Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2017 – 02:11 PM EST

PDB ID	:	5VGJ
Title	:	Crystal Structure of the Human Fab VRC38.01, an HIV-1 V1V2-Directed Neutralizing Antibody Isolated from Donor N90, bound to a scaffolded WITO V1V2 domain
Authors	:	Gorman, J.; Li, J.; Kwong, P.D.
Deposited on	:	unknown
Resolution	:	3.46 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345
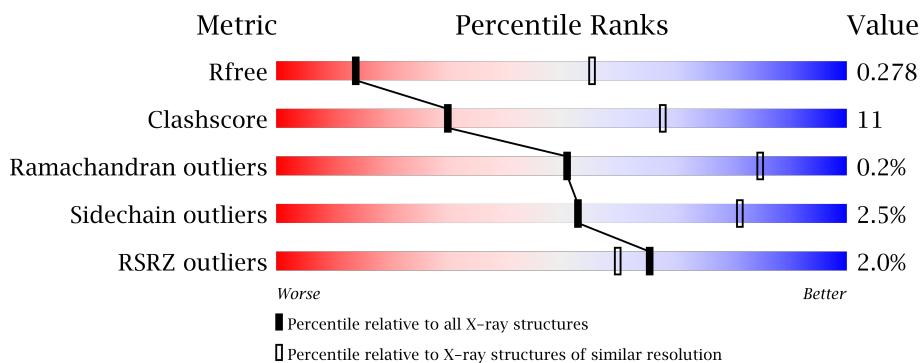
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
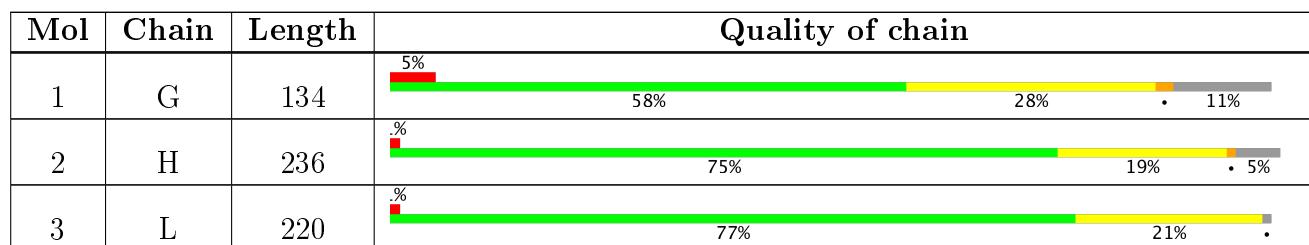
The reported resolution of this entry is 3.46 Å.

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

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)

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.

Mol	Chain	Length	Quality of chain
1	G	134	5% / 58% / 28% · 11%
2	H	236	.% / 75% / 19% · 5%
3	L	220	.% / 77% / 21% ·

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
6	MAN	G	1605	-	-	-	X
6	MAN	G	1653	-	-	-	X

2 Entity composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4724 atoms, of which 204 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 1FD6-V1V2-WITO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	119	929	584	150	188	7	0	0	0
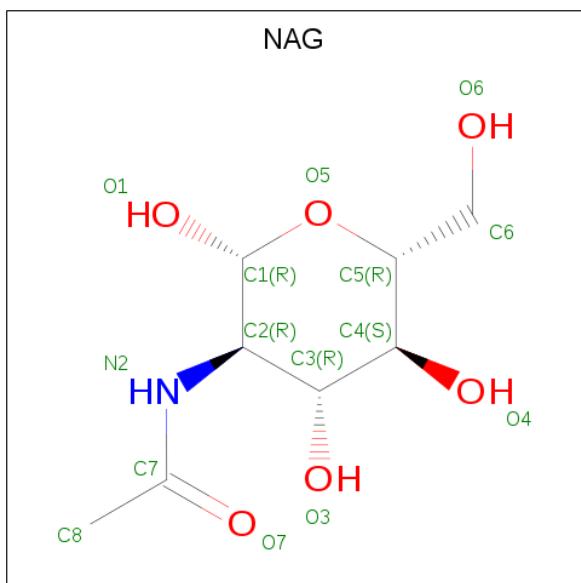
- Molecule 2 is a protein called VRC38.01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	224	1675	1056	285	328	6	0	0	0

