



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:57 am BST

PDB ID : 1TVB  
Title : Crystal structure of Melanoma Antigen gp100(209-217) Bound to Human Class I MHC HLA-A2  
Authors : Borbulevych, O.Y.; Baker, B.M.  
Deposited on : 2004-06-29  
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](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 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

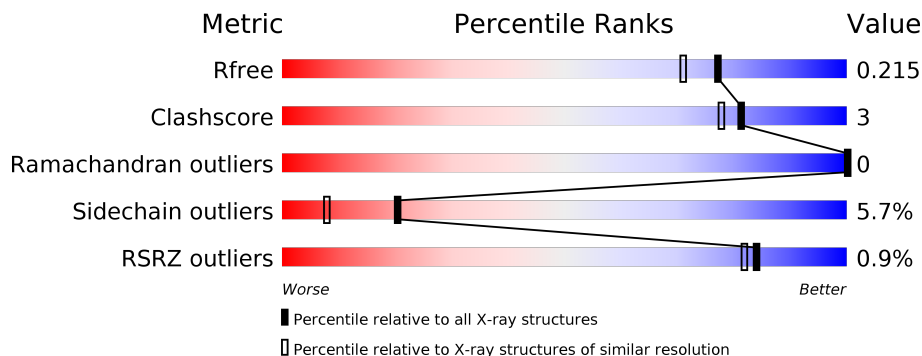
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 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	
1	D	275	
2	B	100	
2	E	100	
3	C	9	
3	F	9	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7378 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	2253	1407	409	427	10	0	2	0
1	D	275	2247	1403	409	426	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0
2	E	100	837	533	141	159	4	0	0	0

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 epitope of Melanocyte protein Pmel 17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	71	46	10	15	0	0	0
3	F	9	71	46	10	15	0	0	0

- 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 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	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	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	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0

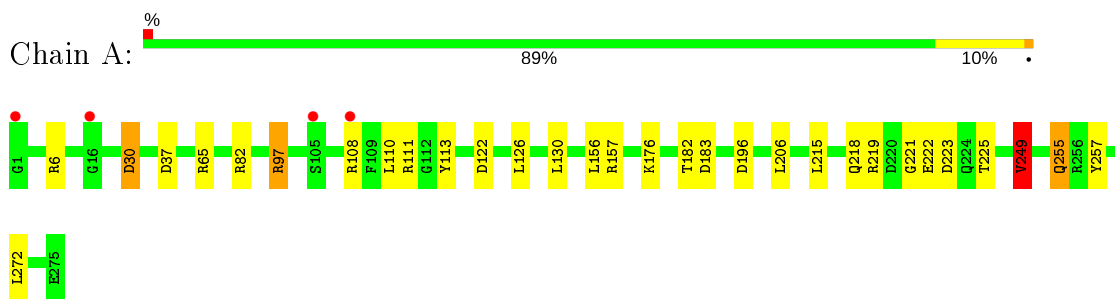
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	312	Total 312	O 312	0	0
5	B	147	Total 147	O 147	0	0
5	C	10	Total 10	O 10	0	0
5	D	307	Total 307	O 307	0	0
5	E	138	Total 138	O 138	0	0
5	F	16	Total 16	O 16	0	0

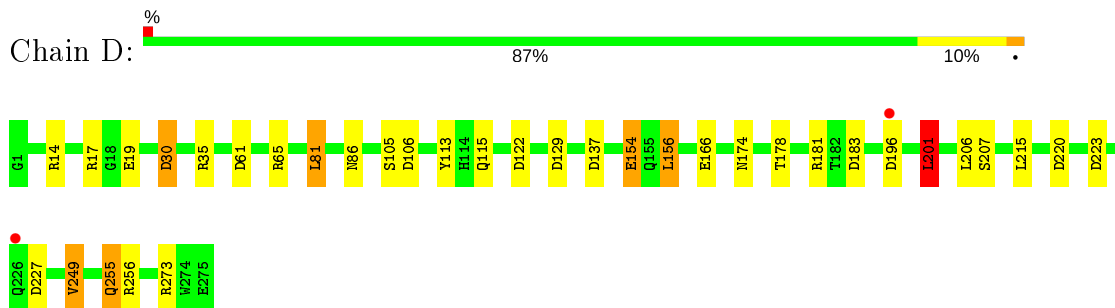
### 3 Residue-property plots [i](#)

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.

