Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 10:59 AM EDT

PDB ID	:	4JAN
Title	:	crystal structure of broadly neutralizing antibody CH103 in complex with HIV-1 gp120
Authors	:	Zhou, T.; Moquin, S.; Zheng, A.; Srivatsan, S.; Kwong, P.D.
Deposited on	:	2013-02-18
Resolution	:	3.15 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

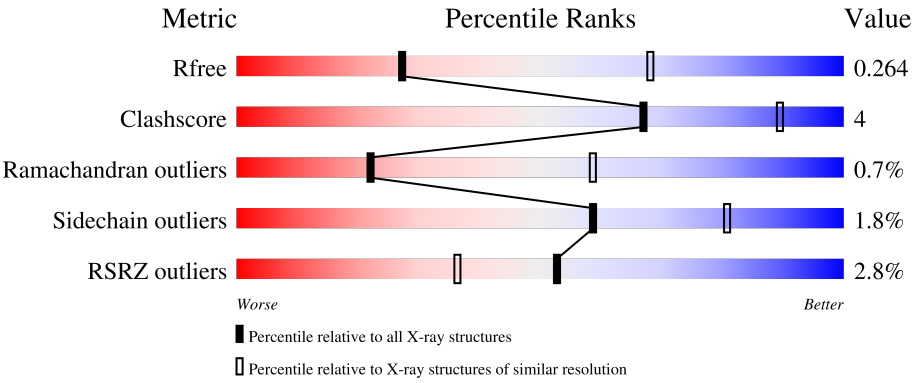
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	355	5% 39% 6% 55%
1	I	355	3% 41% 56%
2	A	226	83% 14%
2	H	226	87% 9%
3	B	209	89% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	209	

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	NAG	I	503	-	-	-	X
4	NAG	I	505	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17823 atoms, of which 8804 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 ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	160	Total	C	H	N	O	S	0	0	0
			2485	779	1233	221	246	6			
1	I	156	Total	C	H	N	O	S	0	0	0
			2418	760	1199	214	239	6			

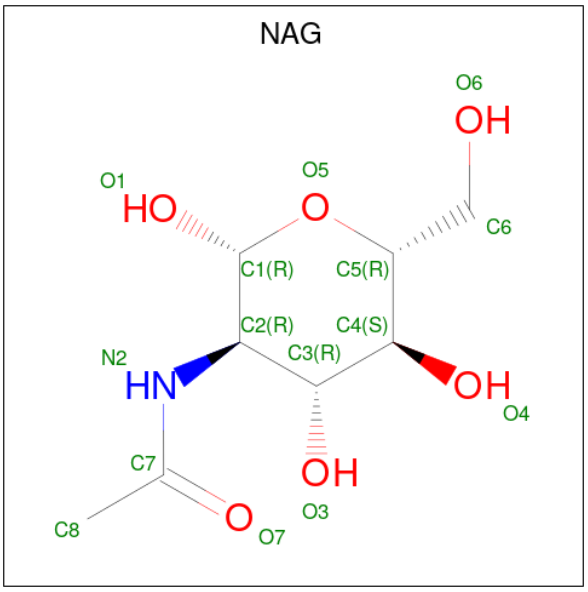
- Molecule 2 is a protein called ANTIGEN BINDING FRAGMENT OF HEAVY CHAIN of CH103.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	218	Total	C	H	N	O	S	0	0	0
			3228	1027	1605	274	317	5			
2	A	218	Total	C	H	N	O	S	0	0	0
			3227	1027	1604	274	317	5			

- Molecule 3 is a protein called ANTIGEN BINDING FRAGMENT OF LIGHT CHAIN of CH103.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	206	Total	C	H	N	O	S	0	0	0
			3072	983	1509	258	317	5			
3	B	206	Total	C	H	N	O	S	0	0	0
			3072	983	1509	258	317	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

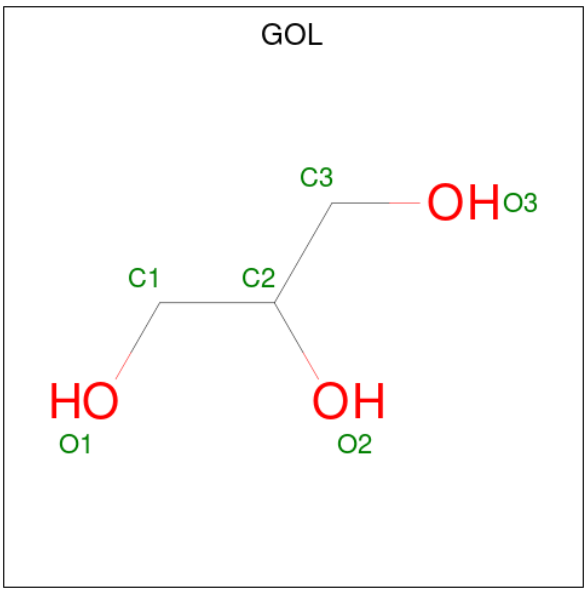


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	L	1	Total	Na	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is water.