- Molecule 3 is a protein called VRC38.01 Fab Light Chain.
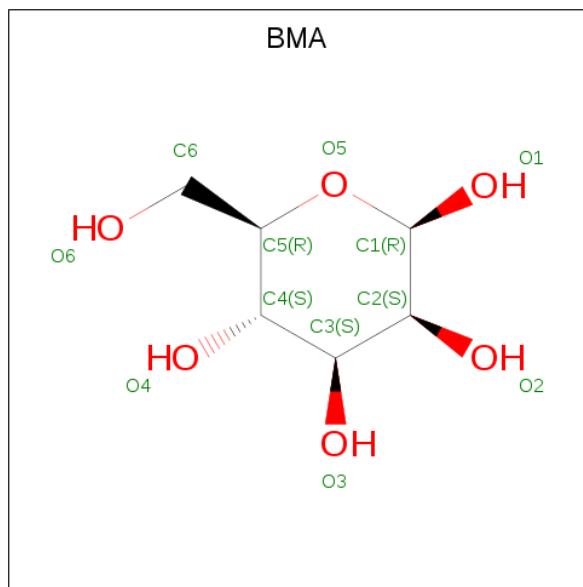
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	217	1675	1048	289	332	6	0	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
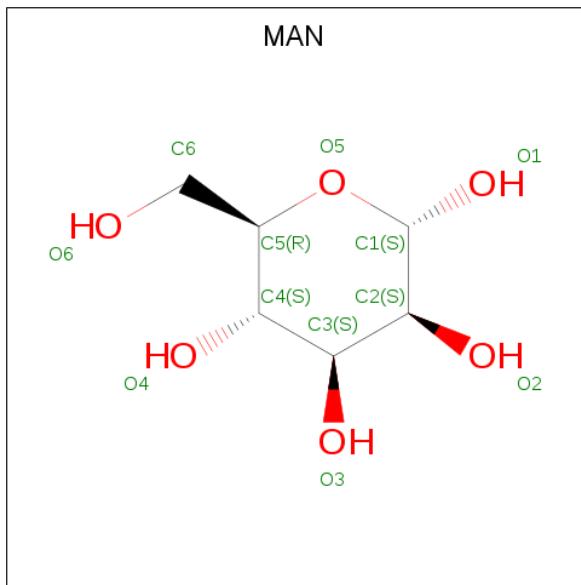
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	H	O	0	0
			19	6	8	5		
5	G	1	Total	C	H	O	0	0
			19	6	8	5		
5	G	1	Total	C	H	O	0	0
			19	6	8	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
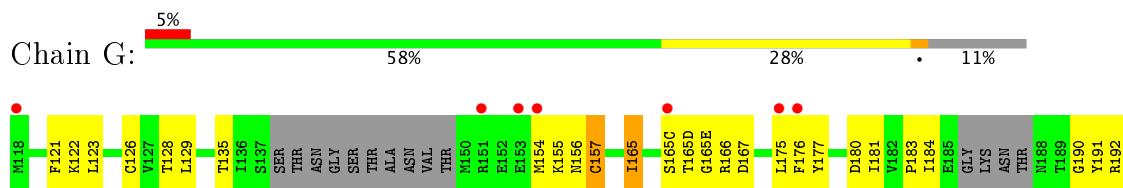
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 19	C 6	H 8	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 18	C 6	H 7	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
6	G	1	Total 21	C 6	H 10	O 5	0	0
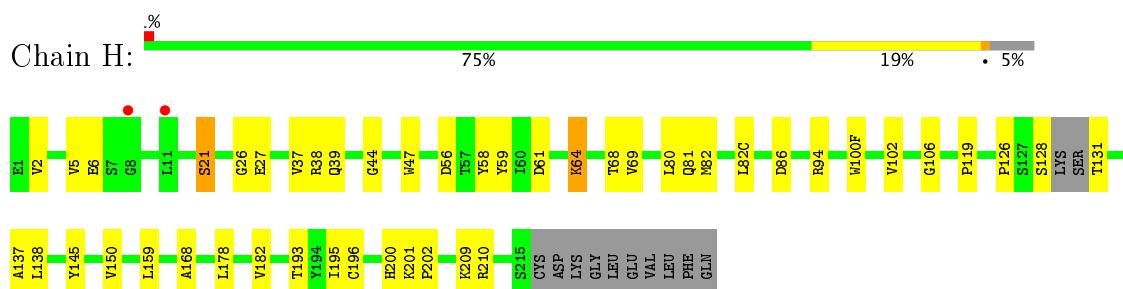
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
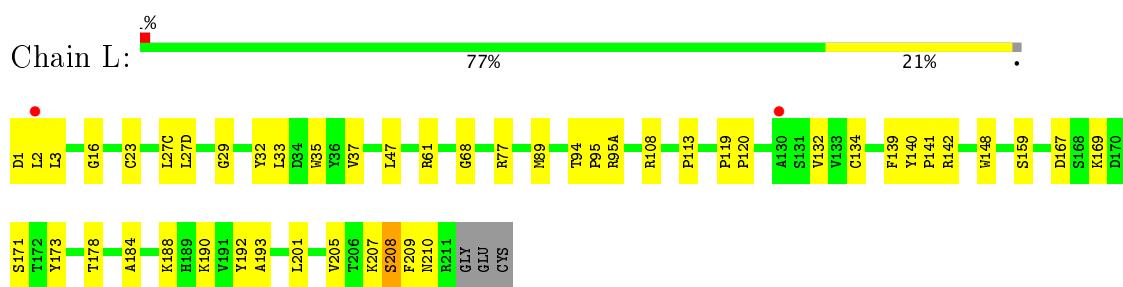
- Molecule 1: 1FD6-V1V2-WITO

