



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:26 pm BST

PDB ID : 6DB7
Title : Crystal structure of anti-HIV-1 V3 Fab 1334 in complex with a HIV-1 gp120 V3 peptide from MN strain
Authors : Chan, K.-W.; Kong, X.-P.
Deposited on : 2018-05-02
Resolution : 2.21 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 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 : 2.11
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) : 2.11

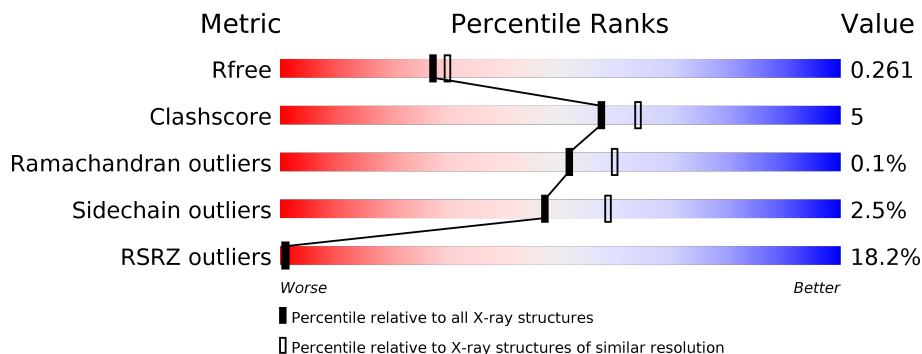
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	238	
1	I	238	
2	L	214	
2	M	214	
3	P	23	
3	Q	23	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7374 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 Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	234	Total	C	N	O	S	0	0	0
			1763	1107	296	351	9			
1	I	233	Total	C	N	O	S	0	0	0
			1757	1104	295	350	8			

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	211	Total	C	N	O	S	0	0	0
			1595	1000	264	326	5			
2	M	210	Total	C	N	O	S	0	0	0
			1590	997	264	324	5			

- Molecule 3 is a protein called HIV-1 gp120 V3 peptide from MN strain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	13	Total	C	N	O	0	0	0
			111	72	25	14			
3	Q	13	Total	C	N	O	0	0	0
			111	72	25	14			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

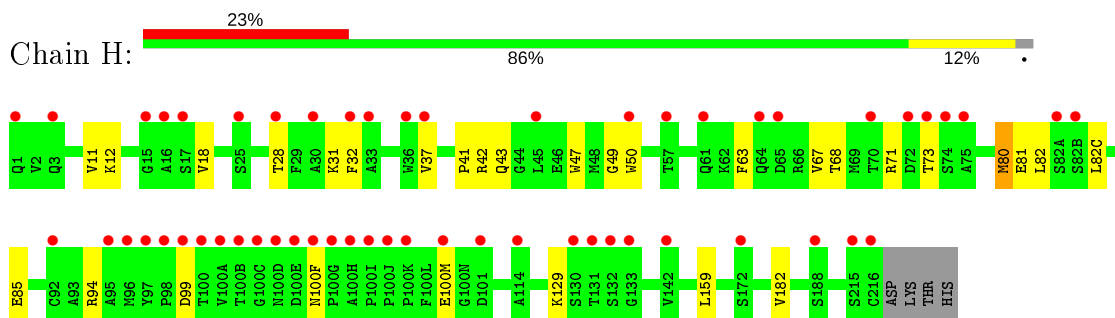
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	95	Total 95	O 95	0	0
5	L	90	Total 90	O 90	0	0
5	P	4	Total 4	O 4	0	0
5	I	104	Total 104	O 104	0	0
5	M	77	Total 77	O 77	0	0
5	Q	5	Total 5	O 5	0	0