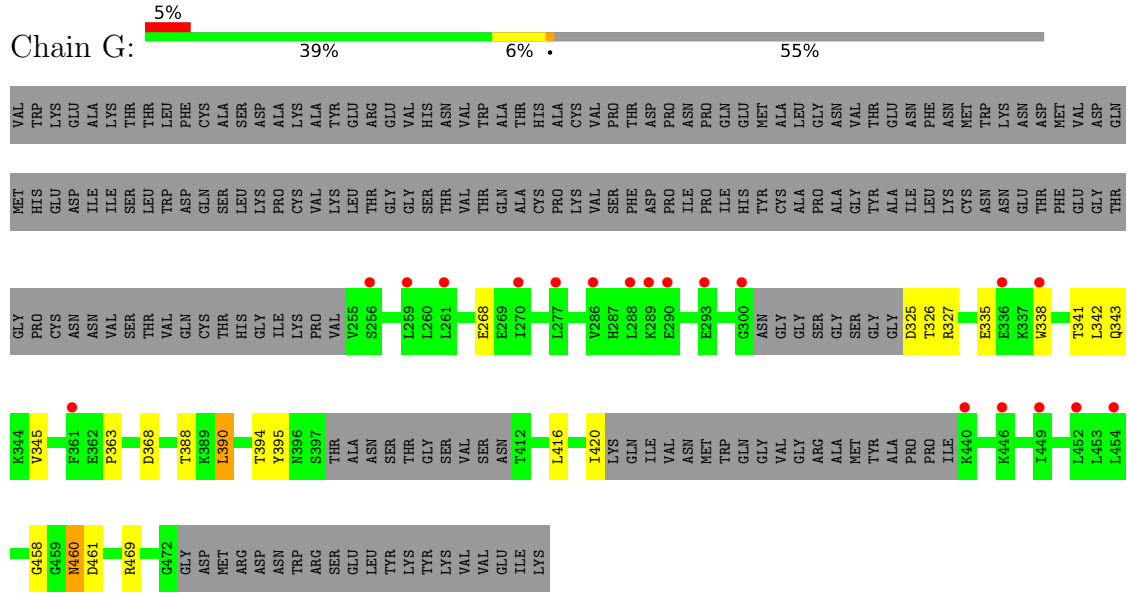
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	5	Total O 5 5	0	0
7	H	3	Total O 3 3	0	0
7	L	3	Total O 3 3	0	0
7	I	1	Total O 1 1	0	0
7	A	6	Total O 6 6	0	0
7	B	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

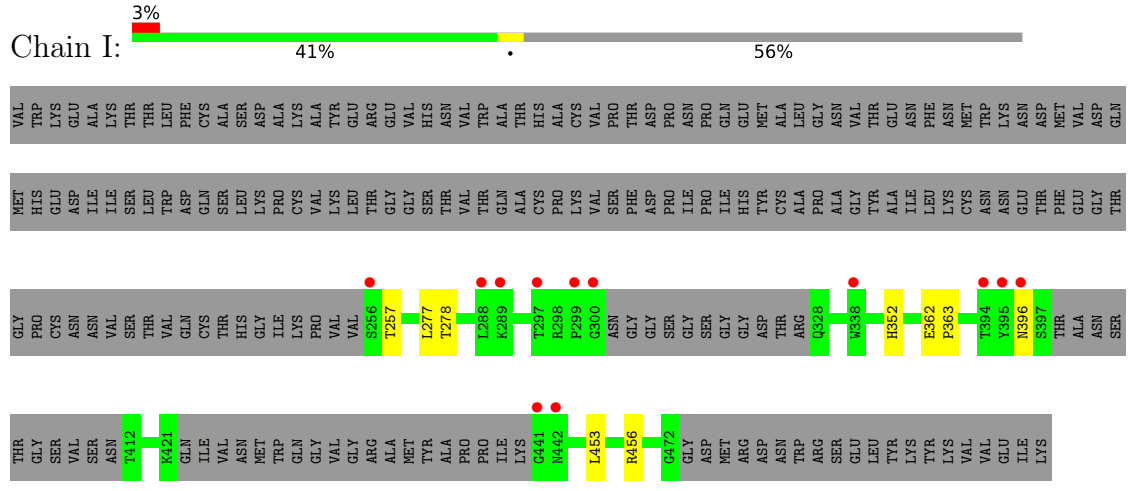
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C

