



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2022 – 03:53 AM EST

PDB ID : 6P64
Title : Alpha-beta TCR Binding to Neoantigen KQWLVLFL Presented by HLA-A206
Authors : Devlin, J.R.; Baker, B.M.
Deposited on : 2019-05-31
Resolution : 3.05 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 ⓘ 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 : 2.27
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) : 2.27

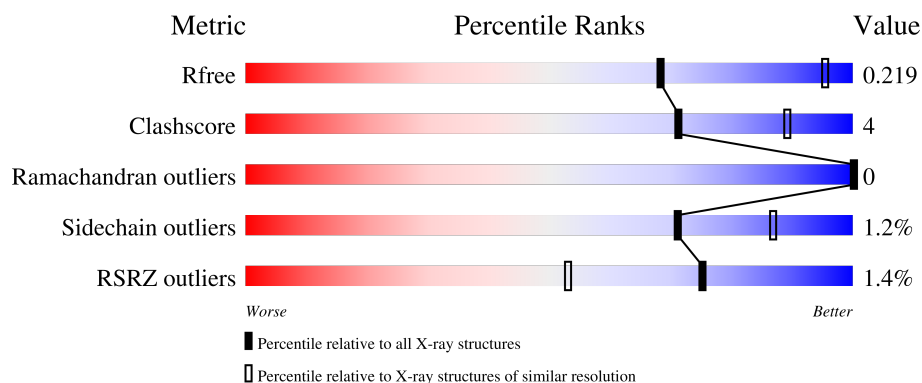
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




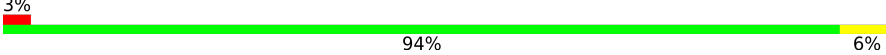

The reported resolution of this entry is 3.05 Å.

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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 $\leq 5\%$. 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	276	 91% 8%
1	F	276	 4% 88% 7%
2	B	100	 88% 11%
2	G	100	 3% 94% 6%
3	D	208	 78% 12% 9%

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Mol	Chain	Length	Quality of chain
3	I	208	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>88%</div><div>9%</div><div></div></div></div>
4	E	245	<div><div><div></div><div></div><div></div></div><div>91%</div><div>9%</div></div>
4	J	245	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>92%</div><div>7%</div><div></div></div></div>
5	C	9	<div><div><div></div><div></div><div></div></div><div>100%</div></div>
5	H	9	<div><div><div></div><div></div><div></div></div><div>100%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13284 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2248	1403	409	427	9			
1	F	256	Total	C	N	O	S	0	0	0
			2102	1318	381	394	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP U5YJP1
F	0	MET	-	initiating methionine	UNP U5YJP1

- 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	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 302TIL TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	S	0	0	0
			1512	959	244	298	11			
3	I	202	Total	C	N	O	S	0	0	0
			1608	1010	261	326	11			

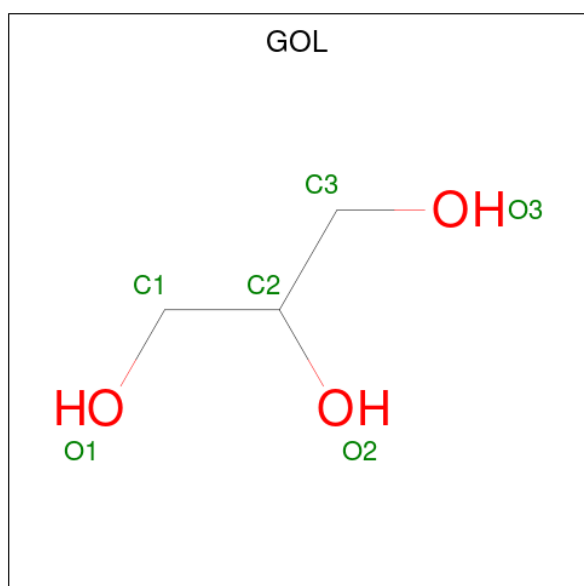
- Molecule 4 is a protein called 302TIL TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	245	Total	C	N	O	S	0	0	0
			1954	1228	339	376	11			
4	J	244	Total	C	N	O	S	0	0	0
			1946	1223	338	375	10			

