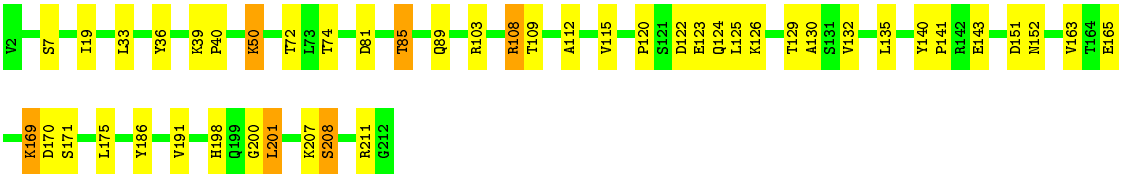
Chain L:





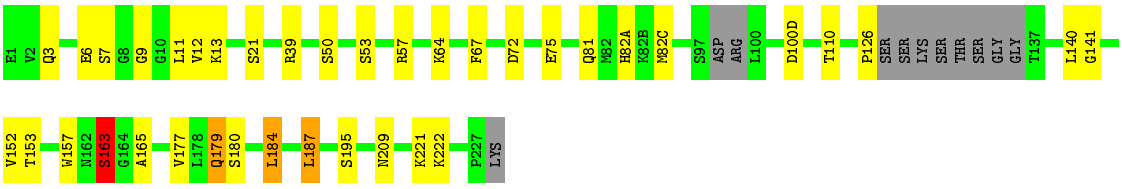
- Molecule 1: FAB 2G12, light chain

Chain K:



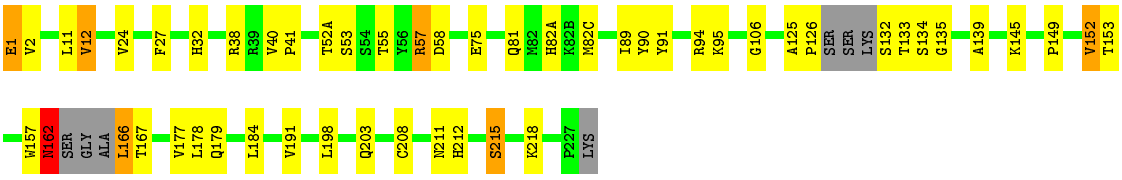
- Molecule 2: FAB 2G12, heavy chain

Chain H:



- Molecule 2: FAB 2G12, heavy chain

Chain M:



4 Data and refinement statistics (i)

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, α, β, γ	44.82Å 131.09Å 169.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33	Depositor
% Data completeness (in resolution range)	99.5 (50.00-2.33)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.210 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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: 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	0.84	1/1647 (0.1%)	0.83	0/2238
1	L	0.84	0/1647	0.83	2/2238 (0.1%)
2	H	0.85	0/1621	0.90	4/2210 (0.2%)
2	M	0.80	1/1662 (0.1%)	0.83	2/2267 (0.1%)
All	All	0.83	2/6577 (0.0%)	0.85	8/8953 (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
2	H	0	1
2	M	0	1
4	H	1	0
4	M	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	208	SER	CB-OG	-6.37	1.33	1.42
2	M	203	GLN	CD-OE1	5.78	1.36	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	187	LEU	CA-CB-CG	6.50	130.26	115.30
2	H	39	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	L	201	LEU	CA-CB-CG	6.04	129.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	94	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	M	57	ARG	NE-CZ-NH1	5.51	123.05	120.30
2	H	72	ASP	CB-CG-OD1	5.48	123.23	118.30
2	H	163	SER	N-CA-C	-5.41	96.39	111.00
1	L	108	ARG	NE-CZ-NH2	-5.10	117.75	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	232	MAN	C1
4	M	232	MAN	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	163	SER	Peptide
2	M	162	ASN	Peptide

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	K	1611	0	1545	24	0
1	L	1611	0	1545	22	0
2	H	1585	0	1528	22	0
2	M	1624	0	1573	37	0
3	H	22	0	19	2	0
4	H	23	0	20	1	0
4	M	45	0	40	1	0
5	H	18	0	0	0	0
5	K	18	0	0	0	0
5	L	26	0	0	3	0
5	M	15	0	0	0	0
All	All	6598	0	6270	102	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 8.

