Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:22 PM GMT

PDB ID	:	1OP3
Title	:	Crystal Structure of Fab 2G12 bound to Man1->2Man
Authors	:	Calarese, D.A.; Scanlan, C.N.; Zwick, M.B.; Deechongkit, S.; Mimura, Y.; Kunert, R.; Stanfield, R.L.; Kelly, J.W.; Rudd, P.M.; Dwek, R.A.; Katinger, H.; Burton, D.R.; Wilson, I.A.
Deposited on	:	2003-03-04
Resolution	:	1.75 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

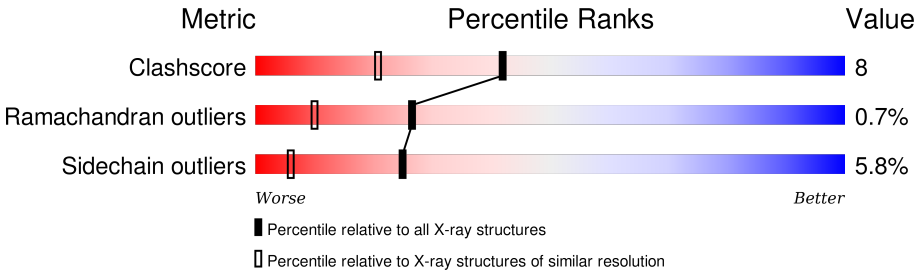
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.75 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	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)

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	212	85% 13% •
1	L	212	82% 15% •
2	H	225	79% 18% •
2	M	225	70% 21% 8%

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
4	MAN	M	503	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7114 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	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

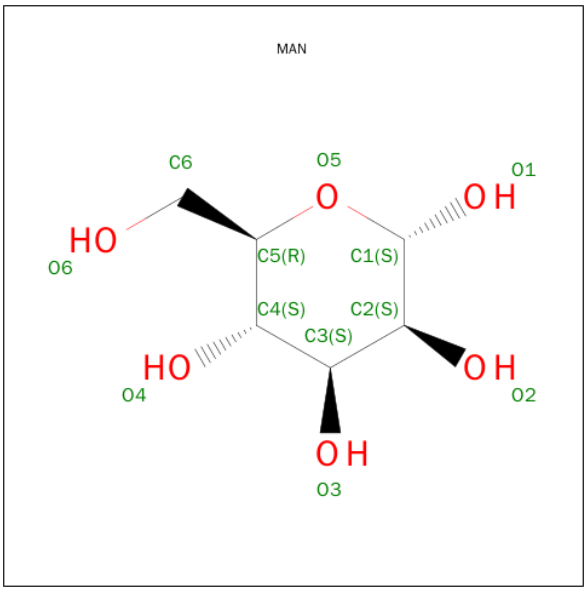
- Molecule 2 is a protein called FAB 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	38	0	0
			1675	1053	286	329	7			
2	M	224	Total	C	N	O	S	51	0	0
			1675	1053	286	329	7			

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

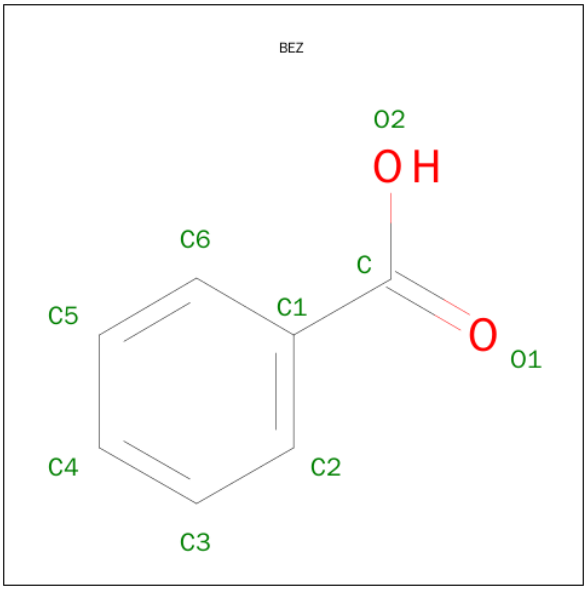
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	2	Total	C	O	0	0
			23	12	11		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O 12 6 6	0	0