- Molecule 5 is a protein called Neoantigen peptide KQWLVLWLFL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	9	Total	C	N	O	0	0	0
			89	65	13	11			
5	H	9	Total	C	N	O	0	0	0
			89	65	13	11			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	1	Total 1	O 1	0	0
7	F	7	Total 7	O 7	0	0
7	D	2	Total 2	O 2	0	0
7	E	4	Total 4	O 4	0	0
7	I	4	Total 4	O 4	0	0
7	J	7	Total 7	O 7	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: MHC class I antigen

Chain A: 




- Molecule 1: MHC class I antigen

Chain F: 



- Molecule 2: Beta-2-microglobulin

Chain B: 




- Molecule 2: Beta-2-microglobulin

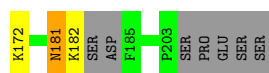
Chain G: 



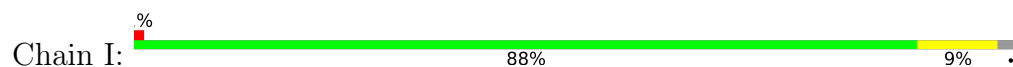
- Molecule 3: 302TIL TCR alpha chain

Chain D: 

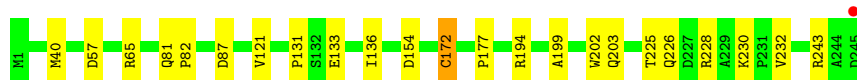




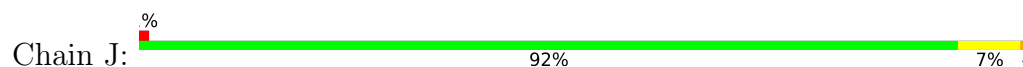
- Molecule 3: 302TIL TCR alpha chain



- Molecule 4: 302TIL TCR beta chain



- Molecule 4: 302TIL TCR beta chain



- Molecule 5: Neoantigen peptide KQWLVLWLFL



There are no outlier residues recorded for this chain.

- Molecule 5: Neoantigen peptide KQWLVLWLFL



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	276.64Å 276.64Å 112.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.38 – 3.05 49.38 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.7 (49.38-3.05) 93.5 (49.38-3.05)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.194 , 0.219 0.194 , 0.219	Depositor DCC
R_{free} test set	2000 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13284	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	A	0.23	0/2313	0.43	0/3139
1	F	0.24	0/2159	0.46	0/2923
2	B	0.31	0/860	0.47	0/1162
2	G	0.27	0/860	0.47	0/1162
3	D	0.28	0/1544	0.47	0/2087
3	I	0.29	0/1643	0.53	2/2226 (0.1%)
4	E	0.26	0/2008	0.49	0/2733
4	J	0.28	0/2000	0.51	1/2723 (0.0%)
5	C	0.23	0/93	0.39	0/125
5	H	0.22	0/93	0.47	0/125
All	All	0.27	0/13573	0.48	3/18405 (0.0%)

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
2	B	0	1
3	D	0	1
3	I	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	62	PRO	N-CA-C	6.23	128.29	112.10
3	I	64	ARG	N-CA-C	-6.08	94.59	111.00
3	I	64	ARG	N-CA-CB	5.59	120.67	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	97	ARG	Sidechain
3	D	51	ARG	Sidechain
3	I	64	ARG	Sidechain

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	2248	0	2096	14	0
1	F	2102	0	1970	21	0
2	B	837	0	803	10	0
2	G	837	0	803	5	0
3	D	1512	0	1444	16	0
3	I	1608	0	1523	17	0
4	E	1954	0	1860	16	0
4	J	1946	0	1848	10	0
5	C	89	0	94	0	0
5	H	89	0	94	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	F	6	0	8	0	0
6	I	12	0	16	0	0
7	A	7	0	0	0	0
7	B	1	0	0	0	0
7	D	2	0	0	0	0
7	E	4	0	0	0	0
7	F	7	0	0	0	0
7	I	4	0	0	0	0
7	J	7	0	0	0	0
All	All	13284	0	12575	91	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 4.

