wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 04:46 AM EST

PDB ID	:	3O3A
Title	:	Human Class I MHC HLA-A2 in complex with the Peptidomimetic ELA-1
Authors	:	Borbulevych, O.Y.; Baker, B.M.
Deposited on	:	2010-07-23
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

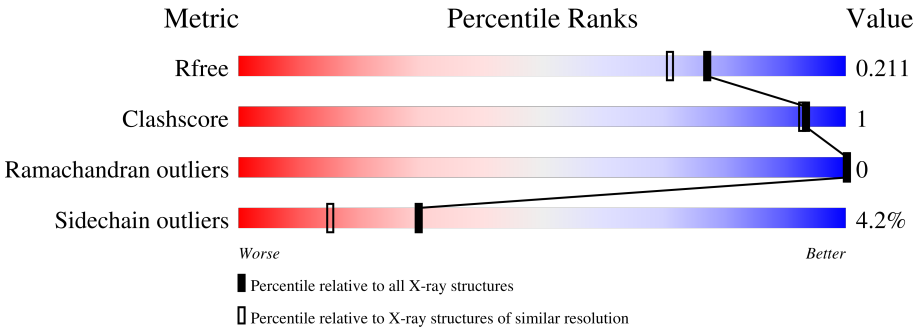
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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)

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%

Mol	Chain	Length	Quality of chain
1	A	275	96% · ·
1	D	275	93% 5% ·
2	B	100	94% 6%
2	E	100	93% 6% ·
3	C	8	62% 25% 12%
3	F	8	50% 25% 25%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7141 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	6	0
			2268	1418	412	429	9			
1	D	275	Total	C	N	O	S	0	10	0
			2282	1425	414	434	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	2	0
			845	538	141	161	5			
2	E	100	Total	C	N	O	S	0	1	0
			841	536	141	159	5			

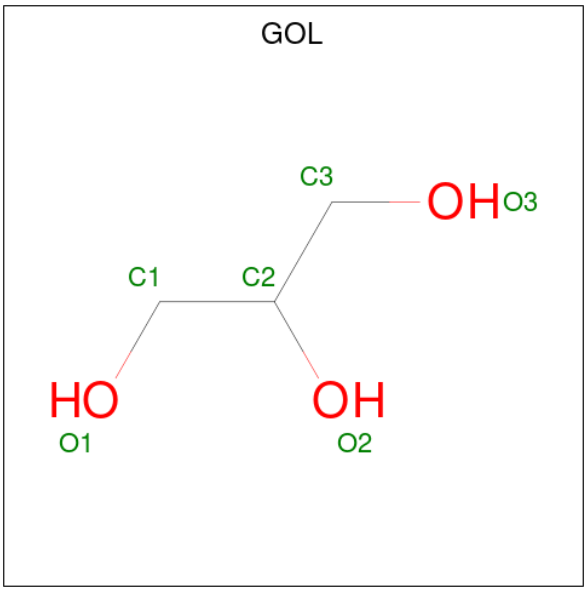
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Peptidomimetic ELA-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			70	49	10	11			
3	F	8	Total	C	N	O	0	1	0
			73	51	10	12			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	B	109	Total O 109 109	0	0
5	C	3	Total O 3 3	0	0

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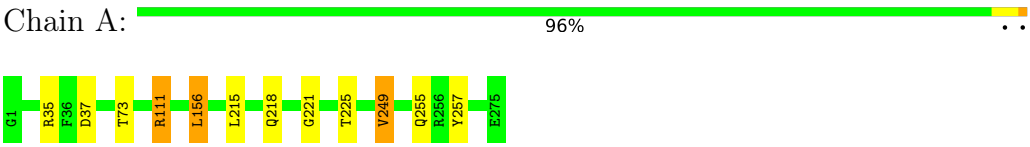
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	252	Total O 252 252	0	0
5	E	116	Total O 116 116	0	0
5	F	4	Total O 4 4	0	0

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. 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. 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.