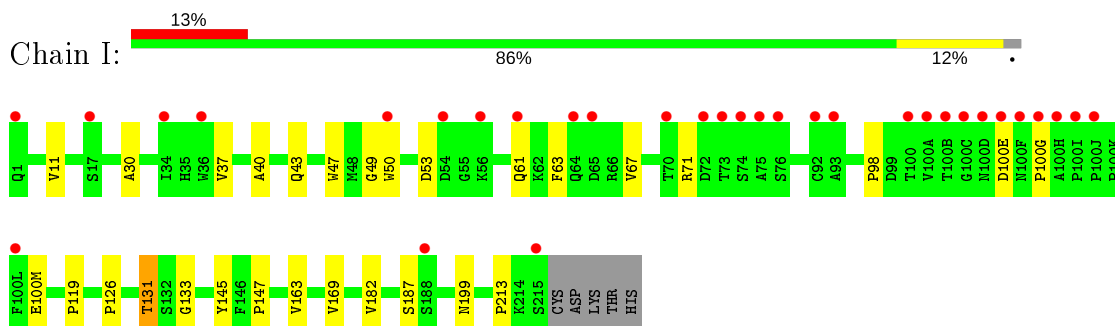
3 Residue-property plots

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

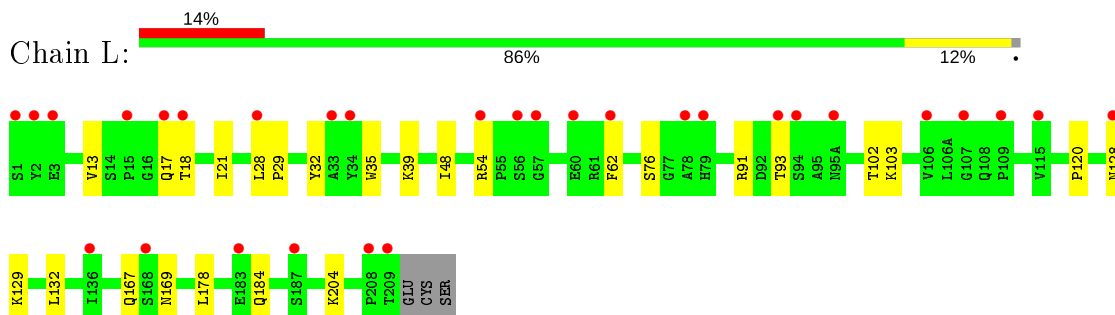
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab heavy chain



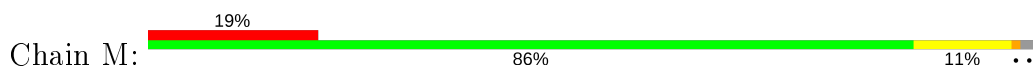
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab heavy chain

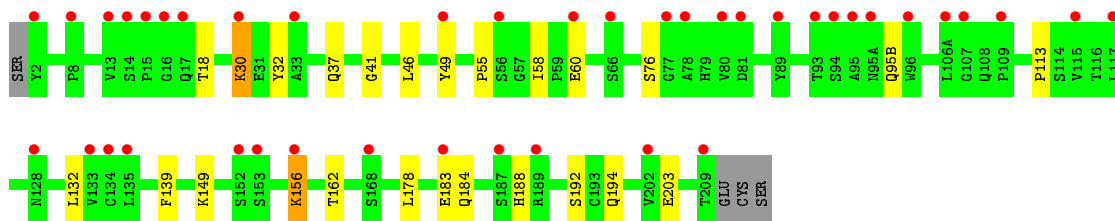


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab light chain

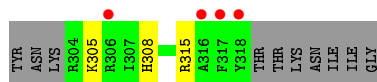
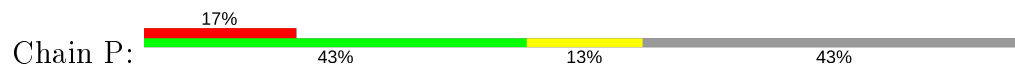


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 1334 Fab light chain





- Molecule 3: HIV-1 gp120 V3 peptide from MN strain



- Molecule 3: HIV-1 gp120 V3 peptide from MN strain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.80Å 69.63Å 97.19Å 90.00° 97.47° 90.00°	Depositor
Resolution (Å)	29.17 – 2.21 29.17 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.17-2.21) 99.3 (29.17-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.22Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.213 , 0.260 0.213 , 0.261	Depositor DCC
R_{free} test set	1998 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7374	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	H	0.26	0/1808	0.47	0/2466
1	I	0.25	0/1802	0.46	0/2458
2	L	0.25	0/1637	0.46	0/2238
2	M	0.25	0/1632	0.44	0/2232
3	P	0.24	0/114	0.38	0/150
3	Q	0.24	0/114	0.39	0/150
All	All	0.25	0/7107	0.46	0/9694