The worst 5 of 91 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)
3:D:181:ASN:OD1	3:D:181:ASN:N	2.15	0.80
1:F:201:LEU:HB2	1:F:247:VAL:CG1	2.12	0.78
3:I:51:ARG:NH1	3:I:53:GLU:OE2	2.21	0.73
1:F:201:LEU:HB2	1:F:247:VAL:HG12	1.70	0.73
1:F:201:LEU:O	1:F:217:TRP:CZ2	2.43	0.72

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	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	F	246/276 (89%)	241 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	G	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	D	181/208 (87%)	174 (96%)	7 (4%)	0	100	100
3	I	200/208 (96%)	190 (95%)	10 (5%)	0	100	100
4	E	243/245 (99%)	232 (96%)	11 (4%)	0	100	100
4	J	242/245 (99%)	234 (97%)	8 (3%)	0	100	100
5	C	7/9 (78%)	7 (100%)	0	0	100	100
5	H	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1595/1676 (95%)	1541 (97%)	54 (3%)	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	231/232 (100%)	230 (100%)	1 (0%)	91	95
1	F	215/232 (93%)	214 (100%)	1 (0%)	88	94
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	77
2	G	95/95 (100%)	94 (99%)	1 (1%)	73	88
3	D	172/189 (91%)	170 (99%)	2 (1%)	71	87
3	I	184/189 (97%)	181 (98%)	3 (2%)	62	83
4	E	217/217 (100%)	214 (99%)	3 (1%)	67	84
4	J	216/217 (100%)	212 (98%)	4 (2%)	57	79
5	C	9/9 (100%)	9 (100%)	0	100	100
5	H	9/9 (100%)	9 (100%)	0	100	100
All	All	1443/1484 (97%)	1426 (99%)	17 (1%)	71	87

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	63	GLU
4	J	194	ARG
4	E	40	MET
4	E	172	CYS
4	E	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
6	GOL	I	301	-	5,5,5	0.38	0	5,5,5	0.28	0
6	GOL	A	301	-	5,5,5	0.39	0	5,5,5	0.28	0
6	GOL	F	301	-	5,5,5	0.36	0	5,5,5	0.31	0
6	GOL	B	101	-	5,5,5	0.37	0	5,5,5	0.23	0
6	GOL	I	302	-	5,5,5	0.39	0	5,5,5	0.87	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
6	GOL	I	301	-	-	2/4/4/4	-
6	GOL	A	301	-	-	2/4/4/4	-
6	GOL	F	301	-	-	2/4/4/4	-
6	GOL	B	101	-	-	4/4/4/4	-
6	GOL	I	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	GOL	C1-C2-C3-O3
6	B	101	GOL	O1-C1-C2-C3
6	I	302	GOL	O1-C1-C2-O2
6	I	302	GOL	O1-C1-C2-C3
6	B	101	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/276 (99%)	-0.26	1 (0%) 92 82	35, 51, 102, 127	0
1	F	256/276 (92%)	-0.04	12 (4%) 31 14	31, 50, 146, 174	0
2	B	100/100 (100%)	-0.14	0 100 100	41, 65, 99, 111	0
2	G	100/100 (100%)	0.31	3 (3%) 50 25	46, 97, 144, 175	0
3	D	189/208 (90%)	0.06	1 (0%) 91 79	48, 93, 123, 140	0
3	I	202/208 (97%)	-0.22	3 (1%) 73 51	33, 54, 99, 118	0
4	E	245/245 (100%)	-0.19	1 (0%) 92 82	38, 63, 103, 126	0
4	J	244/245 (99%)	-0.24	2 (0%) 86 70	26, 52, 89, 140	0
5	C	9/9 (100%)	-0.43	0 100 100	39, 42, 48, 49	0
5	H	9/9 (100%)	-0.43	0 100 100	32, 34, 39, 44	0
All	All	1629/1676 (97%)	-0.13	23 (1%) 75 53	26, 60, 119, 175	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	61	THR	5.6
4	J	245	ASP	4.0
1	F	247	VAL	4.0
3	D	130	LYS	3.3
1	A	275	GLU	3.3

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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	101	6/6	0.82	0.29	52,63,67,69	0
6	GOL	F	301	6/6	0.83	0.24	62,67,77,81	0
6	GOL	I	302	6/6	0.84	0.52	50,80,83,83	0
6	GOL	A	301	6/6	0.87	0.25	46,54,59,69	0
6	GOL	I	301	6/6	0.89	0.29	37,77,84,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.