Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:34 am BST

PDB ID	:	4M1D
Title	:	Crystal structure of anti-HIV-1 Fab 447-52D in complex with V3 cyclic peptide MN
Authors	:	Killikelly, A.; Kong, X.P.
Deposited on	:	2013-08-02
Resolution	:	1.80 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:

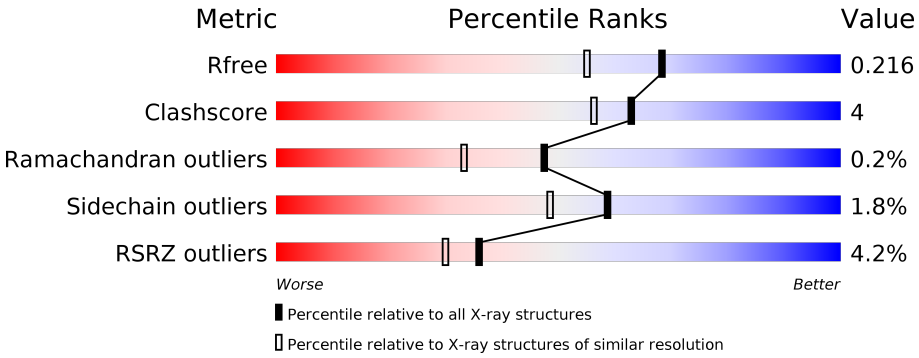
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	L	216	2% 93% 7%
1	M	216	6% 90% 9%
2	H	231	3% 91% 9%
2	I	231	5% 91% 7%
3	P	14	100%
3	Q	14	7% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8039 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 mAb 447-52D Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1603	1007	266	325	5			
1	M	213	Total	C	N	O	S	0	0	0
			1579	994	262	319	4			

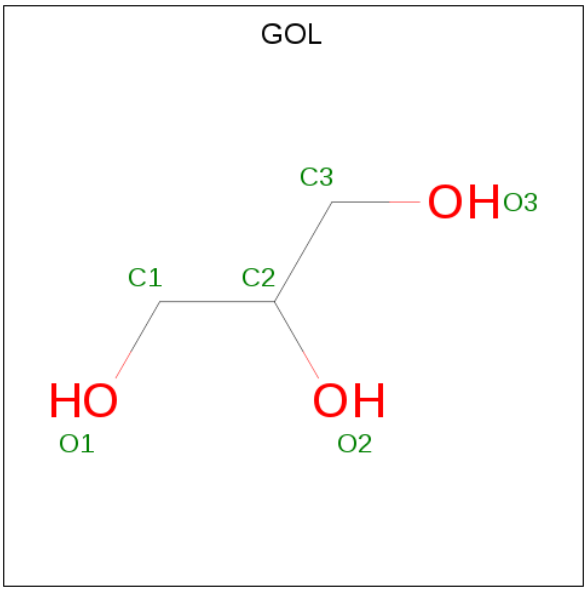
- Molecule 2 is a protein called Fab mAb 447-52D Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	231	Total	C	N	O	S	0	0	0
			1735	1092	290	345	8			
2	I	231	Total	C	N	O	S	0	0	0
			1739	1095	291	345	8			

- Molecule 3 is a protein called Cyclic V3 Arch Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	S	0	0	0
			111	70	22	17	2			
3	Q	14	Total	C	N	O	S	0	0	0
			111	70	22	17	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 5 3 2	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	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	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	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

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

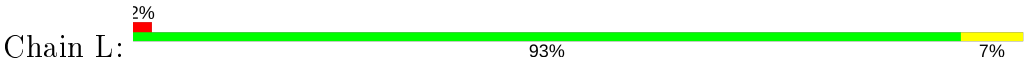
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	291	Total O 291 291	0	0
5	H	311	Total O 311 311	0	0
5	P	18	Total O 18 18	0	0
5	M	213	Total O 213 213	0	0
5	I	213	Total O 213 213	0	0
5	Q	14	Total O 14 14	0	0

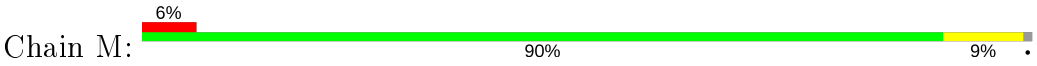
3 Residue-property plots (i)

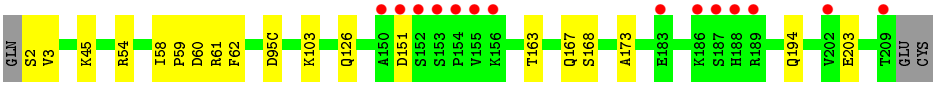
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Fab mAb 447-52D Light Chain