- Molecule 5 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	113	Total O 113 113	0	0
6	K	157	Total O 157 157	0	0
6	L	108	Total O 108 108	0	0
6	M	106	Total O 106 106	0	0

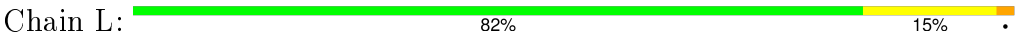
3 Residue-property plots (i)

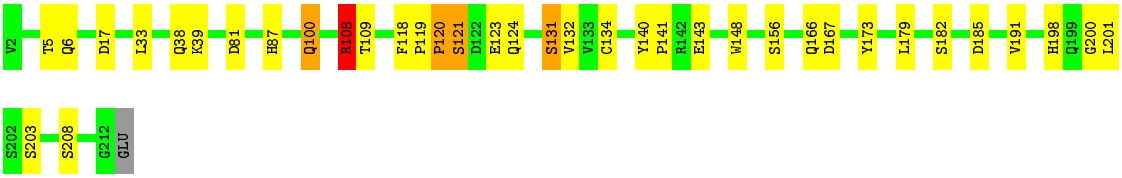
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

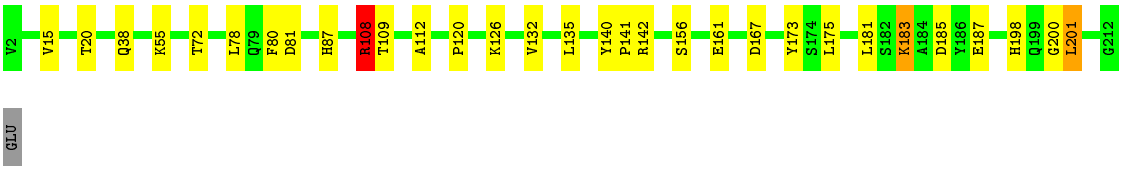
Chain L:





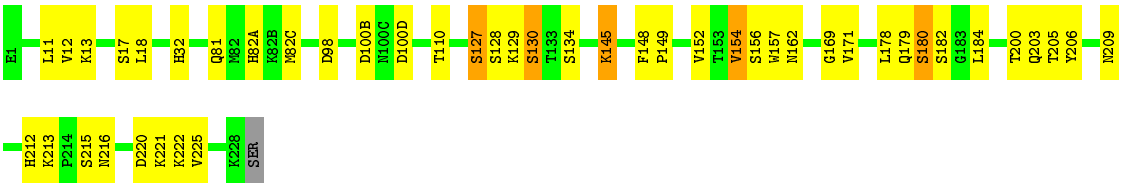
- Molecule 1: FAB 2G12, light chain

Chain K:



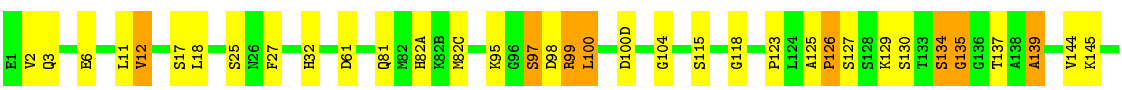
- Molecule 2: FAB 2G12, heavy chain

Chain H:



- Molecule 2: FAB 2G12, heavy chain

Chain M:




P149
V152
T153
V154
S156
W157
N162
L166
G169
V171
L178
Q179
S180
S182
G183
L184
L187
V191
T192
V193
T200
Q203
T205
Y206
I207
C208
N209
Y210
N211
H212
S215
D220
K221
K222
V225
K228
SER

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	81.72Å 94.03Å 169.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75	Depositor
% Data completeness (in resolution range)	95.7 (50.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: BEZ, 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	0.53	1/1654 (0.1%)	0.85	4/2246 (0.2%)
1	L	0.97	6/1654 (0.4%)	0.80	6/2246 (0.3%)
2	H	0.96	4/1708 (0.2%)	0.84	5/2316 (0.2%)
2	M	1.37	11/1709 (0.6%)	1.00	13/2319 (0.6%)
All	All	1.00	22/6725 (0.3%)	0.88	28/9127 (0.3%)