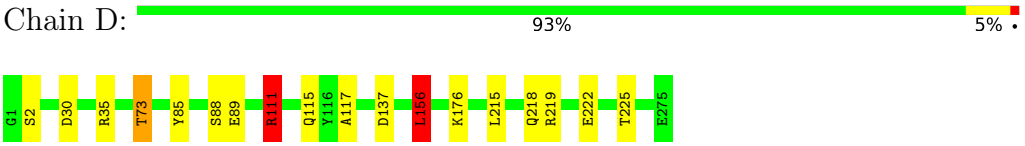
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



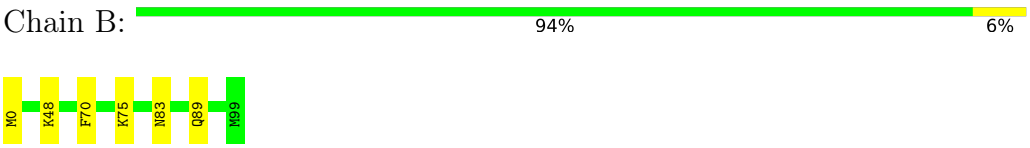
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain D:



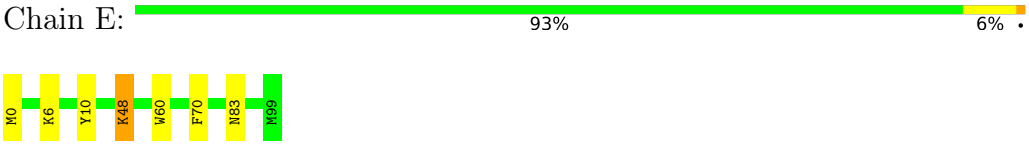
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain E:

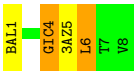


• Molecule 3: Peptidomimetic ELA-1

Chain C:

• Molecule 3: Peptidomimetic ELA-1

Chain F:


BAL1
G1C4
3A25
L6
T7
V8

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.21Å 84.22Å 83.95Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.80) 99.5 (19.82-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.212 0.192 , 0.211	Depositor DCC
R_{free} test set	3786 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.009 for -h,l,k 0.138 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7141	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: 3AZ, GOL, GIC, BAL

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	A	0.78	0/2357	0.87	5/3198 (0.2%)
1	D	0.80	0/2387	0.88	2/3240 (0.1%)
2	B	0.81	0/876	0.85	0/1183
2	E	0.85	1/868 (0.1%)	0.81	0/1172
3	C	0.90	0/34	0.91	0/43
3	F	0.95	0/41	0.88	0/53
All	All	0.81	1/6563 (0.0%)	0.87	7/8889 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10	TYR	CD2-CE2	5.64	1.47	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	111	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	37	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	249	VAL	CG1-CB-CG2	7.25	122.49	110.90
1	A	111	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	249	VAL	CA-CB-CG1	5.44	119.06	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	1	BAL	Peptide

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	A	2268	0	2122	4	0
1	D	2282	0	2127	11	0
2	B	845	0	806	1	0
2	E	841	0	806	2	0
3	C	70	0	62	1	0
3	F	73	0	65	2	0
4	A	18	0	24	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	18	0	24	1	0
4	F	6	0	8	0	0
5	A	224	0	0	0	0
5	B	109	0	0	1	0
5	C	3	0	0	0	0
5	D	252	0	0	2	0
5	E	116	0	0	0	0
5	F	4	0	0	0	0
All	All	7141	0	6060	18	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 1.

The worst 5 of 18 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:D:111:ARG:HH21	1:D:111:ARG:HG2	1.64	0.62
1:D:30:ASP:OD1	4:D:276:GOL:H31	2.01	0.60
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:NZ	5:B:648:HOH:O	2.38	0.57
1:A:156:LEU:HD13	3:C:4:GIC:H10	1.87	0.56

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	A	279/275 (102%)	275 (99%)	4 (1%)	0	100	100
1	D	283/275 (103%)	279 (99%)	4 (1%)	0	100	100
2	B	99/100 (99%)	99 (100%)	0	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	4/8 (50%)	4 (100%)	0	0	100	100
3	F	5/8 (62%)	4 (80%)	1 (20%)	0	100	100
All	All	768/766 (100%)	758 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	237/231 (103%)	230 (97%)	7 (3%)	41	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	241/231 (104%)	232 (96%)	9 (4%)	34 19
2	B	97/95 (102%)	91 (94%)	6 (6%)	18 6
2	E	96/95 (101%)	90 (94%)	6 (6%)	18 6
3	C	4/4 (100%)	3 (75%)	1 (25%)	0 0
3	F	5/4 (125%)	4 (80%)	1 (20%)	1 0
All	All	680/660 (103%)	650 (96%)	30 (4%)	30 14