All (102) 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:H:12:VAL:HG11	2:H:82(C):MET:CE	1.65	1.25
2:H:12:VAL:HG11	2:H:82(C):MET:HE3	1.14	1.09
2:M:212:HIS:HD2	2:M:215:SER:HB2	1.19	1.07
2:M:212:HIS:CD2	2:M:215:SER:HB2	1.96	1.01
4:M:230:MAN:C1	4:M:231:MAN:HO2	1.65	1.01
1:L:6:GLN:H	1:L:100:GLN:HE22	0.95	0.94
2:H:12:VAL:CG1	2:H:82(C):MET:HE3	1.99	0.93
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.49	0.92
1:L:6:GLN:N	1:L:100:GLN:HE22	1.78	0.80
2:M:1:GLU:HG2	2:M:2:VAL:H	1.48	0.78
1:L:198:HIS:CD2	1:L:200:GLY:H	2.03	0.77
2:H:12:VAL:CG1	2:H:82(C):MET:CE	2.57	0.75
1:L:6:GLN:H	1:L:100:GLN:NE2	1.78	0.73
2:H:12:VAL:HG21	2:H:82(C):MET:HE1	1.70	0.71
1:L:199:GLN:HB2	5:L:226:HOH:O	1.93	0.69
1:K:198:HIS:CD2	1:K:200:GLY:H	2.10	0.68
2:M:12:VAL:HG21	2:M:82(C):MET:CE	2.24	0.68
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.42	0.65
2:H:141:GLY:HA2	2:H:157:TRP:CH2	2.31	0.65
1:K:85:THR:HG22	1:K:103:ARG:HG3	1.78	0.65
1:L:198:HIS:HD2	1:L:200:GLY:H	1.49	0.60
2:M:81:GLN:NE2	2:M:82(A):HIS:HE1	1.98	0.60
2:M:12:VAL:HG21	2:M:82(C):MET:HE3	1.84	0.60
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.37	0.60
2:H:179:GLN:HG2	2:H:184:LEU:O	2.02	0.60
2:M:211:ASN:HD21	2:M:218:LYS:NZ	2.00	0.60
1:L:108:ARG:HD3	1:L:109:THR:O	2.03	0.58
1:L:87:HIS:HD2	5:L:214:HOH:O	1.87	0.57
2:H:81:GLN:NE2	2:H:82(A):HIS:HE1	2.01	0.57
2:M:1:GLU:CG	2:M:2:VAL:H	2.18	0.57
2:M:145:LYS:HE2	2:M:179:GLN:HE22	1.71	0.56
2:M:132:SER:HA	2:M:198:LEU:HB2	1.88	0.56
2:M:149:PRO:O	2:M:212:HIS:HE1	1.88	0.56
1:L:100:GLN:H	1:L:100:GLN:CD	2.09	0.55
2:M:2:VAL:HG13	2:M:27:PHE:CE2	2.42	0.55
2:M:157:TRP:C	2:M:166:LEU:H	2.11	0.54
1:K:124:GLN:HG2	1:K:129:THR:O	2.09	0.53
1:K:36:TYR:OH	1:K:89:GLN:NE2	2.41	0.52
2:H:12:VAL:HG21	2:H:82(C):MET:CE	2.39	0.52
2:H:81:GLN:HE21	2:H:82(A):HIS:CE1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:PRO:O	1:K:198:HIS:HE1	1.92	0.52
3:H:230:MAN:O5	4:H:231:MAN:O2	2.24	0.52
1:L:87:HIS:CD2	5:L:214:HOH:O	2.60	0.52
1:L:141:PRO:O	1:L:198:HIS:HE1	1.93	0.51
2:M:81:GLN:HE21	2:M:82(A):HIS:CE1	2.30	0.50
2:M:211:ASN:HD21	2:M:218:LYS:HZ2	1.58	0.50
1:K:39:LYS:NZ	1:K:81:ASP:O	2.44	0.50
2:H:57:ARG:NH2	2:M:75:GLU:HG2	2.27	0.50
1:L:100:GLN:H	1:L:100:GLN:NE2	2.09	0.50
2:M:81:GLN:HE21	2:M:82(A):HIS:HE1	1.59	0.50
1:L:160:GLN:HB3	2:M:177:VAL:HG21	1.93	0.49
1:K:169:LYS:HG3	1:K:170:ASP:N	2.27	0.49
2:H:141:GLY:HA2	2:H:157:TRP:CZ2	2.47	0.48
1:L:33:LEU:HG	1:L:34:ALA:N	2.29	0.47
2:M:157:TRP:CH2	2:M:208:CYS:HB3	2.49	0.47
1:L:189:HIS:O	1:L:211:ARG:NH2	2.47	0.47