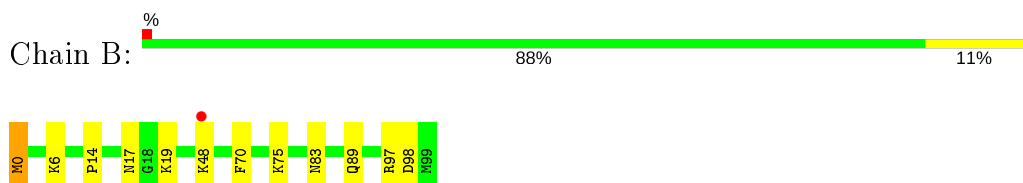
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



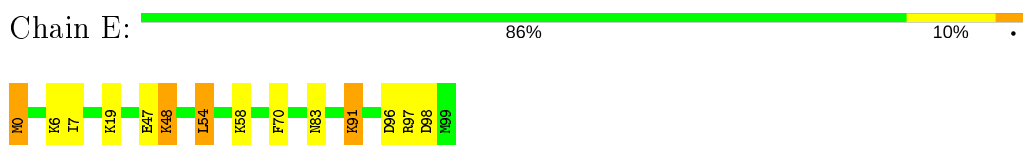
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: epitope of Melanocyte protein Pmel 17

Chain C:  89% 11%



- Molecule 3: epitope of Melanocyte protein Pmel 17

Chain F:  78% 22%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.39Å 84.45Å 84.02Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 9.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-1.80) 99.0 (9.96-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.165 , 0.216 0.166 , 0.215	Depositor DCC
$R_{free}$ test set	3748 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.002 for -h,l,k 0.129 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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:  
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	A	0.87	1/2326 (0.0%)	1.06	13/3155 (0.4%)
1	D	0.82	0/2312	1.09	17/3137 (0.5%)
2	B	0.88	0/860	0.97	2/1162 (0.2%)
2	E	0.86	1/860 (0.1%)	1.06	5/1162 (0.4%)
3	C	0.94	0/72	1.12	1/97 (1.0%)
3	F	0.86	0/72	1.09	1/97 (1.0%)
All	All	0.85	2/6502 (0.0%)	1.06	39/8810 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	CB-CG	-6.26	1.35	1.52
2	E	91	LYS	CE-NZ	5.37	1.62	1.49

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	223	ASP	CB-CG-OD2	8.75	126.18	118.30
1	A	249	VAL	CG1-CB-CG2	7.77	123.34	110.90
1	D	30	ASP	CB-CG-OD2	7.74	125.26	118.30
2	E	54	LEU	CB-CG-CD2	7.65	124.01	111.00
1	D	106	ASP	CB-CG-OD2	7.32	124.89	118.30
1	D	137	ASP	CB-CG-OD1	-7.26	111.76	118.30
1	A	30	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	97	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	D	201	LEU	CB-CG-CD1	6.85	122.64	111.00
1	D	137	ASP	CB-CG-OD2	6.82	124.44	118.30
1	D	122	ASP	CB-CG-OD2	6.73	124.36	118.30
2	E	96	ASP	CB-CG-OD2	6.71	124.34	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	CA-CB-CG1	6.70	120.94	110.90
1	A	37	ASP	CB-CG-OD1	6.56	124.20	118.30
1	D	61	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	97	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	D	183	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	81	LEU	CB-CG-CD1	6.34	121.78	111.00
1	D	223	ASP	CB-CG-OD2	6.29	123.96	118.30
2	B	98	ASP	CB-CG-OD2	6.24	123.92	118.30
2	E	97	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	D	129	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	181	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	E	0	MET	CG-SD-CE	-5.82	90.89	100.20
1	A	249	VAL	N-CA-CB	-5.75	98.84	111.50
1	D	156	LEU	CB-CG-CD1	5.63	120.57	111.00
3	F	3	ASP	CB-CG-OD2	5.63	123.36	118.30
3	C	3	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	196	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	183	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	110	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	249	VAL	CA-CB-CG1	5.33	118.89	110.90
2	B	0	MET	CG-SD-CE	-5.31	91.71	100.20
1	A	182	THR	OG1-CB-CG2	-5.28	97.86	110.00
1	A	196	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	220	ASP	C-N-CA	-5.14	111.51	122.30
1	D	227	ASP	CB-CG-OD2	5.13	122.92	118.30
2	E	98	ASP	CB-CG-OD2	5.07	122.86	118.30