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	4
2	M	0	3
All	All	0	7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	125	ALA	C-N	-29.64	0.78	1.34
2	M	180	SER	C-N	27.89	1.98	1.34
1	L	121	SER	CB-OG	24.66	1.74	1.42
2	H	180	SER	C-N	23.28	1.87	1.34
2	M	154	VAL	C-N	22.67	1.86	1.34
2	H	154	VAL	C-N	16.80	1.72	1.34
2	H	127	SER	C-N	-14.71	1.00	1.34
1	L	119	PRO	C-O	12.46	1.48	1.23
1	L	131	SER	CB-OG	11.96	1.57	1.42
2	H	128	SER	N-CA	-8.91	1.28	1.46
1	L	182	SER	CB-OG	8.25	1.52	1.42
2	M	135	GLY	C-N	-7.29	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	137	THR	C-O	6.98	1.36	1.23
2	M	139	ALA	C-O	6.76	1.36	1.23
1	L	119	PRO	C-N	6.24	1.46	1.34
1	K	183	LYS	C-O	6.24	1.35	1.23
1	L	120	PRO	N-CD	5.95	1.56	1.47
2	M	208	CYS	CB-SG	5.80	1.92	1.82
2	M	206	TYR	CG-CD2	5.59	1.46	1.39
2	M	206	TYR	CE1-CZ	5.48	1.45	1.38
2	M	123	PRO	C-O	5.47	1.34	1.23
2	M	137	THR	C-N	5.27	1.46	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	125	ALA	O-C-N	-14.18	94.16	121.10
1	K	108	ARG	NE-CZ-NH2	-13.51	113.55	120.30
1	L	108	ARG	NE-CZ-NH1	12.05	126.32	120.30
1	L	108	ARG	NE-CZ-NH2	-11.99	114.31	120.30
2	M	135	GLY	C-N-CA	11.22	145.86	122.30
2	H	127	SER	O-C-N	-10.60	105.73	122.70
1	K	108	ARG	NE-CZ-NH1	10.52	125.56	120.30
2	M	125	ALA	CA-C-N	10.13	145.48	117.10
2	H	180	SER	O-C-N	-8.37	109.31	122.70
2	M	135	GLY	O-C-N	-7.60	110.28	123.20
2	M	125	ALA	C-N-CD	-7.56	103.96	120.60
2	M	154	VAL	C-N-CA	-6.47	105.52	121.70
2	H	100(D)	ASP	CB-CG-OD2	6.38	124.05	118.30
2	M	180	SER	O-C-N	-6.38	112.49	122.70
1	K	81	ASP	CB-CG-OD2	6.17	123.85	118.30
1	L	81	ASP	CB-CG-OD2	6.10	123.79	118.30
2	M	134	SER	CB-CA-C	5.81	121.14	110.10
2	M	126	PRO	CB-CA-C	-5.78	97.56	112.00
2	M	98	ASP	CB-CG-OD2	5.62	123.36	118.30
2	M	220	ASP	CB-CG-OD2	5.61	123.35	118.30
2	H	220	ASP	CB-CG-OD2	5.44	123.20	118.30
2	M	100(D)	ASP	CB-CG-OD2	5.29	123.06	118.30
1	L	185	ASP	CB-CG-OD2	5.21	122.99	118.30
2	M	61	ASP	CB-CG-OD2	5.13	122.91	118.30
1	L	167	ASP	CB-CG-OD2	5.06	122.86	118.30
1	K	167	ASP	CB-CG-OD2	5.06	122.86	118.30
1	L	17	ASP	CB-CG-OD2	5.04	122.84	118.30
2	H	98	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	127	SER	Mainchain,Peptide
2	H	129	LYS	Peptide
2	H	130	SER	Peptide
2	M	129	LYS	Peptide
2	M	130	SER	Peptide
2	M	135	GLY	Mainchain