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	SER
2	E	70	PHE
1	D	111	ARG
3	F	6	LEU
2	E	0[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	218	GLN
1	D	255	GLN
2	E	83	ASN
1	D	72	GLN
1	D	115	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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BAL	F	1	3	4,4,5	0.60	0	3,3,5	0.53	0
3	3AZ	C	5	3	10,10,11	0.47	0	12,12,14	1.75	3 (25%)
3	3AZ	F	5	3	10,10,11	0.35	0	12,12,14	2.12	4 (33%)
3	GIC	F	4	3	19,20,21	1.44	1 (5%)	19,26,28	2.33	8 (42%)
3	GIC	C	4	3	19,20,21	1.45	1 (5%)	19,26,28	2.05	8 (42%)
3	BAL	C	1	3	4,4,5	0.71	0	3,3,5	0.70	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
3	BAL	F	1	3	-	0/1/2/3	-
3	3AZ	C	5	3	-	2/4/4/6	0/1/1/1
3	3AZ	F	5	3	-	2/4/4/6	0/1/1/1
3	GIC	F	4	3	-	5/13/14/15	0/2/2/2
3	GIC	C	4	3	-	11/13/14/15	0/2/2/2
3	BAL	C	1	3	-	0/1/2/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	GIC	C1-N1	-5.09	1.33	1.47
3	C	4	GIC	C1-N1	-4.94	1.34	1.47

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	GIC	O1-C3-C4	-5.19	113.14	121.60
3	C	4	GIC	C5-C4-C3	4.69	119.79	112.49
3	F	5	3AZ	O-C-C3	-4.37	110.44	124.59
3	F	4	GIC	C2-C1-N1	4.27	121.20	113.11
3	F	5	3AZ	C3-C2-C1	-4.21	116.54	121.64

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	GIC	C2-C1-N1-C3
3	C	4	GIC	C4-C3-N1-CC
3	C	4	GIC	C-CC-N1-C3
3	C	4	GIC	N1-C1-C2-N
3	F	4	GIC	C-CC-N1-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	GIC	1	0
3	C	4	GIC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	A	276	-	5,5,5	0.48	0	5,5,5	1.30	1 (20%)
4	GOL	D	276	-	5,5,5	0.45	0	5,5,5	1.10	1 (20%)
4	GOL	A	277	-	5,5,5	0.36	0	5,5,5	0.60	0
4	GOL	A	278	-	5,5,5	0.28	0	5,5,5	0.71	0
4	GOL	D	278	-	5,5,5	0.35	0	5,5,5	0.57	0
4	GOL	D	277	-	5,5,5	0.44	0	5,5,5	0.69	0
4	GOL	C	9	-	5,5,5	0.37	0	5,5,5	0.51	0
4	GOL	F	9	-	5,5,5	0.29	0	5,5,5	0.80	0
4	GOL	B	100	-	5,5,5	0.40	0	5,5,5	1.14	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	A	276	-	-	1/4/4/4	-
4	GOL	D	276	-	-	0/4/4/4	-
4	GOL	A	277	-	-	0/4/4/4	-
4	GOL	A	278	-	-	4/4/4/4	-
4	GOL	D	278	-	-	1/4/4/4	-
4	GOL	D	277	-	-	4/4/4/4	-
4	GOL	C	9	-	-	3/4/4/4	-
4	GOL	F	9	-	-	2/4/4/4	-
4	GOL	B	100	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	276	GOL	C3-C2-C1	-2.38	102.45	111.70
4	D	276	GOL	C3-C2-C1	-2.08	103.60	111.70

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	100	GOL	C1-C2-C3-O3
4	C	9	GOL	C1-C2-C3-O3
4	D	277	GOL	O1-C1-C2-C3
4	D	277	GOL	C1-C2-C3-O3
4	F	9	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	276	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.