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	A	2253	0	2102	13	0
1	D	2247	0	2096	11	0
2	B	837	0	803	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	837	0	803	3	0
3	C	71	0	71	0	0
3	F	71	0	71	1	0
4	A	30	0	40	4	0
4	B	24	0	32	0	0
4	D	66	0	87	8	0
4	E	12	0	16	0	0
5	A	312	0	0	3	0
5	B	147	0	0	0	0
5	C	10	0	0	0	0
5	D	307	0	0	2	0
5	E	138	0	0	1	0
5	F	16	0	0	0	0
All	All	7378	0	6121	32	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 3.

All (32) 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:A:30:ASP:OD1	4:A:1002:GOL:H31	1.92	0.69
1:D:256:ARG:HG3	4:D:1010:GOL:H12	1.76	0.66
1:D:207:SER:HB2	4:D:1021:GOL:O2	1.96	0.65
1:D:206:LEU:HD13	4:D:1021:GOL:H31	1.80	0.64
4:D:1021:GOL:H2	5:E:1055:HOH:O	1.99	0.63
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.65	0.61
1:A:108:ARG:NH1	1:D:174:ASN:OD1	2.35	0.60
1:A:219:ARG:O	1:A:222:GLU:HG2	2.05	0.56
1:A:65:ARG:NH2	5:A:1231:HOH:O	2.38	0.55
1:D:65:ARG:NH2	5:D:1276:HOH:O	2.40	0.54
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.44	0.52
2:B:17:ASN:HD21	2:B:97:ARG:HH12	1.57	0.51
1:A:97:ARG:NH1	5:A:1278:HOH:O	2.43	0.51
1:D:154:GLU:HB3	4:D:1022:GOL:H12	1.92	0.51
1:D:30:ASP:OD1	4:D:1003:GOL:O3	2.29	0.50
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.94	0.50
1:A:6:ARG:HD2	4:A:1002:GOL:O1	2.12	0.49
1:A:126:LEU:HG	1:A:130:LEU:HA	1.94	0.49
2:B:17:ASN:ND2	2:B:97:ARG:HH22	2.11	0.49
1:A:206:LEU:HB3	4:A:1013:GOL:H11	1.97	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ILE:HD12	2:E:91:LYS:HE2	1.97	0.47
2:E:47:GLU:H	2:E:48:LYS:NZ	2.13	0.46
1:A:255:GLN:NE2	1:A:255:GLN:H	2.13	0.46
4:A:1013:GOL:H12	2:B:14:PRO:HD3	1.97	0.46
1:A:157:ARG:NH1	5:A:1046:HOH:O	2.39	0.43
1:A:218:GLN:NE2	1:A:221:GLY:HA2	2.33	0.43
1:D:14:ARG:HB2	1:D:17:ARG:HB2	2.00	0.43
1:D:255:GLN:NE2	1:D:255:GLN:H	2.19	0.41
4:D:1022:GOL:H11	5:D:1308:HOH:O	2.21	0.40
3:F:1:ILE:HD13	3:F:1:ILE:HG21	1.83	0.40
1:D:273:ARG:HH12	4:D:1007:GOL:H31	1.85	0.40
2:E:6:LYS:N	2:E:6:LYS:HD2	2.36	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	275/275 (100%)	269 (98%)	6 (2%)	0	100	100
1	D	273/275 (99%)	269 (98%)	4 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	758/768 (99%)	746 (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	233/231 (101%)	224 (96%)	9 (4%)	32	17
1	D	231/231 (100%)	217 (94%)	14 (6%)	18	7
2	B	95/95 (100%)	87 (92%)	8 (8%)	11	3
2	E	95/95 (100%)	88 (93%)	7 (7%)	13	4
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
All	All	672/670 (100%)	634 (94%)	38 (6%)	20	8