- Molecule 2: VRC38.01 Fab Heavy Chain

- Molecule 3: VRC38.01 Fab Light Chain

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.57Å　　106.57Å　　129.86Å 90.00°　　　90.00°　　　120.00°	Depositor
Resolution (Å)	37.61　–　3.46 37.61　–　3.46	Depositor EDS
% Data completeness (in resolution range)	90.1 (37.61-3.46) 90.1 (37.61-3.46)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX (dev_2776: ???)	Depositor
R, R_{free}	0.214　,　0.273 0.212　,　0.278	Depositor DCC
R_{free} test set	511 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	106.2	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 29.4	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4724	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	G	0.27	0/941	0.49	0/1274
2	H	0.24	0/1716	0.46	0/2335
3	L	0.25	0/1711	0.45	0/2320
All	All	0.25	0/4368	0.46	0/5929

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	929	0	899	30	0
2	H	1675	0	1631	37	0
3	L	1675	0	1639	27	0
4	G	98	85	85	6	0
5	G	33	24	24	0	0
6	G	110	95	96	2	0
All	All	4520	204	4374	94	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 11.

All (94) 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)
4:G:1330:NAG:H81	3:L:29:GLY:HA3	1.52	0.89
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.63	0.79
2:H:61:ASP:OD1	2:H:64:LYS:NZ	2.16	0.75
1:G:225:GLU:O	1:G:237:VAL:HA	1.87	0.73
1:G:129:LEU:HB3	1:G:157:CYS:SG	2.31	0.70
2:H:59:TYR:O	3:L:95(A):ARG:NH2	2.24	0.70
1:G:165(C):SER:O	1:G:165(D):THR:OG1	2.10	0.69
1:G:184:ILE:HG22	1:G:190:GLY:O	1.93	0.69
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.76	0.66
1:G:210:ALA:O	1:G:214:LYS:HG3	1.95	0.66
3:L:61:ARG:NH1	3:L:77:ARG:O	2.29	0.65
6:G:1605:MAN:O3	2:H:27:GLU:OE2	2.18	0.62
2:H:131:THR:CG2	2:H:137:ALA:H	2.12	0.62
2:H:26:GLY:O	2:H:27:GLU:HG3	1.99	0.61
3:L:16:GLY:HA2	3:L:77:ARG:HG3	1.82	0.60
2:H:6:GLU:HA	2:H:21:SER:O	2.01	0.60
4:G:1561:NAG:H83	4:G:1561:NAG:H3	1.82	0.60
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.83	0.59
1:G:126:CYS:SG	1:G:192:ARG:NH1	2.76	0.58
1:G:156:ASN:HD22	4:G:1560:NAG:C7	2.15	0.58
1:G:183:PRO:HA	1:G:191:TYR:HA	1.86	0.57
2:H:2:VAL:HG22	2:H:27:GLU:HB2	1.87	0.56
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.88	0.56
3:L:27(D):LEU:HD12	3:L:32:TYR:CE1	2.40	0.56
2:H:131:THR:HG21	2:H:137:ALA:O	2.06	0.56
1:G:165:ILE:HG22	4:G:1650:NAG:O7	2.06	0.55
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.89	0.55
1:G:155:LYS:O	1:G:175:LEU:HA	2.07	0.54
2:H:68:THR:HG23	2:H:81:GLN:HB3	1.89	0.54
1:G:197:GLN:OE1	1:G:197:GLN:HA	2.08	0.54
2:H:39:GLN:HG3	2:H:44:GLY:O	2.08	0.54
2:H:193:THR:HG23	2:H:210:ARG:NE	2.22	0.54
2:H:131:THR:O	2:H:131:THR:HG22	2.06	0.54
1:G:123:LEU:HB3	1:G:199:THR:HG23	1.89	0.53
1:G:176:PHE:HB2	1:G:181:ILE:HD11	1.90	0.53
3:L:27(C):LEU:HD11	3:L:29:GLY:HA2	1.91	0.53
2:H:59:TYR:CE1	2:H:69:VAL:HG23	2.45	0.52
2:H:131:THR:HG22	2:H:137:ALA:H	1.74	0.52
1:G:192:ARG:NH1	1:G:196:CYS:SG	2.83	0.51
1:G:122:LYS:HG2	1:G:200:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:190:LYS:HE2	3:L:210:ASN:ND2	2.25	0.51
2:H:69:VAL:HG22	2:H:80:LEU:CD1	2.41	0.51
3:L:37:VAL:HB	3:L:47:LEU:HD11	1.91	0.50