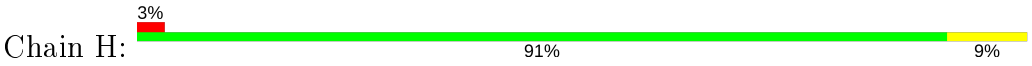


• Molecule 1: Fab mAb 447-52D Light Chain

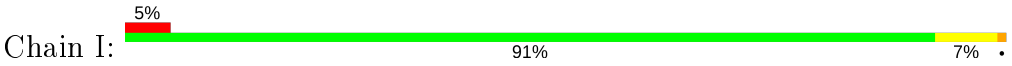


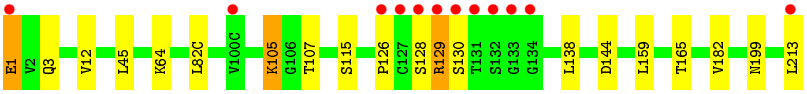


• Molecule 2: Fab mAb 447-52D Heavy Chain



• Molecule 2: Fab mAb 447-52D Heavy Chain



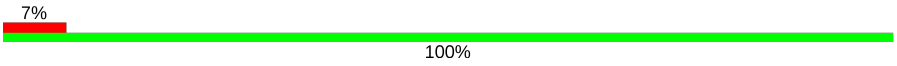


• Molecule 3: Cyclic V3 Arch Peptide

There are no outlier residues recorded for this chain.

• Molecule 3: Cyclic V3 Arch Peptide

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.84Å 59.78Å 137.07Å 90.00° 127.35° 90.00°	Depositor
Resolution (Å)	45.34 – 1.80 45.34 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.34-1.80) 98.9 (45.34-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.216 0.186 , 0.216	Depositor DCC
R_{free} test set	5302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8039	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: 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	L	0.42	0/1644	0.60	0/2247
1	M	0.32	0/1620	0.52	0/2215
2	H	0.40	0/1774	0.60	1/2417 (0.0%)
2	I	0.34	0/1778	0.54	0/2421
3	P	0.45	0/114	0.64	0/151
3	Q	0.37	0/114	0.49	0/151
All	All	0.38	0/7044	0.57	1/9602 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	138	LEU	CA-CB-CG	6.50	130.24	115.30

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	L	1603	0	1556	13	1
1	M	1579	0	1535	14	0
2	H	1735	0	1694	20	0
2	I	1739	0	1706	12	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	111	0	105	0	0
3	Q	111	0	105	0	0
4	H	36	0	48	6	0
4	I	12	0	16	5	0
4	L	35	0	45	6	0
4	M	18	0	24	3	0
5	H	311	0	0	10	4
5	I	213	0	0	3	3
5	L	291	0	0	4	5
5	M	213	0	0	7	3
5	P	18	0	0	0	0
5	Q	14	0	0	0	1
All	All	8039	0	6834	60	9