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	113	TYR
1	A	156	LEU
1	A	176	LYS
1	A	215	LEU
1	A	225	THR
1	A	249	VAL
1	A	255	GLN
1	A	272	LEU
2	B	0	MET
2	B	6	LYS
2	B	19	LYS
2	B	48	LYS
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN
2	B	89	GLN
1	D	19	GLU
1	D	35	ARG
1	D	81	LEU
1	D	86	ASN
1	D	105	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	113	TYR
1	D	115	GLN
1	D	154	GLU
1	D	156	LEU
1	D	166	GLU
1	D	178	THR
1	D	201	LEU
1	D	215	LEU
1	D	255	GLN
2	E	0	MET
2	E	19	LYS
2	E	48	LYS
2	E	54	LEU
2	E	58	LYS
2	E	70	PHE
2	E	83	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	218	GLN
1	A	255	GLN
2	B	17	ASN
2	B	83	ASN
1	D	115	GLN
2	E	17	ASN
2	E	83	ASN

### 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

22 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	1001	-	5,5,5	0.28	0	5,5,5	0.75	0
4	GOL	D	1010	-	5,5,5	0.74	0	5,5,5	1.11	1 (20%)
4	GOL	D	1007	-	5,5,5	0.26	0	5,5,5	1.07	1 (20%)
4	GOL	A	1004	-	5,5,5	0.37	0	5,5,5	0.46	0
4	GOL	D	1021	-	5,5,5	0.98	0	5,5,5	0.79	0
4	GOL	A	1013	-	5,5,5	0.81	0	5,5,5	2.21	2 (40%)
4	GOL	D	1022	-	5,5,5	0.53	0	5,5,5	1.03	0
4	GOL	D	1020	-	5,5,5	0.43	0	5,5,5	1.05	0
4	GOL	E	1016	-	5,5,5	0.30	0	5,5,5	0.66	0
4	GOL	B	1008	-	5,5,5	0.38	0	5,5,5	1.37	1 (20%)
4	GOL	B	1019	-	5,5,5	1.03	0	5,5,5	2.12	1 (20%)
4	GOL	B	1006	-	5,5,5	0.33	0	5,5,5	1.66	2 (40%)
4	GOL	D	1011	-	5,5,5	0.33	0	5,5,5	0.74	0
4	GOL	D	1018	-	5,5,5	0.54	0	5,5,5	1.35	1 (20%)
4	GOL	D	1003	-	5,5,5	0.38	0	5,5,5	0.94	1 (20%)
4	GOL	D	1014	-	5,5,5	0.36	0	5,5,5	1.13	0
4	GOL	B	1012	-	5,5,5	0.48	0	5,5,5	0.68	0
4	GOL	A	1005	-	5,5,5	0.68	0	5,5,5	1.30	1 (20%)
4	GOL	A	1002	-	5,5,5	0.20	0	5,5,5	1.32	1 (20%)
4	GOL	E	1009	-	5,5,5	0.41	0	5,5,5	1.16	1 (20%)
4	GOL	D	1017	-	5,5,5	0.36	0	5,5,5	0.81	0
4	GOL	D	1015	-	5,5,5	1.19	1 (20%)	5,5,5	1.21	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	A	1001	-	-	3/4/4/4	-
4	GOL	D	1010	-	-	2/4/4/4	-
4	GOL	D	1007	-	-	2/4/4/4	-
4	GOL	A	1004	-	-	0/4/4/4	-
4	GOL	D	1021	-	-	2/4/4/4	-
4	GOL	A	1013	-	-	2/4/4/4	-
4	GOL	D	1022	-	-	4/4/4/4	-
4	GOL	D	1020	-	-	4/4/4/4	-
4	GOL	E	1016	-	-	4/4/4/4	-
4	GOL	B	1008	-	-	2/4/4/4	-
4	GOL	B	1019	-	-	2/4/4/4	-
4	GOL	B	1006	-	-	1/4/4/4	-
4	GOL	D	1011	-	-	3/4/4/4	-
4	GOL	D	1018	-	-	4/4/4/4	-
4	GOL	D	1003	-	-	4/4/4/4	-
4	GOL	D	1014	-	-	4/4/4/4	-
4	GOL	B	1012	-	-	4/4/4/4	-
4	GOL	A	1005	-	-	4/4/4/4	-
4	GOL	A	1002	-	-	0/4/4/4	-
4	GOL	E	1009	-	-	2/4/4/4	-
4	GOL	D	1017	-	-	2/4/4/4	-
4	GOL	D	1015	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1015	GOL	O2-C2	-2.45	1.36	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1019	GOL	C3-C2-C1	-4.23	95.24	111.70
4	A	1013	GOL	O2-C2-C1	3.40	124.09	109.12
4	E	1009	GOL	C3-C2-C1	-2.55	101.80	111.70
4	B	1006	GOL	C3-C2-C1	-2.52	101.89	111.70
4	D	1018	GOL	O2-C2-C3	2.52	120.21	109.12
4	A	1013	GOL	O1-C1-C2	2.50	122.21	110.20
4	A	1002	GOL	C3-C2-C1	-2.36	102.52	111.70
4	A	1005	GOL	O1-C1-C2	-2.26	99.36	110.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1010	GOL	O1-C1-C2	2.23	120.91	110.20
4	B	1008	GOL	O2-C2-C3	2.19	118.77	109.12
4	B	1006	GOL	O2-C2-C1	2.09	118.33	109.12
4	D	1007	GOL	O3-C3-C2	2.01	119.86	110.20
4	D	1003	GOL	C3-C2-C1	-2.01	103.90	111.70