3:L:159:SER:HA	3:L:178:THR:O	2.12	0.50
1:G:165(E):GLY:O	1:G:166:ARG:HB2	2.11	0.50
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.93	0.49
1:G:183:PRO:HB3	1:G:191:TYR:CD2	2.48	0.48
1:G:128:THR:H	1:G:240:GLY:H	1.60	0.48
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.29	0.48
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.95	0.48
3:L:140:TYR:CG	3:L:141:PRO:HA	2.49	0.48
3:L:2:LEU:HD23	3:L:3:LEU:N	2.29	0.47
1:G:192:ARG:NH1	1:G:193:LEU:O	2.47	0.47
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.96	0.47
3:L:192:TYR:O	3:L:208:SER:HA	2.14	0.47
1:G:135:THR:HG22	4:G:1560:NAG:O7	2.15	0.47
1:G:122:LYS:HA	1:G:200:THR:HG22	1.97	0.47
1:G:128:THR:HB	1:G:240:GLY:HA2	1.97	0.47
2:H:59:TYR:HE1	2:H:69:VAL:HG23	1.80	0.47
1:G:222:ILE:HG23	1:G:239:GLU:OE1	2.16	0.46
3:L:184:ALA:O	3:L:188:LYS:HG3	2.16	0.46
2:H:201:LYS:N	2:H:202:PRO:CD	2.78	0.46
1:G:217:ALA:HA	1:G:222:ILE:HD12	1.96	0.46
6:G:1606:MAN:O5	2:H:100(F):TRP:HD1	1.99	0.46
3:L:201:LEU:HD13	3:L:205:VAL:HG23	1.98	0.45
2:H:2:VAL:HG21	2:H:94:ARG:NH1	2.32	0.45
1:G:123:LEU:HD12	1:G:235:PHE:O	2.17	0.45
1:G:122:LYS:HG2	1:G:200:THR:CG2	2.46	0.44
3:L:33:LEU:HD22	3:L:89:MET:O	2.16	0.44
2:H:68:THR:CG2	2:H:81:GLN:HB3	2.46	0.44
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.82	0.44
2:H:178:LEU:HD12	2:H:178:LEU:C	2.38	0.43
3:L:193:ALA:HA	3:L:207:LYS:O	2.18	0.43
2:H:6:GLU:CD	2:H:106:GLY:H	2.21	0.43
2:H:58:TYR:CE1	3:L:95:PRO:HG2	2.53	0.43
1:G:184:ILE:O	1:G:184:ILE:HG23	2.18	0.43
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	2.00	0.43
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.53	0.43
1:G:154:MET:HG2	1:G:177:TYR:CD1	2.54	0.43
1:G:183:PRO:HB3	1:G:191:TYR:CE2	2.54	0.42
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:PHE:O	1:G:200:THR:HA	2.20	0.42
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.55	0.41
2:H:94:ARG:HB3	2:H:102:VAL:HB	2.01	0.41
2:H:150:VAL:HG22	2:H:200:HIS:HB2	2.02	0.41
3:L:94:THR:HG23	3:L:95:PRO:HA	2.02	0.41
4:G:1560:NAG:H62	4:G:1561:NAG:C1	2.51	0.41
2:H:69:VAL:HG22	2:H:80:LEU:HD13	2.01	0.41
3:L:142:ARG:HB3	3:L:173:TYR:CE2	2.56	0.41
3:L:167:ASP:C	3:L:169:LYS:H	2.23	0.41
2:H:56:ASP:N	2:H:56:ASP:OD1	2.54	0.41
2:H:195:ILE:HA	2:H:209:LYS:O	2.21	0.40
3:L:119:PRO:HB3	3:L:209:PHE:CZ	2.56	0.40
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.03	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	G	113/134 (84%)	106 (94%)	7 (6%)	0	100	100
2	H	220/236 (93%)	215 (98%)	5 (2%)	0	100	100
3	L	215/220 (98%)	209 (97%)	5 (2%)	1 (0%)	32	73
All	All	548/590 (93%)	530 (97%)	17 (3%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	68	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	G	103/115 (90%)	98 (95%)	5 (5%)	29	65
2	H	187/198 (94%)	182 (97%)	5 (3%)	50	80
3	L	189/191 (99%)	187 (99%)	2 (1%)	78	91
All	All	479/504 (95%)	467 (98%)	12 (2%)	53	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	157	CYS
1	G	165	ILE
1	G	167	ASP
1	G	180	ASP
1	G	222	ILE
2	H	5	VAL
2	H	21	SER
2	H	64	LYS
2	H	128	SER
2	H	196	CYS
3	L	1	ASP
3	L	208	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	32	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