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	H	1763	0	1709	18	0
1	I	1757	0	1704	13	0
2	L	1595	0	1529	18	0
2	M	1590	0	1525	19	0
3	P	111	0	116	3	0
3	Q	111	0	116	4	0
4	H	18	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	6	0	8	0	0
4	L	18	0	24	1	0
4	M	30	0	40	3	0
5	H	95	0	0	0	0
5	I	104	0	0	0	0
5	L	90	0	0	5	0
5	M	77	0	0	1	0
5	P	4	0	0	0	0
5	Q	5	0	0	0	0
All	All	7374	0	6795	68	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 5.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:184:GLN:HE21	4:M:305:GOL:H11	1.61	0.65
2:M:156:LYS:H	2:M:156:LYS:HD3	1.62	0.65
1:H:99:ASP:OD2	3:P:315:ARG:NH1	2.31	0.64
2:M:30:LYS:HD3	3:Q:306:ARG:HG3	1.78	0.64
1:I:131:THR:HG23	1:I:133:GLY:H	1.63	0.63
1:H:12:LYS:HG3	1:H:18:VAL:HG12	1.80	0.63
2:L:128:ASN:ND2	5:L:403:HOH:O	2.32	0.62
2:L:129:LYS:NZ	5:L:406:HOH:O	2.33	0.61
2:L:18:THR:HG22	2:L:76:SER:HA	1.86	0.57
1:H:28:THR:HB	1:H:31:LYS:HG2	1.87	0.57
2:M:46:LEU:HD21	2:M:49:TYR:HB3	1.88	0.56
2:L:13:VAL:HG22	2:L:17:GLN:HG3	1.87	0.55
1:I:11:VAL:HB	1:I:147:PRO:HG3	1.88	0.54
1:H:41:PRO:O	1:H:42:ARG:HG2	2.07	0.54
2:L:54:ARG:NE	2:L:62:PHE:O	2.39	0.53
2:M:132:LEU:HD12	2:M:178:LEU:HD23	1.91	0.53
1:H:80:MET:HE1	1:H:82:LEU:HB2	1.91	0.52
2:L:132:LEU:HD12	2:L:178:LEU:HD23	1.91	0.51
2:M:149:LYS:HB2	2:M:192:SER:HB2	1.91	0.51
2:M:37:GLN:NE2	5:M:402:HOH:O	2.43	0.51
2:M:113:PRO:HB3	2:M:139:PHE:HB3	1.93	0.51
2:M:32:TYR:CZ	3:Q:305:LYS:HB2	2.45	0.51
1:H:18:VAL:HG13	1:H:82(C):LEU:HD11	1.91	0.50
1:I:30:ALA:HB1	1:I:53:ASP:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:132:LEU:HB2	2:M:178:LEU:HB3	1.93	0.50
2:L:204:LYS:NZ	5:L:413:HOH:O	2.44	0.50
1:I:98:PRO:HD3	1:I:100(M):GLU:HG3	1.94	0.49
2:M:55:PRO:HD2	2:M:58:ILE:HG13	1.94	0.49
1:I:40:ALA:HB3	1:I:43:GLN:HG3	1.96	0.48
2:M:194:GLN:HG2	2:M:203:GLU:HG2	1.95	0.48
2:L:39:LYS:NZ	5:L:404:HOH:O	2.32	0.48
2:L:103:LYS:NZ	5:L:414:HOH:O	2.45	0.47
2:L:184:GLN:HE21	4:L:301:GOL:H2	1.79	0.47
1:H:63:PHE:O	1:H:67:VAL:HG12	2.16	0.46
2:L:167:GLN:NE2	2:L:169:ASN:OD1	2.41	0.46
2:L:28:LEU:N	2:L:29:PRO:HD2	2.30	0.46
2:M:188:HIS:CE1	4:M:305:GOL:H2	2.51	0.46
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.97	0.46
1:H:159:LEU:HD21	1:H:182:VAL:HG11	1.96	0.46
1:I:61:GLN:HG2	2:M:95(B):GLN:HE22	1.81	0.45