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 (60) 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:L:54:ARG:NH1	5:L:628:HOH:O	2.06	0.87
1:M:60:ASP:OD2	5:M:569:HOH:O	2.09	0.69
2:H:192:GLN:NE2	5:H:661:HOH:O	1.90	0.68
1:M:45:LYS:HE2	5:M:602:HOH:O	1.92	0.68
2:H:28:THR:H	4:H:302:GOL:H12	1.60	0.67
2:H:115:SER:H	1:M:126:GLN:NE2	1.93	0.66
2:I:144:ASP:OD2	5:I:553:HOH:O	2.14	0.65
1:M:61:ARG:NH2	4:M:303:GOL:O3	2.18	0.65
2:H:100(E):GLU:OE1	5:H:564:HOH:O	2.15	0.64
1:M:61:ARG:HH21	4:M:303:GOL:HO3	1.43	0.64
4:L:302:GOL:H2	5:H:425:HOH:O	1.99	0.62
1:L:126:GLN:NE2	2:I:115:SER:H	1.99	0.61
2:H:27:PHE:HB2	4:H:302:GOL:H11	1.85	0.59
1:L:118:PHE:CE2	1:L:135:LEU:HD12	2.37	0.59
2:H:45:LEU:HB2	4:H:301:GOL:H31	1.84	0.58
2:H:21:THR:HG23	5:H:493:HOH:O	2.03	0.58
2:H:28:THR:H	4:H:302:GOL:C1	2.17	0.57
2:H:199:ASN:OD1	5:H:514:HOH:O	2.18	0.56
1:L:182:PRO:O	1:L:186:LYS:HG2	2.06	0.55
1:L:118:PHE:HE2	1:L:135:LEU:HD12	1.70	0.55
1:L:79:GLN:HE22	4:L:301:GOL:H2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:GLU:O	5:I:588:HOH:O	2.18	0.55
1:L:132:LEU:HD12	1:L:178:LEU:HD23	1.90	0.54
1:M:2:SER:HA	5:M:547:HOH:O	2.07	0.54
2:I:105:LYS:NZ	4:I:302:GOL:H32	2.23	0.53
1:L:20:THR:H	4:L:303:GOL:C3	2.22	0.53
2:I:12:VAL:HG11	2:I:82(C):LEU:HD13	1.90	0.52
4:L:303:GOL:H11	5:L:493:HOH:O	2.09	0.52
2:I:159:LEU:HD21	2:I:182:VAL:HG21	1.92	0.51
2:I:128:SER:O	2:I:130:SER:N	2.43	0.50
2:H:171:GLN:NE2	5:H:646:HOH:O	2.46	0.49
2:I:107:THR:OG1	4:I:302:GOL:H31	2.13	0.49
2:I:126:PRO:HD2	2:I:213:LEU:HD22	1.94	0.48
2:H:171:GLN:CD	5:H:681:HOH:O	2.51	0.48
4:L:302:GOL:H11	2:H:45:LEU:HD13	1.97	0.47
1:M:3:VAL:N	5:M:547:HOH:O	2.24	0.47
1:M:103:LYS:HE2	5:M:595:HOH:O	2.14	0.46
1:L:79:GLN:NE2	4:L:301:GOL:H2	2.29	0.46
2:I:138:LEU:HB3	2:I:213:LEU:HD11	1.98	0.46
1:M:45:LYS:HE3	1:M:58:ILE:HD11	1.98	0.45
2:I:45:LEU:HB2	4:I:301:GOL:H32	1.98	0.45
1:L:54:ARG:NH1	5:L:637:HOH:O	2.27	0.45
1:L:54:ARG:CZ	5:L:628:HOH:O	2.59	0.44
2:H:64:LYS:HG3	5:H:642:HOH:O	2.18	0.44
2:H:71:ARG:HG2	4:H:304:GOL:H31	2.00	0.44
1:L:135:LEU:HD13	2:H:181:VAL:HG11	1.99	0.44
1:M:59:PRO:HG3	4:M:303:GOL:H2	2.00	0.44
4:I:302:GOL:O3	5:I:558:HOH:O	2.00	0.43
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	2.00	0.43
1:M:194:GLN:HG2	1:M:203:GLU:HG3	1.99	0.43
1:M:3:VAL:HG23	5:M:547:HOH:O	2.19	0.42
2:H:171:GLN:NE2	5:H:681:HOH:O	2.53	0.42
2:I:64:LYS:HA	2:I:64:LYS:HD2	1.87	0.42
1:M:167:GLN:OE1	1:M:173:ALA:HB2	2.20	0.42
2:H:71:ARG:HG3	4:H:304:GOL:H12	2.01	0.41
2:H:126:PRO:HG3	5:H:605:HOH:O	2.21	0.41
1:M:54:ARG:HD3	1:M:62:PHE:O	2.19	0.41
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.55	0.41
5:M:421:HOH:O	4:I:301:GOL:H11	2.20	0.41
1:L:19:VAL:HG13	1:L:78:LEU:HD11	2.01	0.41

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:685:HOH:O	5:H:691:HOH:O[4_546]	1.86	0.34
5:L:681:HOH:O	5:I:600:HOH:O[3_556]	1.88	0.32
5:L:630:HOH:O	5:Q:412:HOH:O[3_556]	1.94	0.26
5:H:676:HOH:O	5:M:591:HOH:O[3_556]	2.02	0.18
5:L:672:HOH:O	5:I:601:HOH:O[3_556]	2.05	0.15
5:H:643:HOH:O	5:M:588:HOH:O[3_556]	2.09	0.11
2:I:3:GLN:NE2	5:I:503:HOH:O[4_445]	2.11	0.09
1:L:30:ASN:ND2	5:L:583:HOH:O[4_556]	2.13	0.07
5:H:629:HOH:O	5:M:561:HOH:O[3_556]	2.16	0.04