Chain G:



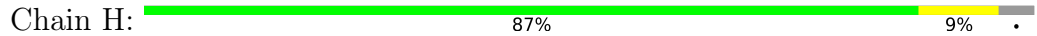
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C

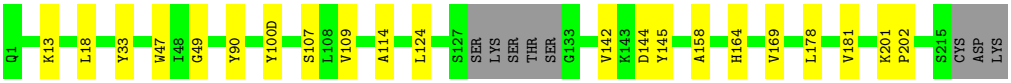
Chain I:



• Molecule 2: ANTIGEN BINDING FRAGMENT OF HEAVY CHAIN of CH103

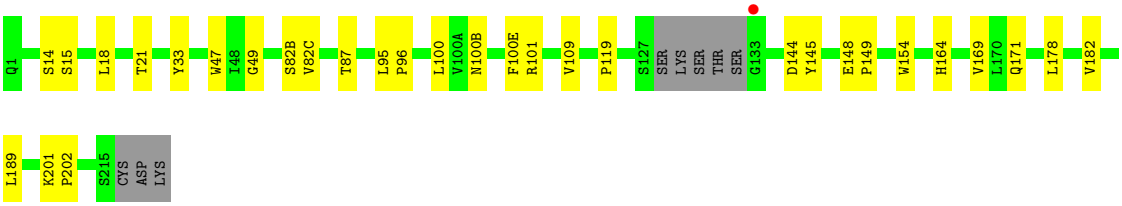
Chain H:





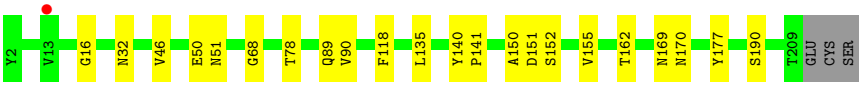
• Molecule 2: ANTIGEN BINDING FRAGMENT OF HEAVY CHAIN of CH103

Chain A:



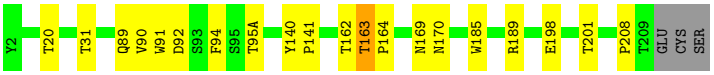
• Molecule 3: ANTIGEN BINDING FRAGMENT OF LIGHT CHAIN of CH103

Chain L:



• Molecule 3: ANTIGEN BINDING FRAGMENT OF LIGHT CHAIN of CH103

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.94Å 208.65Å 69.42Å 90.00° 107.21° 90.00°	Depositor
Resolution (Å)	46.75 – 3.15 46.75 – 3.15	Depositor EDS
% Data completeness (in resolution range)	89.1 (46.75-3.15) 89.2 (46.75-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.196 , 0.256 0.203 , 0.264	Depositor DCC
R_{free} test set	1043 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17823	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.22	0/1269	0.39	0/1710
1	I	0.21	0/1236	0.40	0/1665
2	A	0.23	0/1662	0.42	0/2266
2	H	0.23	0/1662	0.41	0/2266
3	B	0.23	0/1604	0.42	0/2196
3	L	0.22	0/1604	0.41	0/2196
All	All	0.22	0/9037	0.41	0/12299