1:K:163:VAL:HG22	1:K:175:LEU:HD12	1.97	0.47
1:K:123:GLU:HA	1:K:126:LYS:HE2	1.96	0.47
2:H:64:LYS:HB2	2:H:64:LYS:HE3	1.64	0.47
1:K:108:ARG:HD3	1:K:109:THR:O	2.15	0.46
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.51	0.46
2:M:152:VAL:HG22	2:M:212:HIS:HB2	1.98	0.46
1:K:198:HIS:HD2	1:K:200:GLY:H	1.59	0.46
2:H:11:LEU:CD1	2:M:178:LEU:HD21	2.46	0.45
2:M:32:HIS:HD2	2:M:95:LYS:O	1.98	0.45
2:H:75:GLU:HG3	2:M:57:ARG:CZ	2.47	0.44
2:H:12:VAL:HG11	2:H:82(C):MET:HE1	1.82	0.44
1:L:120:PRO:HG3	1:L:130:ALA:HB1	1.99	0.44
1:K:112:ALA:CB	1:K:201:LEU:HD13	2.35	0.44
1:K:186:TYR:CZ	1:K:211:ARG:HG3	2.53	0.44
1:K:120:PRO:HG3	1:K:130:ALA:HB1	1.99	0.43
2:H:57:ARG:CZ	2:M:75:GLU:HG2	2.48	0.43
1:L:143:GLU:CD	1:L:143:GLU:H	2.21	0.43
2:M:212:HIS:HD2	2:M:215:SER:CB	2.09	0.43
2:M:166:LEU:HD21	2:M:191:VAL:HG21	1.99	0.43
2:M:157:TRP:C	2:M:166:LEU:N	2.72	0.43
2:M:90:TYR:O	2:M:106:GLY:HA2	2.19	0.43
2:M:81:GLN:NE2	2:M:82(A):HIS:CE1	2.84	0.43
2:M:52(A):THR:O	2:M:53:SER:HB2	2.18	0.42
2:M:24:VAL:HB	2:M:27:PHE:CE2	2.53	0.42
2:H:126:PRO:HD3	2:H:140:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:ASP:HA	1:K:125:LEU:HD12	2.00	0.42
1:K:50:LYS:HB3	1:K:50:LYS:HE2	1.90	0.42
1:K:108:ARG:HD2	1:K:140:TYR:CB	2.50	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD2	1.88	0.41
1:K:120:PRO:HD3	1:K:132:VAL:HG22	2.01	0.41
2:M:40:VAL:HB	2:M:41:PRO:HD2	2.02	0.41
2:M:38:ARG:HA	2:M:89:ILE:O	2.20	0.41
1:K:115:VAL:HA	1:K:135:LEU:O	2.21	0.41
1:L:67:SER:HA	1:L:71:PHE:CE2	2.56	0.41
2:M:126:PRO:HA	2:M:139:ALA:O	2.21	0.41
2:H:100(D):ASP:OD1	3:H:229:MAN:O3	2.35	0.41
1:L:9:SER:O	1:L:102:THR:HA	2.20	0.41
2:H:6:GLU:HA	2:H:21:SER:O	2.21	0.41
1:L:175:LEU:HD23	1:L:176:SER:N	2.35	0.40
1:K:40:PRO:HG2	1:K:165:GLU:OE1	2.21	0.40
2:M:157:TRP:CZ3	2:M:208:CYS:HB3	2.56	0.40
1:K:170:ASP:O	1:K:171:SER:HB2	2.22	0.40
2:M:125:ALA:HA	2:M:126:PRO:HD2	1.87	0.40
1:K:19:ILE:O	1:K:74:THR:HA	2.21	0.40
2:H:67:PHE:HA	2:H:81:GLN:O	2.21	0.40
1:K:151:ASP:O	1:K:152:ASN:HB2	2.22	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	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
1	L	209/211 (99%)	199 (95%)	8 (4%)	2 (1%)	19	18
2	H	207/224 (92%)	199 (96%)	5 (2%)	3 (1%)	14	11
2	M	213/224 (95%)	200 (94%)	10 (5%)	3 (1%)	14	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	838/870 (96%)	799 (95%)	31 (4%)	8 (1%)	19 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	163	SER
2	H	165	ALA
2	M	134	SER
2	M	162	ASN
1	L	128	GLY
1	L	127	SER
2	M	135	GLY
2	H	9	GLY