20 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	#$|Z| > 2$
4	NAG	G	1330	1	14,14,15	0.43	0	15,19,21	0.44	0
4	NAG	G	1560	1,4	14,14,15	0.85	1 (7%)	15,19,21	0.74	0
4	NAG	G	1561	5,4	14,14,15	0.29	0	15,19,21	1.19	1 (6%)
5	BMA	G	1562	4,6	11,11,12	0.61	0	13,15,17	0.84	0
6	MAN	G	1563	5	11,11,12	0.61	0	13,15,17	0.99	2 (15%)
6	MAN	G	1564	5,6	11,11,12	0.77	1 (9%)	13,15,17	1.04	1 (7%)
6	MAN	G	1565	6	11,11,12	0.94	1 (9%)	13,15,17	0.96	1 (7%)
6	MAN	G	1566	6	11,11,12	0.56	0	13,15,17	1.06	2 (15%)
4	NAG	G	1600	1,4	14,14,15	0.21	0	15,19,21	0.60	0
4	NAG	G	1601	5,4	14,14,15	0.21	0	15,19,21	0.58	0
5	BMA	G	1602	4,6	11,11,12	0.45	0	13,15,17	0.73	0
6	MAN	G	1603	5	11,11,12	0.55	0	13,15,17	1.09	2 (15%)
6	MAN	G	1604	5,6	11,11,12	0.56	0	13,15,17	1.08	2 (15%)
6	MAN	G	1605	6	11,11,12	0.57	0	13,15,17	1.09	2 (15%)
6	MAN	G	1606	6	11,11,12	0.78	0	13,15,17	1.16	2 (15%)
4	NAG	G	1650	1,4	14,14,15	0.38	0	15,19,21	0.85	0
4	NAG	G	1651	5,4	14,14,15	0.22	0	15,19,21	0.50	0
5	BMA	G	1652	4,6	11,11,12	0.60	0	13,15,17	0.69	0
6	MAN	G	1653	5	11,11,12	0.54	0	13,15,17	1.12	2 (15%)
6	MAN	G	1654	5	11,11,12	0.60	0	13,15,17	1.08	2 (15%)