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

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	1252	1233	1233	22	0
1	I	1219	1199	1200	5	0
2	A	1623	1604	1604	16	0
2	H	1623	1605	1604	16	0
3	B	1563	1509	1509	8	0
3	L	1563	1509	1509	14	0
4	G	70	64	65	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	70	65	65	1	0
5	H	1	0	0	0	0
5	L	1	0	0	0	0
6	B	6	8	8	0	0
6	L	6	8	8	0	0
7	A	6	0	0	4	0
7	B	4	0	0	0	0
7	G	5	0	0	0	0
7	H	3	0	0	0	0
7	I	1	0	0	0	0
7	L	3	0	0	0	0
All	All	9019	8804	8805	70	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 4.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:GLU:CD	4:G:503:NAG:H82	1.82	0.99
2:A:82(C):VAL:N	7:A:305:HOH:O	2.12	0.82
1:G:335:GLU:OE1	4:G:503:NAG:H82	1.79	0.81
2:A:82(C):VAL:O	7:A:305:HOH:O	2.09	0.71
1:G:327:ARG:NH1	1:G:420:ILE:O	2.25	0.69
1:G:460:ASN:CG	1:G:460:ASN:O	2.32	0.67
1:G:325:ASP:O	1:G:326:THR:OG1	2.11	0.67
1:G:338:TRP:CE2	1:G:390:LEU:HD23	2.31	0.65
1:G:388:THR:HG22	4:G:505:NAG:H81	1.79	0.65
1:G:390:LEU:HD11	1:G:416:LEU:HD11	1.81	0.62
1:I:396:ASN:H	4:I:503:NAG:H81	1.65	0.61
1:G:335:GLU:OE2	4:G:503:NAG:H82	2.03	0.58
2:A:171:GLN:NE2	7:A:302:HOH:O	2.36	0.58
1:G:460:ASN:O	1:G:460:ASN:ND2	2.38	0.57
1:G:458:GLY:O	3:L:32:ASN:ND2	2.39	0.55
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.42	0.55
2:A:14:SER:O	2:A:15:SER:OG	2.22	0.54
1:G:338:TRP:CZ2	1:G:342:LEU:HD11	2.43	0.53
2:A:201:LYS:N	2:A:202:PRO:CD	2.72	0.53
1:G:338:TRP:CD2	1:G:390:LEU:HD23	2.43	0.53
2:H:181:VAL:HG21	3:L:135:LEU:CD1	2.39	0.52
2:A:33:TYR:HB2	2:A:95:LEU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:VAL:HG21	3:L:177:TYR:CD1	2.44	0.52
1:G:335:GLU:OE1	4:G:503:NAG:C8	2.55	0.52
2:H:107:SER:HA	3:B:189:ARG:HE	1.76	0.51
1:G:368:ASP:OD1	2:H:33:TYR:OH	2.22	0.51
1:G:390:LEU:CD1	1:G:416:LEU:HD11	2.41	0.49
2:H:169:VAL:HG22	3:L:162:THR:HG23	1.94	0.49
3:L:89:GLN:HG2	3:L:90:VAL:N	2.27	0.49
2:H:90:TYR:N	2:H:107:SER:O	2.45	0.48
3:B:169:ASN:O	3:B:170:ASN:HB2	2.13	0.47
2:H:201:LYS:N	2:H:202:PRO:CD	2.76	0.47
3:L:140:TYR:CD2	3:L:141:PRO:HA	2.49	0.47
3:B:185:TRP:CZ2	3:B:208:PRO:HB3	2.50	0.47
1:G:341:THR:O	1:G:345:VAL:HG21	2.15	0.46
2:A:18:LEU:HD13	2:A:109:VAL:HG11	1.96	0.46
2:A:96:PRO:HG3	2:A:101:ARG:NH1	2.31	0.46
1:I:277:LEU:HD21	1:I:352:HIS:CG	2.50	0.46
1:I:257:THR:O	1:I:453:LEU:HD12	2.16	0.46
2:H:178:LEU:C	2:H:178:LEU:HD12	2.36	0.45
1:I:278:THR:O	1:I:456:ARG:NH2	2.50	0.45
2:A:148:GLU:CB	2:A:149:PRO:HA	2.46	0.45
1:G:390:LEU:HD11	1:G:416:LEU:CD1	2.47	0.45
2:A:15:SER:HA	7:A:305:HOH:O	2.16	0.45
3:L:169:ASN:O	3:L:170:ASN:HB2	2.16	0.45
3:L:150:ALA:O	3:L:152:SER:N	2.51	0.44
2:H:124:LEU:HB3	3:L:118:PHE:CD1	2.53	0.44
3:B:90:VAL:HG22	3:B:91:TRP:N	2.32	0.44
1:I:362:GLU:HB3	1:I:363:PRO:HD2	2.00	0.43
2:H:181:VAL:HG21	3:L:135:LEU:HD13	2.00	0.43
1:G:343:GLN:HG2	1:G:395:TYR:HB3	2.00	0.43
2:H:13:LYS:HE2	2:H:114:ALA:HA	2.00	0.43