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1010	GOL	C1-C2-C3-O3
4	D	1007	GOL	C1-C2-C3-O3
4	D	1007	GOL	O2-C2-C3-O3
4	D	1021	GOL	C1-C2-C3-O3
4	A	1013	GOL	O2-C2-C3-O3
4	D	1022	GOL	O1-C1-C2-O2
4	D	1022	GOL	O1-C1-C2-C3
4	D	1022	GOL	C1-C2-C3-O3
4	D	1020	GOL	O1-C1-C2-C3
4	E	1016	GOL	O1-C1-C2-C3
4	B	1019	GOL	O1-C1-C2-C3
4	D	1011	GOL	O1-C1-C2-O2
4	D	1018	GOL	O1-C1-C2-C3
4	D	1003	GOL	O1-C1-C2-O2
4	D	1003	GOL	O1-C1-C2-C3
4	D	1003	GOL	C1-C2-C3-O3
4	D	1014	GOL	O1-C1-C2-C3
4	D	1014	GOL	C1-C2-C3-O3
4	B	1012	GOL	O1-C1-C2-C3
4	B	1012	GOL	C1-C2-C3-O3
4	A	1005	GOL	O1-C1-C2-C3
4	A	1005	GOL	C1-C2-C3-O3
4	E	1009	GOL	O1-C1-C2-O2
4	E	1009	GOL	O1-C1-C2-C3
4	D	1015	GOL	C1-C2-C3-O3
4	D	1022	GOL	O2-C2-C3-O3
4	B	1012	GOL	O1-C1-C2-O2
4	D	1017	GOL	O1-C1-C2-O2
4	A	1001	GOL	C1-C2-C3-O3
4	A	1013	GOL	C1-C2-C3-O3
4	D	1020	GOL	C1-C2-C3-O3
4	E	1016	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	1008	GOL	O1-C1-C2-C3
4	D	1011	GOL	O1-C1-C2-C3
4	D	1017	GOL	O1-C1-C2-C3
4	D	1015	GOL	O1-C1-C2-C3
4	D	1010	GOL	O2-C2-C3-O3
4	D	1021	GOL	O2-C2-C3-O3
4	D	1020	GOL	O1-C1-C2-O2
4	E	1016	GOL	O1-C1-C2-O2
4	B	1008	GOL	O1-C1-C2-O2
4	B	1019	GOL	O1-C1-C2-O2
4	D	1018	GOL	O1-C1-C2-O2
4	D	1003	GOL	O2-C2-C3-O3
4	D	1014	GOL	O2-C2-C3-O3
4	A	1005	GOL	O2-C2-C3-O3
4	D	1015	GOL	O2-C2-C3-O3
4	D	1020	GOL	O2-C2-C3-O3
4	D	1018	GOL	O2-C2-C3-O3
4	B	1012	GOL	O2-C2-C3-O3
4	A	1005	GOL	O1-C1-C2-O2
4	B	1006	GOL	O1-C1-C2-O2
4	D	1011	GOL	O2-C2-C3-O3
4	E	1016	GOL	O2-C2-C3-O3
4	D	1015	GOL	O1-C1-C2-O2
4	A	1001	GOL	O1-C1-C2-O2
4	D	1018	GOL	C1-C2-C3-O3
4	D	1014	GOL	O1-C1-C2-O2
4	A	1001	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1010	GOL	1	0
4	D	1007	GOL	1	0
4	D	1021	GOL	3	0