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	175/182 (96%)	163 (93%)	12 (7%)	19 21
1	L	175/182 (96%)	166 (95%)	9 (5%)	29 36
2	H	172/189 (91%)	155 (90%)	17 (10%)	10 9
2	M	179/189 (95%)	165 (92%)	14 (8%)	16 16
All	All	701/742 (94%)	649 (93%)	52 (7%)	17 18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	100	GLN
1	L	105	GLU
1	L	108	ARG
1	L	114	SER
1	L	125	LEU
1	L	143	GLU

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Mol	Chain	Res	Type
1	L	191	VAL
1	L	201	LEU
2	H	3	GLN
2	H	7	SER
2	H	13	LYS
2	H	50	SER
2	H	53	SER
2	H	110	THR
2	H	152	VAL
2	H	153	THR
2	H	177	VAL
2	H	179	GLN
2	H	180	SER
2	H	184	LEU
2	H	187	LEU
2	H	195	SER
2	H	209	ASN
2	H	221	LYS
2	H	222	LYS
1	K	7	SER
1	K	33	LEU
1	K	50	LYS
1	K	72	THR
1	K	85	THR
1	K	108	ARG
1	K	143	GLU
1	K	169	LYS
1	K	191	VAL
1	K	201	LEU
1	K	207	LYS
1	K	208	SER
2	M	1	GLU
2	M	11	LEU
2	M	12	VAL
2	M	55	THR
2	M	58	ASP
2	M	91	TYR
2	M	133	THR
2	M	152	VAL
2	M	153	THR
2	M	162	ASN
2	M	166	LEU

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Mol	Chain	Res	Type
2	M	167	THR
2	M	184	LEU
2	M	215	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	87	HIS
1	L	89	GLN
1	L	90	HIS
1	L	100	GLN
1	L	138	ASN
1	L	198	HIS
2	H	32	HIS
2	H	81	GLN
2	H	82(A)	HIS
2	H	209	ASN
1	K	87	HIS
1	K	89	GLN
1	K	138	ASN
1	K	152	ASN
1	K	198	HIS
2	M	32	HIS
2	M	35	ASN
2	M	81	GLN
2	M	82(A)	HIS
2	M	179	GLN
2	M	211	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 (i)