3:L:50:GLU:O	3:L:51:ASN:HB2	2.19	0.43
3:B:163:THR:HG22	3:B:164:PRO:HD2	2.00	0.43
2:A:47:TRP:CZ2	2:A:49:GLY:HA2	2.54	0.42
1:G:394:THR:HG22	1:G:395:TYR:N	2.34	0.42
2:H:142:VAL:HG12	2:H:145:TYR:CD2	2.55	0.42
3:L:140:TYR:CG	3:L:141:PRO:HA	2.55	0.42
3:B:140:TYR:CG	3:B:141:PRO:HA	2.54	0.42
1:G:368:ASP:OD1	1:G:368:ASP:N	2.53	0.41
2:H:100(D):TYR:CE1	3:L:46:VAL:HG11	2.55	0.41
3:L:16:GLY:N	3:L:78:THR:O	2.51	0.41
2:A:119:PRO:HB3	2:A:145:TYR:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HD13	2:H:109:VAL:HG11	2.03	0.41
1:G:363:PRO:O	1:G:469:ARG:NH1	2.54	0.41
2:A:95:LEU:HD11	2:A:100(E):PHE:CE1	2.56	0.41
2:A:169:VAL:HG13	3:B:162:THR:CG2	2.50	0.40
2:A:178:LEU:C	2:A:178:LEU:HD12	2.41	0.40
2:H:158:ALA:CB	3:B:94:PHE:HB3	2.51	0.40
2:A:154:TRP:CE2	2:A:182:VAL:CG2	3.05	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	152/355 (43%)	132 (87%)	19 (12%)	1 (1%)	22	59
1	I	148/355 (42%)	129 (87%)	19 (13%)	0	100	100
2	A	214/226 (95%)	206 (96%)	5 (2%)	3 (1%)	11	43
2	H	214/226 (95%)	194 (91%)	19 (9%)	1 (0%)	29	65
3	B	204/209 (98%)	195 (96%)	8 (4%)	1 (0%)	29	65
3	L	204/209 (98%)	187 (92%)	15 (7%)	2 (1%)	15	51
All	All	1136/1580 (72%)	1043 (92%)	85 (8%)	8 (1%)	22	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	151	ASP
2	A	82(B)	SER
2	A	87	THR
2	H	144	ASP
2	A	144	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	268	GLU
3	B	198	GLU
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	144/309 (47%)	141 (98%)	3 (2%)	53 78
1	I	140/309 (45%)	140 (100%)	0	100 100
2	A	184/192 (96%)	179 (97%)	5 (3%)	44 73
2	H	184/192 (96%)	183 (100%)	1 (0%)	88 95
3	B	179/182 (98%)	172 (96%)	7 (4%)	32 64
3	L	179/182 (98%)	177 (99%)	2 (1%)	73 88
All	All	1010/1366 (74%)	992 (98%)	18 (2%)	59 81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	390	LEU
1	G	460	ASN
1	G	461	ASP
2	H	164	HIS
3	L	155	VAL
3	L	190	SER
2	A	21	THR
2	A	100	LEU
2	A	100(B)	ASN
2	A	164	HIS
2	A	189	LEU
3	B	20	THR
3	B	31	THR
3	B	89	GLN
3	B	92	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	95(A)	THR
3	B	163	THR
3	B	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	460	ASN
2	A	99	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	I	502	1	14,14,15	0.51	0	17,19,21	0.75	0
4	NAG	I	504	1	14,14,15	0.54	0	17,19,21	0.59	0
4	NAG	G	503	1	14,14,15	0.49	0	17,19,21	1.42	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	I	505	1	14,14,15	0.51	0	17,19,21	0.74	0
6	GOL	L	302	-	5,5,5	0.37	0	5,5,5	0.29	0
4	NAG	I	503	1	14,14,15	0.49	0	17,19,21	0.75	0
4	NAG	G	501	1	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
4	NAG	G	502	1	14,14,15	0.49	0	17,19,21	0.69	0
4	NAG	I	501	1	14,14,15	0.55	0	17,19,21	0.82	1 (5%)
4	NAG	G	504	1	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
6	GOL	B	301	-	5,5,5	0.37	0	5,5,5	0.24	0
4	NAG	G	505	1	14,14,15	0.52	0	17,19,21	0.69	0