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	1618	0	1580	20	0
1	L	1618	0	1580	24	0
2	H	1675	0	1639	27	0
2	M	1675	0	1640	43	0
3	H	23	0	21	0	0
4	M	12	0	12	0	0
5	L	9	0	5	0	0
6	H	113	0	0	1	0
6	K	157	0	0	2	0
6	L	108	0	0	0	0
6	M	106	0	0	1	0
All	All	7114	0	6477	109	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 (109) 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:154:VAL:C	2:H:156:SER:N	1.72	1.43
1:L:121:SER:OG	1:L:121:SER:CB	1.74	1.33
2:M:154:VAL:C	2:M:156:SER:N	1.86	1.27
2:H:180:SER:C	2:H:182:SER:N	1.87	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:180:SER:C	2:M:182:SER:N	1.98	1.16
2:H:169:GLY:C	2:H:171:VAL:N	2.17	0.97
1:K:20:THR:HG23	1:K:72:THR:HG23	1.48	0.92
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.50	0.91
1:K:108:ARG:HD3	1:K:109:THR:O	1.74	0.88
1:K:20:THR:HG23	1:K:72:THR:CG2	2.04	0.88
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.23	0.83
2:H:222:LYS:HA	2:H:225:VAL:N	1.94	0.82
1:L:6:GLN:H	1:L:100:GLN:HE22	1.27	0.80
1:L:108:ARG:HD3	1:L:109:THR:O	1.83	0.78
1:L:198:HIS:CD2	1:L:200:GLY:H	2.04	0.76
2:M:81:GLN:HE21	2:M:82(A):HIS:HE1	1.33	0.75
2:H:81:GLN:HE21	2:H:82(A):HIS:CE1	2.07	0.71
1:K:198:HIS:HD2	1:K:200:GLY:H	1.39	0.71
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.73	0.71
1:K:198:HIS:CD2	1:K:200:GLY:H	2.08	0.71
2:M:12:VAL:HG11	2:M:82(C):MET:HE3	1.72	0.70
2:H:81:GLN:NE2	2:H:82(A):HIS:HE1	1.91	0.68
2:H:149:PRO:O	2:H:212:HIS:HE1	1.75	0.68
1:K:20:THR:CG2	1:K:72:THR:HG23	2.24	0.67
2:M:145:LYS:HE2	2:M:179:GLN:HE22	1.58	0.66
2:M:81:GLN:HE21	2:M:82(A):HIS:CE1	2.13	0.66
2:H:12:VAL:HG11	2:H:82(C):MET:CE	2.26	0.65
2:M:154:VAL:C	2:M:156:SER:CA	2.65	0.65
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.79	0.64
1:L:5:THR:HA	1:L:100:GLN:HE22	1.64	0.63
2:M:12:VAL:HG11	2:M:82(C):MET:CE	2.30	0.62
2:M:169:GLY:C	2:M:171:VAL:N	2.51	0.62
1:L:100:GLN:H	1:L:100:GLN:CD	2.02	0.61
1:K:55:LYS:HE3	6:K:312:HOH:O	2.01	0.61
2:H:32:HIS:HE1	6:H:614:HOH:O	1.82	0.61
2:M:81:GLN:NE2	2:M:82(A):HIS:HE1	1.98	0.60
2:H:157:TRP:C	2:H:162:ASN:N	2.55	0.59
2:M:203:GLN:OE1	2:M:205:THR:N	2.36	0.59
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.38	0.58
1:L:5:THR:HA	1:L:100:GLN:NE2	2.19	0.58
2:H:145:LYS:HE2	2:H:179:GLN:OE1	2.03	0.57
2:M:166:LEU:HD21	2:M:191:VAL:HG21	1.87	0.57
1:L:132:VAL:CG2	1:L:179:LEU:HB3	2.33	0.57
2:H:222:LYS:CA	2:H:225:VAL:N	2.67	0.57
2:M:118:GLY:HA2	2:M:212:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:LYS:O	1:K:187:GLU:HG3	2.04	0.56
2:H:12:VAL:HG11	2:H:82(C):MET:HE1	1.87	0.56
2:M:162:ASN:N	2:M:162:ASN:OD1	2.38	0.56
2:H:169:GLY:O	2:H:171:VAL:N	2.38	0.56
2:M:153:THR:HG22	2:M:211:ASN:HB3	1.87	0.55
2:H:203:GLN:HB2	2:H:206:TYR:CZ	2.42	0.55
2:H:11:LEU:HD11	2:M:178:LEU:HD21	1.88	0.55
1:L:6:GLN:N	1:L:100:GLN:HE22	2.02	0.54
2:M:32:HIS:HE1	6:M:607:HOH:O	1.90	0.54
2:H:12:VAL:HG11	2:H:82(C):MET:HE3	1.90	0.54
