



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 12:22 AM EST

PDB ID : 3O3B  
Title : Human Class I MHC HLA-A2 in complex with the Peptidomimetic ELA-1.1  
Authors : Borbulevych, O.Y.; Baker, B.M.  
Deposited on : 2010-07-23  
Resolution : 1.90 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](mailto: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>.

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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 : 2.36  
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

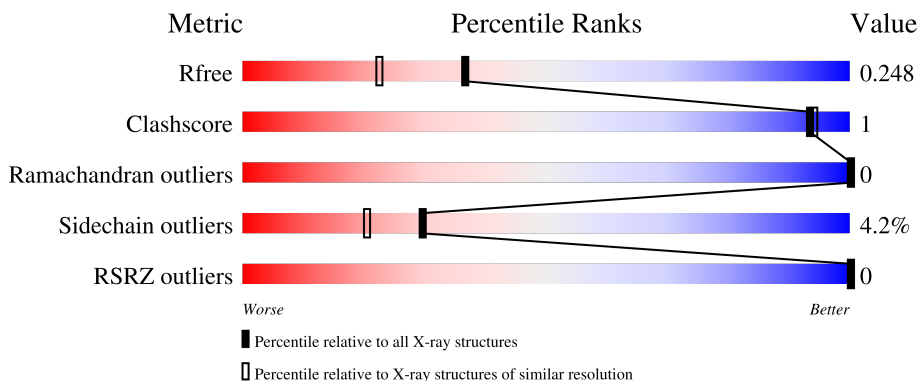
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	A	275	94% (green), 5% (yellow), 5% (orange), 0% (red)
1	D	275	92% (green), 7% (yellow), 0% (orange), 0% (red)
2	B	100	94% (green), 6% (yellow), 0% (orange), 0% (red)
2	E	100	93% (green), 7% (yellow), 0% (orange), 0% (red)
3	C	8	62% (green), 25% (yellow), 12% (orange), 0% (red)

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Mol	Chain	Length	Quality of chain
3	F	8	 62% 25% 12%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7077 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
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	11	0
			2289	1433	414	433	9			
1	D	275	Total	C	N	O	S	0	12	0
			2289	1430	414	436	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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-1.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	Total	C	N	O	0	0	0
			74	51	10	13			
3	F	8	Total	C	N	O	0	1	0
			74	51	10	13			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 12 6 6	0	1
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	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	E	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	212	Total O 212 212	0	0
5	B	87	Total O 87 87	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	C	5	Total O 5 5	0	0
5	D	199	Total O 199 199	0	0
5	E	88	Total O 88 88	0	0
5	F	8	Total O 8 8	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: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:  94% 5%



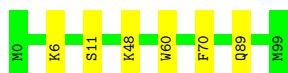
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain D:  92% 7%



- Molecule 2: Beta-2-microglobulin

Chain B:  94% 6%



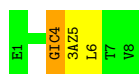
- Molecule 2: Beta-2-microglobulin

Chain E:  93% 7%



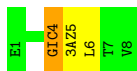
- Molecule 3: Peptidomimetic ELA-1.1

Chain C:  62% 25% 12%



- Molecule 3: Peptidomimetic ELA-1.1

Chain F:  62% 25% 12%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.12Å 84.25Å 83.95Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-1.90) 96.7 (19.82-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.186 , 0.238 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	3116 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 13.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for -h,-l,-k 0.011 for -h,l,k 0.179 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3AZ, GOL, GIC