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	NAG	G	1330	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1560	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1561	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	1562	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1563	5	-	0/2/19/22	0/1/1/1
6	MAN	G	1564	5,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1565	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1566	6	-	0/2/19/22	0/1/1/1
4	NAG	G	1600	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1601	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	1602	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1603	5	-	0/2/19/22	0/1/1/1
6	MAN	G	1604	5,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1605	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1606	6	-	0/2/19/22	0/1/1/1
4	NAG	G	1650	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1651	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	1652	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1653	5	-	0/2/19/22	0/1/1/1
6	MAN	G	1654	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1560	NAG	C1-C2	-2.63	1.48	1.52
6	G	1565	MAN	O5-C1	-2.44	1.39	1.43
6	G	1564	MAN	O5-C1	-2.14	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	1606	MAN	O2-C2-C3	-2.28	105.69	110.17
6	G	1605	MAN	O2-C2-C3	-2.28	105.69	110.17
6	G	1653	MAN	O2-C2-C3	-2.26	105.74	110.17
6	G	1604	MAN	O2-C2-C3	-2.19	105.88	110.17
6	G	1563	MAN	O2-C2-C3	-2.18	105.90	110.17
6	G	1654	MAN	O2-C2-C3	-2.18	105.90	110.17
6	G	1566	MAN	O2-C2-C3	-2.16	105.94	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	1565	MAN	O2-C2-C3	-2.15	105.95	110.17
6	G	1603	MAN	O2-C2-C3	-2.09	106.08	110.17
6	G	1564	MAN	O2-C2-C3	-2.05	106.14	110.17
6	G	1563	MAN	C1-O5-C5	2.14	115.12	112.17
6	G	1605	MAN	C1-O5-C5	2.25	115.26	112.17
6	G	1566	MAN	C1-O5-C5	2.30	115.34	112.17
6	G	1604	MAN	C1-O5-C5	2.36	115.42	112.17
6	G	1603	MAN	C1-O5-C5	2.42	115.50	112.17
6	G	1654	MAN	C1-O5-C5	2.45	115.55	112.17
6	G	1653	MAN	C1-O5-C5	2.67	115.85	112.17
6	G	1606	MAN	C1-O5-C5	2.88	116.14	112.17
4	G	1561	NAG	C2-N2-C7	2.89	127.17	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1330	NAG	1	0
4	G	1560	NAG	3	0
4	G	1561	NAG	2	0
6	G	1605	MAN	1	0
6	G	1606	MAN	1	0
4	G	1650	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	G	119/134 (88%)	0.06	7 (5%)	23	21	86, 116, 166, 186	0
2	H	224/236 (94%)	-0.03	2 (0%)	84	78	80, 107, 133, 151	0
3	L	217/220 (98%)	-0.06	2 (0%)	84	78	71, 97, 126, 144	0
All	All	560/590 (94%)	-0.02	11 (1%)	65	60	71, 105, 139, 186	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	8	GLY	3.2
2	H	11	LEU	3.0
1	G	154	MET	2.8
1	G	153	GLU	2.8
3	L	2	LEU	2.7
1	G	118	MET	2.6
1	G	165(C)	SER	2.5
3	L	130	ALA	2.4
1	G	176	PHE	2.3
1	G	151	ARG	2.3
1	G	175	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MAN	G	1605	11/12	0.69	0.47	2.59	171,204,242,260	0
6	MAN	G	1653	11/12	0.85	0.52	2.00	165,181,218,218	0
4	NAG	G	1650	14/15	0.80	0.35	0.87	113,188,228,238	0
6	MAN	G	1566	11/12	0.89	0.24	0.31	125,143,169,179	0
4	NAG	G	1600	14/15	0.90	0.22	-0.21	109,131,166,178	0
4	NAG	G	1560	14/15	0.91	0.27	-0.28	119,144,177,177	0
4	NAG	G	1330	14/15	0.81	0.28	-0.32	157,173,202,210	0
6	MAN	G	1606	11/12	0.90	0.21	-1.14	112,135,158,165	0
6	MAN	G	1603	11/12	0.97	0.10	-1.71	118,136,164,166	0
6	MAN	G	1563	11/12	0.92	0.16	-2.13	90,140,169,181	0
5	BMA	G	1562	11/12	0.93	0.14	-2.27	122,138,158,168	0
4	NAG	G	1561	14/15	0.94	0.14	-3.10	92,138,167,182	0
6	MAN	G	1654	11/12	0.86	0.37	-	165,191,230,230	0
4	NAG	G	1601	14/15	0.95	0.20	-	102,123,171,171	0
5	BMA	G	1652	11/12	0.84	0.49	-	177,194,234,234	0
6	MAN	G	1604	11/12	0.93	0.33	-	115,131,161,161	0
5	BMA	G	1602	11/12	0.95	0.23	-	100,119,144,144	0
6	MAN	G	1565	11/12	0.89	0.27	-	155,175,206,216	0
6	MAN	G	1564	11/12	0.96	0.19	-	116,142,171,172	0
4	NAG	G	1651	14/15	0.87	0.41	-	151,195,235,248	0

6.5 Other polymers (i)

There are no such residues in this entry.