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	L	214/216 (99%)	203 (95%)	11 (5%)	0	100 100
1	M	211/216 (98%)	204 (97%)	6 (3%)	1 (0%)	29 15
2	H	229/231 (99%)	226 (99%)	3 (1%)	0	100 100
2	I	229/231 (99%)	222 (97%)	6 (3%)	1 (0%)	34 21
3	P	12/14 (86%)	12 (100%)	0	0	100 100
3	Q	12/14 (86%)	12 (100%)	0	0	100 100
All	All	907/922 (98%)	879 (97%)	26 (3%)	2 (0%)	47 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	129	ARG
1	M	151	ASP

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	L	180/180 (100%)	178 (99%)	2 (1%)	73	68
1	M	177/180 (98%)	174 (98%)	3 (2%)	60	51
2	H	195/196 (100%)	191 (98%)	4 (2%)	53	42
2	I	196/196 (100%)	191 (97%)	5 (3%)	46	32
3	P	11/11 (100%)	11 (100%)	0	100	100
3	Q	11/11 (100%)	11 (100%)	0	100	100
All	All	770/774 (100%)	756 (98%)	14 (2%)	59	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	95(C)	ASP
1	L	103	LYS
2	H	76	ASN
2	H	127	CYS
2	H	131	THR
2	H	138	LEU
1	M	95(C)	ASP
1	M	163	THR
1	M	168	SER
2	I	1	GLU
2	I	105	LYS
2	I	129	ARG
2	I	165	THR
2	I	199	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	126	GLN
2	H	76	ASN

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Mol	Chain	Res	Type
1	M	126	GLN
2	I	76	ASN
2	I	164	HIS
2	I	199	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

17 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	L	303	-	3,4,5	0.48	0	1,4,5	0.24	0
4	GOL	H	303	-	5,5,5	0.35	0	5,5,5	0.60	0
4	GOL	H	304	-	5,5,5	0.45	0	5,5,5	0.64	0
4	GOL	M	302	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	H	301	-	5,5,5	0.19	0	5,5,5	0.81	0
4	GOL	L	304	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	I	302	-	5,5,5	0.33	0	5,5,5	0.56	0
4	GOL	M	301	-	5,5,5	0.30	0	5,5,5	0.31	0
4	GOL	L	301	-	5,5,5	0.49	0	5,5,5	0.68	0
4	GOL	I	301	-	5,5,5	0.49	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	L	302	-	5,5,5	0.53	0	5,5,5	0.48	0
4	GOL	L	305	-	5,5,5	0.34	0	5,5,5	0.55	0
4	GOL	H	305	-	5,5,5	0.40	0	5,5,5	0.36	0
4	GOL	L	306	-	5,5,5	0.31	0	5,5,5	0.45	0
4	GOL	H	306	-	5,5,5	0.63	0	5,5,5	0.45	0
4	GOL	H	302	-	5,5,5	0.29	0	5,5,5	0.66	0
4	GOL	M	303	-	5,5,5	0.36	0	5,5,5	0.47	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	GOL	L	303	-	-	2/2/2/4	-
4	GOL	H	303	-	-	0/4/4/4	-
4	GOL	H	304	-	-	2/4/4/4	-
4	GOL	M	302	-	-	2/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	L	304	-	-	2/4/4/4	-
4	GOL	I	302	-	-	4/4/4/4	-
4	GOL	M	301	-	-	2/4/4/4	-
4	GOL	L	301	-	-	4/4/4/4	-
4	GOL	I	301	-	-	4/4/4/4	-
4	GOL	L	302	-	-	2/4/4/4	-
4	GOL	L	305	-	-	2/4/4/4	-
4	GOL	H	305	-	-	2/4/4/4	-
4	GOL	L	306	-	-	2/4/4/4	-
4	GOL	H	306	-	-	2/4/4/4	-
4	GOL	H	302	-	-	0/4/4/4	-
4	GOL	M	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	303	GOL	O1-C1-C2-O2
4	L	303	GOL	O1-C1-C2-C3
4	H	304	GOL	C1-C2-C3-O3
4	H	301	GOL	C1-C2-C3-O3
4	L	304	GOL	O1-C1-C2-C3
4	I	302	GOL	O1-C1-C2-C3
4	L	301	GOL	C1-C2-C3-O3
4	I	301	GOL	O1-C1-C2-C3
4	L	305	GOL	O1-C1-C2-C3
4	H	305	GOL	O1-C1-C2-C3
4	L	306	GOL	O1-C1-C2-O2
4	M	303	GOL	O1-C1-C2-C3
4	L	301	GOL	O2-C2-C3-O3
4	M	302	GOL	O1-C1-C2-C3
4	I	302	GOL	C1-C2-C3-O3
4	M	301	GOL	O1-C1-C2-C3
4	L	301	GOL	O1-C1-C2-C3
4	L	306	GOL	O1-C1-C2-C3
4	H	306	GOL	C1-C2-C3-O3
4	H	304	GOL	O2-C2-C3-O3
4	H	301	GOL	O2-C2-C3-O3
4	L	304	GOL	O1-C1-C2-O2
4	I	302	GOL	O1-C1-C2-O2
4	I	302	GOL	O2-C2-C3-O3
4	I	301	GOL	O1-C1-C2-O2
4	L	305	GOL	O1-C1-C2-O2
4	M	303	GOL	O1-C1-C2-O2
4	M	301	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-O2
4	H	305	GOL	O1-C1-C2-O2
4	H	306	GOL	O2-C2-C3-O3
4	L	302	GOL	O1-C1-C2-O2
4	M	302	GOL	O1-C1-C2-O2
4	I	301	GOL	C1-C2-C3-O3
4	L	302	GOL	O1-C1-C2-C3
4	I	301	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	303	GOL	2	0
4	H	304	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	GOL	1	0
4	I	302	GOL	3	0
4	L	301	GOL	2	0
4	I	301	GOL	2	0
4	L	302	GOL	2	0
4	H	302	GOL	3	0
4	M	303	GOL	3	0