6 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	$\#\|Z\| > 2$
4	MAN	H	231	3,4	11,11,12	0.71	0	14,15,17	1.76	3 (21%)
4	MAN	H	232	4	12,12,12	0.82	0	17,17,17	3.00	9 (52%)
4	MAN	M	229	4	11,11,12	0.69	0	14,15,17	1.32	2 (14%)
4	MAN	M	230	4	11,11,12	0.67	0	14,15,17	1.42	3 (21%)
4	MAN	M	231	4	11,11,12	0.73	0	14,15,17	1.75	4 (28%)
4	MAN	M	232	4	12,12,12	0.84	0	17,17,17	2.43	8 (47%)

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	H	231	3,4	-	0/2/19/22	0/1/1/1
4	MAN	H	232	4	1/1/5/5	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	-	0/2/19/22	0/1/1/1
4	MAN	M	232	4	1/1/5/5	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	232	MAN	O3-C3-C4	-5.69	97.52	110.34
4	M	231	MAN	O5-C1-C2	-2.71	106.46	110.86
4	H	231	MAN	O2-C2-C3	-2.59	104.91	110.12
4	H	232	MAN	C1-C2-C3	-2.52	106.69	110.43
4	H	231	MAN	O5-C1-C2	-2.38	106.99	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	230	MAN	O6-C6-C5	-2.30	103.72	111.33
4	H	232	MAN	C1-O5-C5	-2.26	109.29	113.47
4	M	232	MAN	O3-C3-C4	-2.21	105.36	110.34
4	M	231	MAN	O2-C2-C3	-2.18	105.73	110.12
4	M	232	MAN	O4-C4-C3	-2.14	105.51	110.34
4	H	232	MAN	O5-C5-C4	2.05	113.52	109.68
4	M	232	MAN	O2-C2-C3	2.07	115.00	110.34
4	H	232	MAN	O5-C5-C6	2.27	112.09	106.36
4	M	231	MAN	C3-C4-C5	2.29	114.18	110.20
4	M	230	MAN	O4-C4-C5	2.30	115.34	109.24
4	M	230	MAN	C1-O5-C5	2.35	115.23	112.25
4	M	229	MAN	O3-C3-C2	2.39	114.31	110.00
4	H	232	MAN	C4-C3-C2	2.41	115.30	110.79
4	M	232	MAN	O5-C5-C6	2.57	112.85	106.36
4	H	232	MAN	O1-C1-C2	2.60	116.18	109.21
4	M	232	MAN	C3-C4-C5	2.80	115.08	110.20
4	M	232	MAN	C4-C3-C2	3.02	116.42	110.79
4	M	229	MAN	C1-O5-C5	3.21	116.33	112.25
4	M	231	MAN	C1-O5-C5	4.00	117.32	112.25
4	M	232	MAN	C1-C2-C3	4.37	116.92	110.43
4	H	231	MAN	C1-C2-C3	4.46	114.81	109.54
4	H	232	MAN	C3-C4-C5	6.13	120.88	110.20
4	H	232	MAN	O3-C3-C2	6.14	124.16	110.34
4	M	232	MAN	O3-C3-C2	6.32	124.57	110.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	232	MAN	C1
4	M	232	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	231	MAN	1	0
4	M	230	MAN	1	0
4	M	231	MAN	1	0

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	MAN	H	229	3	11,11,12	0.75	0	14,15,17	1.66	2 (14%)
3	MAN	H	230	3,4	11,11,12	0.70	0	14,15,17	1.52	3 (21%)

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	3,4	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	229	MAN	O2-C2-C1	-2.95	103.30	109.21
3	H	230	MAN	O5-C1-C2	-2.06	107.51	110.86
3	H	230	MAN	C3-C4-C5	2.34	114.28	110.20
3	H	230	MAN	C1-O5-C5	2.92	115.95	112.25
3	H	229	MAN	C1-O5-C5	4.42	117.86	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	230	MAN	C1

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
3	H	229	MAN	1	0
3	H	230	MAN	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

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.