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	0.87	0/2393	0.91	5/3248 (0.2%)
1	D	0.86	0/2400	0.90	4/3258 (0.1%)
2	B	0.83	0/876	0.84	0/1183
2	E	0.87	0/868	0.87	2/1172 (0.2%)
3	C	0.81	0/43	0.96	0/55
3	F	1.13	0/43	1.06	0/55
All	All	0.86	0/6623	0.89	11/8971 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	111	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	D	37	ASP	CB-CG-OD1	7.96	125.47	118.30
1	A	6	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	121	LYS	CD-CE-NZ	5.95	125.39	111.70
2	E	59	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	37	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	111	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	A	6	ARG	NE-CZ-NH1	-5.38	117.61	120.30
2	E	96	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	37	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	170	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	A	2289	0	2155	7	0
1	D	2289	0	2139	9	0
2	B	845	0	806	2	0
2	E	841	0	806	1	0
3	C	74	0	65	1	0
3	F	74	0	62	1	0
4	A	36	0	48	4	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
5	A	212	0	0	0	0
5	B	87	0	0	0	0
5	C	5	0	0	0	0
5	D	199	0	0	3	0
5	E	88	0	0	0	0
5	F	8	0	0	1	0
All	All	7077	0	6121	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.

All (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:274:TRP:O	5:D:343:HOH:O	2.17	0.58
1:D:73:THR:HG23	5:D:367:HOH:O	2.07	0.53
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.52
1:A:156:LEU:HD13	3:C:4:GIC:H10	1.91	0.52
1:A:234:ARG:HH22	4:A:278:GOL:H2	1.76	0.51
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.95	0.49
1:A:234:ARG:HH12	4:A:278:GOL:H2	1.77	0.49
1:A:6:ARG:NH1	1:A:102:ASP:OD1	2.48	0.47
1:D:216[B]:THR:HG23	5:D:285:HOH:O	2.15	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:GIC:H6	5:F:274:HOH:O	2.17	0.44
1:D:88[B]:SER:OG	1:D:89:GLU:N	2.51	0.44
1:D:11[A]:SER:HB3	1:D:95[A]:VAL:CG2	2.49	0.42
4:A:276:GOL:H31	2:B:11:SER:O	2.19	0.42
1:A:249[A]:VAL:HG22	1:A:257:TYR:CZ	2.56	0.41
1:A:234:ARG:HH12	4:A:278:GOL:C2	2.34	0.40
1:D:111:ARG:HG2	1:D:111:ARG:HH21	1.86	0.40
1:D:255:GLN:H	1:D:255:GLN:NE2	2.20	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	A	284/275 (103%)	280 (99%)	4 (1%)	0	100	100
1	D	285/275 (104%)	280 (98%)	5 (2%)	0	100	100
2	B	99/100 (99%)	97 (98%)	2 (2%)	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	4/8 (50%)	4 (100%)	0	0	100	100
All	All	774/766 (101%)	762 (98%)	12 (2%)	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	242/231 (105%)	234 (97%)	8 (3%)	38	29
1	D	243/231 (105%)	232 (96%)	11 (4%)	27	18
2	B	97/95 (102%)	93 (96%)	4 (4%)	30	21
2	E	96/95 (101%)	91 (95%)	5 (5%)	23	14
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	0
3	F	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	688/662 (104%)	658 (96%)	30 (4%)	30	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	82	ARG
1	A	111	ARG
1	A	156	LEU
1	A	177	GLU
1	A	215	LEU
1	A	225	THR
1	A	255	GLN
2	B	6	LYS
2	B	48	LYS
2	B	70	PHE
2	B	89	GLN
3	C	6	LEU
1	D	2	SER
1	D	35	ARG
1	D	67	VAL
1	D	72	GLN
1	D	73	THR
1	D	105	SER
1	D	156	LEU
1	D	225[A]	THR
1	D	225[B]	THR
1	D	255	GLN
1	D	268	LYS
2	E	0[A]	MET
2	E	0[B]	MET
2	E	6	LYS

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Mol	Chain	Res	Type
2	E	48	LYS
2	E	70	PHE
3	F	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
2	B	13	HIS
1	D	72	GLN
1	D	115	GLN
1	D	255	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](#)