1:H:18:VAL:O	1:H:81:GLU:HA	2.16	0.45
2:L:32:TYR:CZ	3:P:305:LYS:HB2	2.50	0.45
2:L:91:ARG:HG2	3:P:308:HIS:CE1	2.52	0.45
1:H:31:LYS:HG3	1:H:32:PHE:CD2	2.51	0.45
2:L:21:ILE:HD12	2:L:102:THR:HG21	1.98	0.45
2:M:60:GLU:CD	2:M:60:GLU:H	2.20	0.44
2:M:156:LYS:N	2:M:156:LYS:HD3	2.31	0.44
2:L:120:PRO:HD3	2:L:132:LEU:HD23	1.99	0.44
2:M:18:THR:HA	2:M:76:SER:HA	2.01	0.43
1:H:82:LEU:HD22	1:H:82(C):LEU:HD23	2.00	0.43
1:H:12:LYS:HG3	1:H:18:VAL:CG1	2.48	0.43
1:I:126:PRO:HD2	1:I:213:PRO:HA	2.01	0.43
1:I:63:PHE:O	1:I:67:VAL:HG12	2.18	0.43
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.53	0.42
1:H:67:VAL:HA	1:H:81:GLU:O	2.18	0.42
1:H:94:ARG:NH2	1:H:100(M):GLU:O	2.53	0.42
1:I:47:TRP:CH2	1:I:49:GLY:HA2	2.54	0.42
1:I:163:VAL:HG22	1:I:182:VAL:HG22	2.01	0.42
1:H:129:LYS:HG2	1:H:129:LYS:H	1.66	0.42
1:I:169:VAL:HB	2:M:162:THR:HG22	2.01	0.42
1:H:85:GLU:HG2	1:H:85:GLU:H	1.63	0.41
1:H:80:MET:CE	1:H:82:LEU:HB2	2.49	0.41
3:Q:306:ARG:HD3	3:Q:318:TYR:HD2	1.86	0.41
1:I:119:PRO:HB3	1:I:145:TYR:HB3	2.03	0.41
2:L:167:GLN:HB2	2:L:169:ASN:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:PRO:HB2	1:I:187:SER:HA	2.03	0.40
3:Q:306:ARG:HD3	3:Q:318:TYR:CD2	2.57	0.40
2:M:41:GLY:HA3	4:M:302:GOL:H2	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	H	232/238 (98%)	224 (97%)	8 (3%)	0	100	100
1	I	231/238 (97%)	220 (95%)	10 (4%)	1 (0%)	34	37
2	L	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	M	208/214 (97%)	204 (98%)	4 (2%)	0	100	100
3	P	11/23 (48%)	10 (91%)	1 (9%)	0	100	100
3	Q	11/23 (48%)	10 (91%)	1 (9%)	0	100	100
All	All	902/950 (95%)	870 (96%)	31 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	100(G)	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	H	198/202 (98%)	189 (96%)	9 (4%)	27	33
1	I	197/202 (98%)	191 (97%)	6 (3%)	41	51
2	L	177/181 (98%)	176 (99%)	1 (1%)	86	92
2	M	177/181 (98%)	174 (98%)	3 (2%)	60	73
3	P	10/19 (53%)	10 (100%)	0	100	100
3	Q	10/19 (53%)	10 (100%)	0	100	100
All	All	769/804 (96%)	750 (98%)	19 (2%)	47	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	VAL
1	H	37	VAL
1	H	43	GLN
1	H	50	TRP
1	H	68	THR
1	H	71	ARG
1	H	73	THR
1	H	80	MET
1	H	100(F)	ASN
2	L	93	THR
1	I	37	VAL
1	I	50	TRP
1	I	71	ARG
1	I	100(E)	ASP
1	I	131	THR
1	I	199	ASN
2	M	30	LYS
2	M	156	LYS
2	M	183	GLU