2:H:206:TYR:O	2:H:225:VAL:N	2.41	0.54
1:K:15:VAL:HG21	1:K:80:PHE:CZ	2.42	0.54
2:H:13:LYS:HD3	2:H:148:PHE:CE1	2.42	0.54
2:M:193:VAL:HG11	2:M:206:TYR:CE1	2.43	0.53
2:M:149:PRO:O	2:M:212:HIS:HE1	1.92	0.53
1:L:198:HIS:HD2	1:L:200:GLY:H	1.53	0.53
2:H:212:HIS:HD2	2:H:215:SER:OG	1.92	0.53
2:H:145:LYS:HE3	6:K:241:HOH:O	2.07	0.53
2:H:203:GLN:HA	2:H:205:THR:N	2.24	0.53
1:L:6:GLN:H	1:L:100:GLN:NE2	2.03	0.52
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.91	0.51
1:L:118:PHE:CE1	2:M:139:ALA:O	2.63	0.51
2:M:212:HIS:CD2	2:M:215:SER:OG	2.64	0.51
2:M:18:LEU:HB2	2:M:82(C):MET:HE1	1.93	0.51
2:M:144:VAL:HG11	2:M:152:VAL:HG11	1.93	0.50
2:M:203:GLN:O	2:M:205:THR:HA	2.12	0.49
2:H:203:GLN:O	2:H:205:THR:HA	2.13	0.49
1:K:108:ARG:HD2	1:K:140:TYR:CB	2.43	0.48
2:M:118:GLY:HA2	2:M:212:HIS:HD2	1.77	0.48
2:H:18:LEU:N	2:H:82(C):MET:HE2	2.29	0.47
1:L:124:GLN:NE2	1:L:131:SER:OG	2.40	0.47
2:M:212:HIS:HD2	2:M:215:SER:OG	1.97	0.47
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.49	0.47
2:M:208:CYS:SG	2:M:221:LYS:HB3	2.55	0.46
2:M:32:HIS:HD2	2:M:95:LYS:O	1.97	0.46
2:H:17:SER:OG	2:H:82(A):HIS:HD2	1.99	0.46
2:M:97:SER:C	2:M:99:ARG:H	2.19	0.45
1:K:141:PRO:O	1:K:198:HIS:HE1	2.00	0.45
2:M:200:THR:HB	2:M:203:GLN:N	2.32	0.44
2:M:206:TYR:O	2:M:225:VAL:N	2.51	0.43
2:M:208:CYS:O	2:M:208:CYS:SG	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:VAL:HG21	1:K:80:PHE:CE2	2.54	0.43
2:M:154:VAL:CA	2:M:156:SER:N	2.79	0.42
1:K:142:ARG:HD3	1:K:173:TYR:CE2	2.54	0.42
2:M:222:LYS:HA	2:M:225:VAL:N	2.34	0.42
1:K:161:GLU:HG2	1:K:175:LEU:HD21	2.01	0.42
1:L:118:PHE:HE1	2:M:139:ALA:O	2.03	0.42
1:K:20:THR:CG2	1:K:72:THR:CG2	2.86	0.41
1:K:38:GLN:OE1	1:K:87:HIS:HE1	2.03	0.41
2:H:178:LEU:HD21	2:M:11:LEU:HD11	2.01	0.41
2:M:162:ASN:N	2:M:207:ILE:O	2.53	0.41
1:K:108:ARG:HD2	1:K:140:TYR:HB3	2.03	0.41
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.55	0.41
2:M:187:LEU:HD12	2:M:187:LEU:C	2.41	0.41
1:L:100:GLN:CD	1:L:100:GLN:N	2.71	0.41
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.50	0.41
1:L:38:GLN:OE1	1:L:87:HIS:HE1	2.04	0.41
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.56	0.41
1:L:118:PHE:CZ	2:M:139:ALA:O	2.74	0.41
1:L:141:PRO:O	1:L:198:HIS:HE1	2.02	0.41
2:M:17:SER:OG	2:M:82(A):HIS:HD2	2.04	0.41
1:L:143:GLU:CD	1:L:143:GLU:H	2.24	0.41
2:M:6:GLU:OE1	2:M:104:GLY:HA3	2.22	0.40
2:M:3:GLN:HB2	2:M:25:SER:HB2	2.02	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	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
1	L	209/212 (99%)	199 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	211/225 (94%)	205 (97%)	4 (2%)	2 (1%)	21 6
2	M	213/225 (95%)	199 (93%)	10 (5%)	4 (2%)	10 1
All	All	842/874 (96%)	805 (96%)	31 (4%)	6 (1%)	26 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	134	SER
2	M	134	SER
2	M	127	SER
2	M	100	LEU
2	H	130	SER
2	M	126	PRO