4 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	GIC	C	4	3	19,20,21	1.54	2 (10%)	19,26,28	1.73	4 (21%)
3	3AZ	F	5	3	10,10,11	0.42	0	12,12,14	1.92	3 (25%)
3	3AZ	C	5	3	10,10,11	0.64	0	12,12,14	1.87	3 (25%)
3	GIC	F	4	3	19,20,21	1.54	1 (5%)	19,26,28	2.17	8 (42%)

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
3	GIC	C	4	3	-	8/13/14/15	0/2/2/2
3	3AZ	F	5	3	-	2/4/4/6	0/1/1/1
3	3AZ	C	5	3	-	2/4/4/6	0/1/1/1
3	GIC	F	4	3	-	4/13/14/15	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	GIC	C1-N1	-5.31	1.33	1.47
3	F	4	GIC	C1-N1	-5.02	1.34	1.47
3	C	4	GIC	C4-C3	2.56	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	3AZ	O-C-C3	-4.88	108.79	124.59
3	F	4	GIC	C2-C1-N1	4.36	121.37	113.11
3	F	4	GIC	O1-C3-C4	-4.02	115.05	121.60
3	F	5	3AZ	O-C-C3	-3.97	111.74	124.59
3	F	5	3AZ	C3-C2-C1	-3.57	117.31	121.64
3	F	4	GIC	C1-N1-C3	3.41	133.09	121.03
3	C	4	GIC	C5-C4-C3	3.26	117.57	112.49
3	C	4	GIC	C2-C1-N1	3.23	119.23	113.11
3	F	4	GIC	C4-C3-N1	3.14	123.20	117.74
3	C	4	GIC	C4-C5-C12	3.10	132.58	126.50
3	F	5	3AZ	C6-C1-C2	3.06	122.83	118.54
3	F	4	GIC	C5-C4-C3	2.48	116.35	112.49
3	F	4	GIC	C1-C2-N	2.46	120.77	112.69
3	C	4	GIC	O-C-CC	-2.42	119.09	126.39
3	F	4	GIC	CC-N1-C1	-2.33	113.75	117.06
3	C	5	3AZ	C3-C2-C1	-2.27	118.90	121.64
3	C	5	3AZ	C4-C3-C2	2.16	121.41	118.71
3	F	4	GIC	O-C-CC	-2.09	120.06	126.39

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	GIC	C2-C1-N1-C3
3	C	4	GIC	O1-C3-N1-C1
3	C	4	GIC	C4-C3-N1-C1

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Mol	Chain	Res	Type	Atoms
3	C	4	GIC	C-CC-N1-C3
3	F	4	GIC	C2-C1-N1-C3
3	F	4	GIC	C-CC-N1-C3
3	F	4	GIC	N1-C1-C2-N
3	C	4	GIC	O1-C3-N1-CC
3	F	5	3AZ	O-C-C3-C2
3	C	4	GIC	C4-C3-N1-CC
3	C	5	3AZ	O-C-C3-C2
3	C	4	GIC	C2-C1-N1-CC
3	F	5	3AZ	O-C-C3-C4
3	C	5	3AZ	O-C-C3-C4
3	F	4	GIC	C2-C1-N1-CC
3	C	4	GIC	C-CC-N1-C1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	279	-	5,5,5	0.30	0	5,5,5	1.09	0
4	GOL	A	277[A]	-	5,5,5	0.42	0	5,5,5	0.67	0
4	GOL	A	280	-	5,5,5	0.27	0	5,5,5	1.03	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	D	276	-	5,5,5	0.44	0	5,5,5	1.16	0
4	GOL	A	278	-	5,5,5	0.64	0	5,5,5	0.91	0
4	GOL	F	9	-	5,5,5	0.37	0	5,5,5	0.78	0
4	GOL	A	277[B]	-	5,5,5	0.41	0	5,5,5	0.63	0
4	GOL	E	100	-	5,5,5	0.75	0	5,5,5	2.00	1 (20%)
4	GOL	A	276	-	5,5,5	0.38	0	5,5,5	1.36	1 (20%)
4	GOL	C	9	-	5,5,5	0.37	0	5,5,5	0.72	0
4	GOL	D	277	-	5,5,5	0.29	0	5,5,5	0.49	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	279	-	-	3/4/4/4	-
4	GOL	A	277[A]	-	-	2/4/4/4	-
4	GOL	A	280	-	-	0/4/4/4	-
4	GOL	D	276	-	-	0/4/4/4	-
4	GOL	A	278	-	-	1/4/4/4	-
4	GOL	F	9	-	-	2/4/4/4	-
4	GOL	A	277[B]	-	-	2/4/4/4	-
4	GOL	E	100	-	-	2/4/4/4	-
4	GOL	A	276	-	-	2/4/4/4	-
4	GOL	C	9	-	-	4/4/4/4	-
4	GOL	D	277	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	100	GOL	O3-C3-C2	-3.88	91.60	110.20
4	A	276	GOL	O3-C3-C2	2.06	120.07	110.20