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

Mol	Chain	Res	Type
2	M	184	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	GOL	M	303	-	5,5,5	0.92	0	5,5,5	1.00	0
4	GOL	H	303	-	5,5,5	0.90	0	5,5,5	1.02	0
4	GOL	L	302	-	5,5,5	0.90	0	5,5,5	1.03	0
4	GOL	M	305	-	5,5,5	0.89	0	5,5,5	1.03	0
4	GOL	M	304	-	5,5,5	0.92	0	5,5,5	1.01	0
4	GOL	H	302	-	5,5,5	0.90	0	5,5,5	1.01	0
4	GOL	L	301	-	5,5,5	0.90	0	5,5,5	1.02	0
4	GOL	M	301	-	5,5,5	0.90	0	5,5,5	1.01	0
4	GOL	H	301	-	5,5,5	0.87	0	5,5,5	1.10	0
4	GOL	M	302	-	5,5,5	0.92	0	5,5,5	1.00	0
4	GOL	I	301	-	5,5,5	0.89	0	5,5,5	1.03	0
4	GOL	L	303	-	5,5,5	0.88	0	5,5,5	1.02	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	M	303	-	-	4/4/4/4	-
4	GOL	H	303	-	-	0/4/4/4	-
4	GOL	L	302	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	M	305	-	-	4/4/4/4	-
4	GOL	M	304	-	-	0/4/4/4	-
4	GOL	H	302	-	-	0/4/4/4	-
4	GOL	L	301	-	-	0/4/4/4	-
4	GOL	M	301	-	-	3/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	M	302	-	-	2/4/4/4	-
4	GOL	I	301	-	-	1/4/4/4	-
4	GOL	L	303	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	303	GOL	C1-C2-C3-O3
4	M	305	GOL	O1-C1-C2-C3
4	M	301	GOL	C1-C2-C3-O3
4	H	301	GOL	O1-C1-C2-C3
4	M	302	GOL	O1-C1-C2-C3
4	L	303	GOL	C1-C2-C3-O3
4	M	305	GOL	O2-C2-C3-O3
4	M	303	GOL	O1-C1-C2-C3
4	M	305	GOL	C1-C2-C3-O3
4	L	303	GOL	O1-C1-C2-C3
4	M	303	GOL	O2-C2-C3-O3
4	M	305	GOL	O1-C1-C2-O2
4	M	301	GOL	O2-C2-C3-O3
4	H	301	GOL	O1-C1-C2-O2
4	M	302	GOL	O1-C1-C2-O2
4	L	303	GOL	O2-C2-C3-O3
4	M	301	GOL	O1-C1-C2-C3
4	M	303	GOL	O1-C1-C2-O2
4	L	303	GOL	O1-C1-C2-O2
4	I	301	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	305	GOL	2	0
4	L	301	GOL	1	0
4	M	302	GOL	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	H	234/238 (98%)	1.36	55 (23%) 0 0	27, 52, 88, 115	0
1	I	233/238 (97%)	1.14	32 (13%) 3 2	26, 47, 78, 114	0
2	L	211/214 (98%)	0.99	30 (14%) 2 2	26, 51, 73, 92	0
2	M	210/214 (98%)	1.08	41 (19%) 1 1	28, 50, 70, 80	0
3	P	13/23 (56%)	2.08	4 (30%) 0 0	67, 73, 88, 94	0
3	Q	13/23 (56%)	1.51	4 (30%) 0 0	63, 67, 84, 85	0
All	All	914/950 (96%)	1.17	166 (18%) 1 1	26, 51, 78, 115	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	100(A)	VAL	11.7
1	I	100(B)	THR	10.0
1	I	100(H)	ALA	9.8
1	I	100(E)	ASP	9.1
1	H	100(F)	ASN	9.0
1	H	100(H)	ALA	8.8
1	H	100(G)	PRO	8.6
1	H	100(E)	ASP	8.5
2	L	1	SER	8.0
1	I	100(G)	PRO	7.8
1	I	100(C)	GLY	7.8
1	H	216	CYS	7.6
1	I	100(F)	ASN	7.6
1	H	100(B)	THR	7.5
1	H	100(C)	GLY	7.4
3	P	318	TYR	7.2
1	H	100(D)	ASN	7.2
1	I	100(I)	PRO	6.4
1	I	100(D)	ASN	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	73	THR	6.3
2	L	2	TYR	6.1
1	I	61	GLN	6.1
2	L	168	SER	5.6
1	H	100(I)	PRO	5.3
1	H	16	ALA	5.3
2	M	152	SER	5.1
1	H	74	SER	5.0
1	I	17	SER	5.0
1	H	82(B)	SER	5.0
2	M	94	SER	4.8
1	H	215	SER	4.8
2	M	2	TYR	4.7
1	H	1	GLN	4.7
1	I	100	THR	4.6
3	P	316	ALA	4.6
2	L	94	SER	4.5
1	H	75	ALA	4.5
2	L	209	THR	4.4
1	H	82(A)	SER	4.4
2	L	57	GLY	4.4
2	L	60	GLU	4.4