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	182/183 (100%)	174 (96%)	8 (4%)	35 11
1	L	182/183 (100%)	172 (94%)	10 (6%)	27 7
2	H	189/190 (100%)	179 (95%)	10 (5%)	28 7
2	M	189/190 (100%)	174 (92%)	15 (8%)	15 2
All	All	742/746 (100%)	699 (94%)	43 (6%)	25 6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	39	LYS
1	L	100	GLN
1	L	108	ARG
1	L	123	GLU
1	L	156	SER

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Mol	Chain	Res	Type
1	L	191	VAL
1	L	201	LEU
1	L	203	SER
1	L	208	SER
2	H	100(B)	ASP
2	H	110	THR
2	H	145	LYS
2	H	152	VAL
2	H	184	LEU
2	H	200	THR
2	H	209	ASN
2	H	213	LYS
2	H	216	ASN
2	H	221	LYS
1	K	78	LEU
1	K	108	ARG
1	K	126	LYS
1	K	135	LEU
1	K	156	SER
1	K	181	LEU
1	K	185	ASP
1	K	201	LEU
2	M	12	VAL
2	M	97	SER
2	M	99	ARG
2	M	100	LEU
2	M	115	SER
2	M	152	VAL
2	M	153	THR
2	M	156	SER
2	M	162	ASN
2	M	184	LEU
2	M	187	LEU
2	M	200	THR
2	M	205	THR
2	M	209	ASN
2	M	228	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	HIS

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Mol	Chain	Res	Type
1	L	89	GLN
1	L	100	GLN
1	L	198	HIS
2	H	32	HIS
2	H	81	GLN
2	H	82(A)	HIS
2	H	212	HIS
1	K	87	HIS
1	K	89	GLN
1	K	90	HIS
1	K	198	HIS
1	K	210	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

2 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	501	3	12,12,12	0.51	0	17,17,17	0.88	0
3	MAN	H	502	3	11,11,12	0.38	0	14,15,17	1.04	1 (7%)

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	501	3	-	0/2/22/22	0/1/1/1
3	MAN	H	502	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	502	MAN	C1-O5-C5	2.89	115.92	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
5	BEZ	L	504	-	6,9,9	2.08	2 (33%)	8,11,11	0.94	0
4	MAN	M	503	-	12,12,12	0.57	0	17,17,17	1.36	4 (23%)

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	BEZ	L	504	-	-	0/0/4/4	0/1/1/1
4	MAN	M	503	-	1/1/5/5	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	504	BEZ	C2-C1	2.49	1.44	1.39
5	L	504	BEZ	C3-C2	2.85	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	503	MAN	C1-O5-C5	-3.44	107.11	113.47
4	M	503	MAN	C1-C2-C3	-2.28	107.04	110.43
4	M	503	MAN	O4-C4-C5	2.03	114.63	109.24
4	M	503	MAN	O5-C5-C6	2.27	112.10	106.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	503	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.