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	277[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	278	GOL	O1-C1-C2-C3
4	A	279	GOL	O1-C1-C2-C3
4	C	9	GOL	O1-C1-C2-C3
4	C	9	GOL	C1-C2-C3-O3
4	E	100	GOL	O1-C1-C2-C3
4	F	9	GOL	O1-C1-C2-C3
4	C	9	GOL	O1-C1-C2-O2
4	A	276	GOL	C1-C2-C3-O3
4	A	277[A]	GOL	C1-C2-C3-O3
4	A	279	GOL	O1-C1-C2-O2
4	A	276	GOL	O2-C2-C3-O3
4	A	277[B]	GOL	O1-C1-C2-O2
4	A	279	GOL	O2-C2-C3-O3
4	C	9	GOL	O2-C2-C3-O3
4	F	9	GOL	O1-C1-C2-O2
4	A	277[A]	GOL	O2-C2-C3-O3
4	E	100	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	278	GOL	3	0
4	A	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/275 (100%)	-0.26	0 100 100	9, 19, 33, 47	0
1	D	275/275 (100%)	-0.26	0 100 100	10, 18, 34, 44	0
2	B	100/100 (100%)	-0.33	0 100 100	10, 18, 35, 42	0
2	E	100/100 (100%)	-0.34	0 100 100	10, 18, 31, 37	0
3	C	6/8 (75%)	-0.31	0 100 100	16, 19, 24, 26	0
3	F	6/8 (75%)	-0.18	0 100 100	13, 18, 23, 27	0
All	All	762/766 (99%)	-0.28	0 100 100	9, 18, 34, 47	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GIC	C	4	19/20	0.84	0.20	28,39,52,53	0
3	GIC	F	4	19/20	0.86	0.15	26,35,44,45	0
3	3AZ	C	5	10/11	0.90	0.13	30,34,36,36	0
3	3AZ	F	5	10/11	0.92	0.15	28,32,33,35	0

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	A	278	6/6	0.80	0.30	38,40,44,45	0
4	GOL	E	100	6/6	0.84	0.22	41,48,49,51	0
4	GOL	C	9	6/6	0.87	0.18	38,41,42,44	0
4	GOL	A	280	6/6	0.88	0.19	32,35,38,40	0
4	GOL	A	277[B]	6/6	0.88	0.22	34,36,37,37	6
4	GOL	A	277[A]	6/6	0.88	0.22	25,26,27,27	6
4	GOL	A	276	6/6	0.93	0.09	33,34,35,35	0
4	GOL	D	277	6/6	0.94	0.10	24,30,31,31	0
4	GOL	A	279	6/6	0.94	0.10	26,27,29,31	0
4	GOL	D	276	6/6	0.95	0.15	30,34,35,39	0
4	GOL	F	9	6/6	0.95	0.15	33,35,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.