4	A	1013	GOL	2	0
4	D	1022	GOL	2	0
4	D	1003	GOL	1	0
4	A	1002	GOL	2	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%)	-0.34	4 (1%) 73 70	3, 8, 17, 25	0
1	D	275/275 (100%)	-0.34	2 (0%) 87 86	3, 8, 17, 23	0
2	B	100/100 (100%)	-0.47	1 (1%) 82 80	4, 8, 18, 21	0
2	E	100/100 (100%)	-0.43	0 100 100	4, 8, 16, 18	0
3	C	9/9 (100%)	0.31	0 100 100	5, 8, 12, 14	0
3	F	9/9 (100%)	-0.02	0 100 100	2, 3, 12, 13	0
All	All	768/768 (100%)	-0.36	7 (0%) 84 82	2, 8, 17, 25	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	ASP	4.4
1	A	1	GLY	3.6
1	D	226	GLN	3.3
1	A	105	SER	3.1
2	B	48	LYS	2.6
1	A	108	ARG	2.1
1	A	16	GLY	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<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	B	1012	6/6	0.58	0.24	49,51,52,52	0
4	GOL	E	1016	6/6	0.67	0.20	48,51,52,54	0
4	GOL	A	1013	6/6	0.68	0.27	35,36,37,38	0
4	GOL	D	1020	6/6	0.69	0.22	49,51,51,52	0
4	GOL	D	1010	6/6	0.75	0.33	38,42,44,45	0
4	GOL	D	1007	6/6	0.76	0.20	39,42,45,48	0
4	GOL	B	1008	6/6	0.77	0.21	47,48,49,49	0
4	GOL	D	1021	6/6	0.77	0.30	41,46,49,50	0
4	GOL	A	1002	6/6	0.77	0.17	27,29,31,38	0
4	GOL	D	1014	6/6	0.79	0.26	39,43,44,47	0
4	GOL	D	1003	6/6	0.80	0.17	33,37,39,40	0
4	GOL	D	1022	6/6	0.80	0.21	38,44,45,45	0
4	GOL	D	1018	6/6	0.83	0.19	20,33,33,42	0
4	GOL	E	1009	6/6	0.85	0.16	28,37,39,42	0
4	GOL	A	1005	6/6	0.86	0.23	20,31,32,37	0
4	GOL	B	1006	6/6	0.87	0.20	22,32,34,38	0
4	GOL	D	1015	6/6	0.88	0.23	17,28,32,32	0
4	GOL	B	1019	6/6	0.90	0.22	24,40,43,44	0
4	GOL	A	1001	6/6	0.90	0.18	36,39,42,46	0
4	GOL	D	1017	6/6	0.91	0.19	27,38,40,41	0
4	GOL	D	1011	6/6	0.91	0.17	30,36,37,40	0
4	GOL	A	1004	6/6	0.96	0.09	25,26,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.