1	H	15	GLY	4.3
1	I	75	ALA	4.3
1	I	1	GLN	4.2
2	L	93	THR	4.1
2	L	56	SER	4.1
3	Q	317	PHE	4.0
2	M	93	THR	4.0
1	H	132	SER	3.9
1	I	215	SER	3.9
2	L	3	GLU	3.9
1	H	130	SER	3.9
2	M	15	PRO	3.8
2	L	17	GLN	3.8
2	M	107	GLY	3.8
2	M	106(A)	LEU	3.8
1	I	74	SER	3.8
2	M	17	GLN	3.8
1	I	34	ILE	3.7
2	M	153	SER	3.6
3	Q	318	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	100(A)	VAL	3.5
1	H	100	THR	3.5
2	M	56	SER	3.5
2	M	77	GLY	3.5
2	M	168	SER	3.5
3	Q	306	ARG	3.5
1	H	131	THR	3.4
2	L	107	GLY	3.4
3	P	317	PHE	3.4
2	L	79	HIS	3.3
2	M	183	GLU	3.3
1	H	37	VAL	3.2
2	L	187	SER	3.2
1	H	36	TRP	3.2
2	M	80	VAL	3.2
1	I	73	THR	3.1
1	I	65	ASP	3.1
1	H	57	THR	3.1
1	H	33	ALA	3.0
1	H	172	SER	3.0
2	L	183	GLU	3.0
2	L	109	PRO	2.9
1	H	65	ASP	2.9
1	H	61	GLN	2.9
2	L	115	VAL	2.9
2	M	30	LYS	2.9
1	I	188	SER	2.9
1	H	114	ALA	2.9
1	H	50	TRP	2.8
2	M	202	VAL	2.7
1	H	72	ASP	2.7
1	I	76	SER	2.7
2	L	208	PRO	2.7
2	M	135	LEU	2.7
1	H	3	GLN	2.7
2	M	128	ASN	2.7
2	M	115	VAL	2.6
1	I	36	TRP	2.6
1	H	133	GLY	2.6
2	M	209	THR	2.6
2	M	49	TYR	2.6
2	M	60	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	25	SER	2.6
2	M	78	ALA	2.6
2	M	117	LEU	2.5
1	I	100(L)	PHE	2.5
1	H	30	ALA	2.5
1	H	70	THR	2.5
2	M	66	SER	2.5
2	M	189	ARG	2.5
2	L	106	VAL	2.5
2	M	109	PRO	2.5
1	I	56	LYS	2.5
2	M	33	ALA	2.5
1	H	45	LEU	2.4
2	L	78	ALA	2.4
1	I	72	ASP	2.4
1	H	188	SER	2.4
1	I	92	CYS	2.4
2	L	62	PHE	2.4
2	M	133	VAL	2.4
2	L	54	ARG	2.3
1	H	100(J)	PRO	2.3
2	L	28	LEU	2.3
2	L	15	PRO	2.3
2	M	95	ALA	2.3
1	H	98	PRO	2.3
1	H	95	ALA	2.3
2	M	187	SER	2.3
2	M	14	SER	2.3
2	M	16	GLY	2.3
2	M	96	TRP	2.3
1	H	99	ASP	2.3
1	I	70	THR	2.2
2	L	34	TYR	2.2
1	H	92	CYS	2.2
2	M	8	PRO	2.2
1	H	97	TYR	2.2
2	M	89	TYR	2.2
1	H	64	GLN	2.2
1	I	100(J)	PRO	2.2
2	L	18	THR	2.2
2	M	95(A)	ASN	2.1
1	H	96	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	128	ASN	2.1
2	L	136	ILE	2.1
3	Q	304	ARG	2.1
1	H	101	ASP	2.1
1	H	142	VAL	2.1
2	L	33	ALA	2.1
1	H	100(M)	GLU	2.1
3	P	306	ARG	2.1
1	H	17	SER	2.1
1	H	100(K)	PRO	2.1
2	M	156	LYS	2.1
2	M	81	ASP	2.1
1	H	32	PHE	2.1
1	I	50	TRP	2.1
1	I	54	ASP	2.0
2	M	13	VAL	2.0
2	L	95(A)	ASN	2.0
1	I	64	GLN	2.0
1	I	93	ALA	2.0
2	M	134	CYS	2.0
1	H	28	THR	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 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. 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	B-factors(Å ²)	Q<0.9
4	GOL	M	303	6/6	0.56	0.32	49,57,62,64	0
4	GOL	M	305	6/6	0.59	0.30	56,67,71,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	H	301	6/6	0.59	0.36	45,48,52,52	0
4	GOL	M	304	6/6	0.65	0.29	60,64,70,71	0
4	GOL	H	303	6/6	0.75	0.23	58,61,66,68	0
4	GOL	L	303	6/6	0.77	0.23	47,52,57,63	0
4	GOL	M	302	6/6	0.78	0.27	52,61,61,68	0
4	GOL	M	301	6/6	0.80	0.27	42,47,53,53	0
4	GOL	H	302	6/6	0.86	0.17	38,44,47,50	0
4	GOL	L	301	6/6	0.86	0.20	54,59,61,70	0
4	GOL	L	302	6/6	0.89	0.20	40,41,50,51	0
4	GOL	I	301	6/6	0.92	0.13	48,53,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.