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

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	L	216/216 (100%)	0.05	5 (2%) 60 56	7, 20, 44, 66	0
1	M	213/216 (98%)	0.09	14 (6%) 18 14	13, 30, 51, 70	0
2	H	231/231 (100%)	-0.04	7 (3%) 50 44	8, 23, 43, 55	0
2	I	231/231 (100%)	-0.05	12 (5%) 27 22	14, 28, 50, 101	0
3	P	14/14 (100%)	0.63	0 100 100	9, 13, 31, 32	0
3	Q	14/14 (100%)	0.08	1 (7%) 16 12	17, 24, 34, 37	0
All	All	919/922 (99%)	0.02	39 (4%) 36 30	7, 26, 47, 101	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	131	THR	8.0
2	I	130	SER	6.8
2	H	127	CYS	6.8
1	L	211	CYS	5.6
2	I	127	CYS	5.4
2	H	128	SER	4.8
1	L	209	THR	4.4
2	H	132	SER	4.0
2	H	131	THR	3.9
1	L	210	GLU	3.9
2	I	126	PRO	3.9
1	M	155	VAL	3.8
1	M	209	THR	3.8
1	L	1	GLN	3.7
3	Q	320	CYS	3.6
1	M	189	ARG	3.5
2	I	129	ARG	3.3
1	M	187	SER	3.2
2	I	213	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	151	ASP	3.1
2	I	133	GLY	3.1
1	M	150	ALA	3.0
1	M	156	LYS	3.0
2	I	128	SER	3.0
2	I	1	GLU	3.0
1	M	186	LYS	2.8
1	M	154	PRO	2.7
1	M	152	SER	2.6
2	I	100(C)	VAL	2.5
1	M	188	HIS	2.3
2	H	133	GLY	2.2
1	M	153	SER	2.2
1	M	183	GLU	2.2
2	H	126	PRO	2.2
2	H	129	ARG	2.2
2	I	132	SER	2.2
2	I	134	GLY	2.2
1	M	202	VAL	2.2
1	L	168	SER	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, 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	GOL	L	301	6/6	0.79	0.25	26,27,40,47	0
4	GOL	L	303	5/6	0.80	0.20	10,33,35,36	0
4	GOL	M	302	6/6	0.84	0.14	39,41,43,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	L	305	6/6	0.85	0.21	22,29,40,41	0
4	GOL	H	302	6/6	0.86	0.15	21,30,34,40	0
4	GOL	M	303	6/6	0.86	0.17	37,43,47,55	0
4	GOL	M	301	6/6	0.87	0.14	31,34,37,40	0
4	GOL	L	306	6/6	0.87	0.16	21,27,41,42	0
4	GOL	H	304	6/6	0.88	0.27	21,22,27,29	0
4	GOL	I	301	6/6	0.88	0.20	23,33,41,45	0
4	GOL	I	302	6/6	0.89	0.10	33,34,43,46	0
4	GOL	H	306	6/6	0.89	0.18	26,30,35,38	0
4	GOL	L	302	6/6	0.90	0.14	29,32,34,37	0
4	GOL	H	303	6/6	0.94	0.10	14,20,22,28	0
4	GOL	H	301	6/6	0.94	0.10	17,27,32,33	0
4	GOL	L	304	6/6	0.94	0.10	19,24,31,37	0
4	GOL	H	305	6/6	0.94	0.08	26,33,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.