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	I	502	1	-	2/6/23/26	0/1/1/1
4	NAG	I	504	1	-	3/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	I	505	1	-	2/6/23/26	0/1/1/1
6	GOL	L	302	-	-	2/4/4/4	-
4	NAG	I	503	1	-	3/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	I	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	3/6/23/26	0/1/1/1
6	GOL	B	301	-	-	2/4/4/4	-
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	503	NAG	O5-C5-C6	4.06	113.57	107.20
4	G	503	NAG	C6-C5-C4	-2.58	106.95	113.00
4	G	504	NAG	C1-O5-C5	2.57	115.67	112.19
4	G	501	NAG	O5-C5-C6	2.41	110.98	107.20
4	I	501	NAG	O5-C5-C6	2.38	110.94	107.20
4	G	503	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	503	NAG	C3-C2-N2-C7
4	G	505	NAG	C8-C7-N2-C2
4	G	505	NAG	O7-C7-N2-C2
4	I	503	NAG	C8-C7-N2-C2
4	I	503	NAG	O7-C7-N2-C2
4	I	505	NAG	C8-C7-N2-C2
4	I	505	NAG	O7-C7-N2-C2
6	L	302	GOL	O1-C1-C2-C3
6	B	301	GOL	O1-C1-C2-C3
4	G	504	NAG	C8-C7-N2-C2
4	G	504	NAG	O7-C7-N2-C2
4	I	504	NAG	C8-C7-N2-C2
4	I	504	NAG	O7-C7-N2-C2
4	I	503	NAG	O5-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
6	L	302	GOL	O1-C1-C2-O2
6	B	301	GOL	O1-C1-C2-O2
4	G	503	NAG	O5-C5-C6-O6
4	I	504	NAG	O5-C5-C6-O6
4	G	501	NAG	C8-C7-N2-C2
4	I	502	NAG	C8-C7-N2-C2
4	G	501	NAG	O7-C7-N2-C2
4	I	502	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	NAG	4	0
4	I	503	NAG	1	0
4	G	505	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	160/355 (45%)	0.63	19 (11%) 4 2	77, 126, 171, 215	0
1	I	156/355 (43%)	0.58	12 (7%) 13 6	77, 126, 176, 196	0
2	A	218/226 (96%)	-0.09	1 (0%) 91 86	35, 60, 100, 192	0
2	H	218/226 (96%)	-0.04	0 100 100	31, 69, 106, 141	0
3	B	206/209 (98%)	-0.08	0 100 100	38, 62, 90, 128	0
3	L	206/209 (98%)	0.02	1 (0%) 91 86	36, 67, 106, 136	0
All	All	1164/1580 (73%)	0.13	33 (2%) 53 36	31, 76, 149, 215	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	452	LEU	4.5
1	G	290	GLU	4.3
1	I	441	GLY	4.3
1	G	286	VAL	3.7
1	G	336	GLU	3.6
2	A	133	GLY	3.4
1	I	256	SER	3.2
1	I	395	TYR	3.1
1	I	288	LEU	3.1
1	I	300	GLY	3.1
1	G	449	ILE	3.0
1	G	270	ILE	3.0
1	I	442	ASN	2.8
1	G	259	LEU	2.8
1	I	394	THR	2.8
1	I	338	TRP	2.7
1	G	454	LEU	2.7
1	G	440	LYS	2.7
1	G	277	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	297	THR	2.6
1	G	338	TRP	2.6
1	I	289	LYS	2.5
1	G	256	SER	2.3
1	G	289	LYS	2.3
1	G	361	PHE	2.2
3	L	13	VAL	2.2
1	G	293	GLU	2.2
1	G	300	GLY	2.2
1	G	261	LEU	2.1
1	G	446	LYS	2.1
1	I	396	ASN	2.1
1	I	299	PRO	2.1
1	G	288	LEU	2.0

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
4	NAG	I	503	14/15	0.70	0.61	71,100,120,120	0
4	NAG	G	503	14/15	0.77	0.37	70,89,107,107	0
4	NAG	I	505	14/15	0.77	0.54	101,109,131,131	0
4	NAG	I	502	14/15	0.80	0.35	83,101,122,122	0
4	NAG	G	504	14/15	0.82	0.33	65,80,96,97	0
4	NAG	G	505	14/15	0.83	0.33	80,93,112,112	0
4	NAG	G	501	14/15	0.85	0.27	57,78,94,94	0
4	NAG	G	502	14/15	0.86	0.34	59,78,93,94	0
4	NAG	I	501	14/15	0.87	0.25	62,78,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	L	301	1/1	0.88	0.31	65,65,65,65	0
4	NAG	I	504	14/15	0.89	0.24	65,80,96,99	0
6	GOL	B	301	6/6	0.89	0.23	78,93,98,100	0
6	GOL	L	302	6/6	0.91	0.34	88,105,106,107	0
5	NA	H	301	1/1	0.98	0.11	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.