



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:33 pm GMT

PDB ID : 3PWP  
Title : The complex between TCR A6 and human Class I MHC HLA-A2 with the bound HuD peptide  
Authors : Borbulevych, O.Y.; Baker, B.M.  
Deposited on : 2010-12-08  
Resolution : 2.69 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

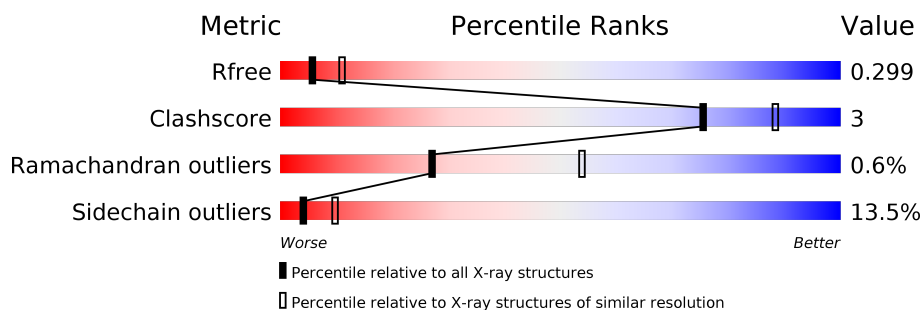
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)

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. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	275	86% 12% .
2	B	100	80% 16% .
3	C	9	67% 33%
4	D	200	79% 17% . .
5	E	245	79% 19% .

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6757 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	0	0
			2247	1403	409	426	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	1	0
			843	537	142	160	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called HuD peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	52	10	13			

- Molecule 4 is a protein called A6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1552	965	255	325	7			

- Molecule 5 is a protein called A6 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1927	1209	338	372	8			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

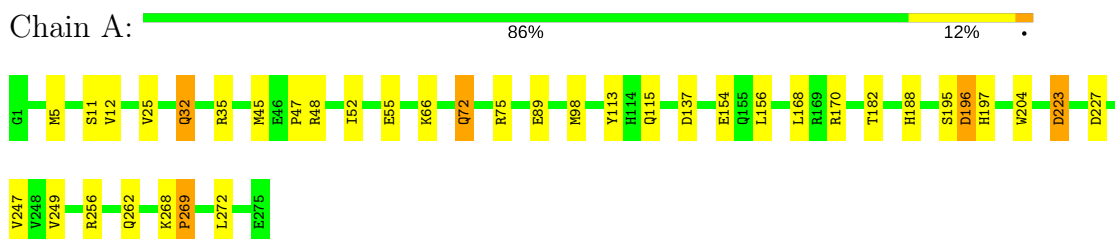
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	16	Total	O	0	0
			16	16		
8	D	7	Total	O	0	0
			7	7		
8	E	24	Total	O	0	0
			24	24		

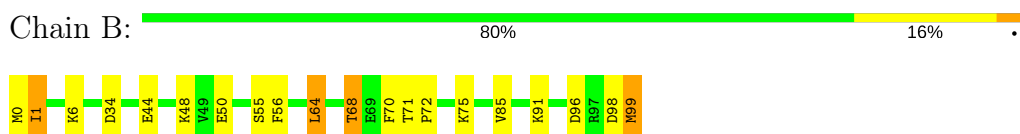
### 3 Residue-property plots

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. 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.

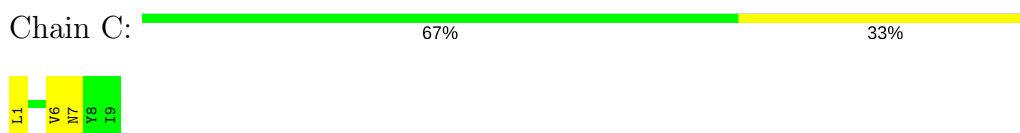
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



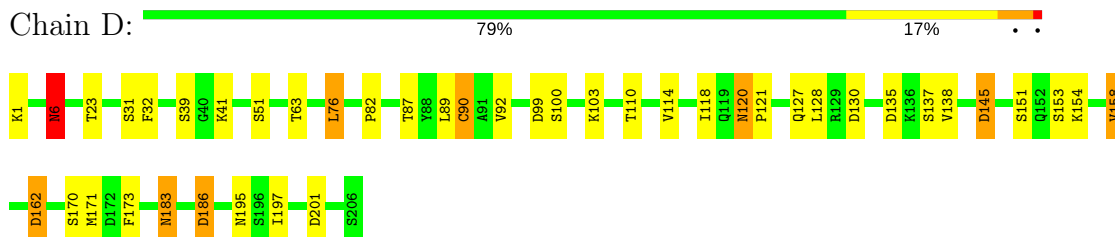
- Molecule 2: Beta-2-microglobulin



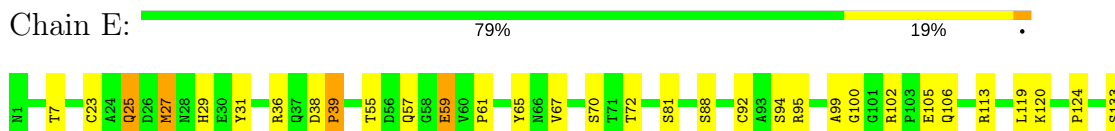
- Molecule 3: HuD peptide

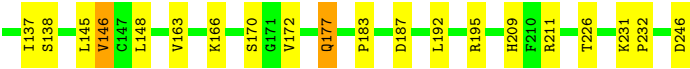


- Molecule 4: A6 TCR alpha chain



- Molecule 5: A6 TCR beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.01Å 49.06Å 93.71Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.69 19.83 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.69) 94.2 (19.83-2.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.198 , 0.259 0.254 , 0.299	Depositor DCC
$R_{free}$ test set	1371 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.66	0/2312	0.80	1/3137 (0.0%)
2	B	0.65	0/869	0.82	0/1174
3	C	0.76	0/77	0.67	0/102
4	D	0.61	1/1585 (0.1%)	0.83	3/2150 (0.1%)
5	E	0.65	1/1980 (0.1%)	0.84	2/2699 (0.1%)
All	All	0.65	2/6823 (0.0%)	0.82	6/9262 (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
5	E	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	CYS	CB-SG	-5.51	1.72	1.81
5	E	92	CYS	CB-SG	-5.12	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	89	LEU	CA-CB-CG	7.14	131.72	115.30
5	E	23	CYS	CA-CB-SG	-5.40	104.27	114.00
4	D	99	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	137	ASP	CB-CG-OD1	5.27	123.05	118.30
4	D	76	LEU	CA-CB-CG	5.11	127.04	115.30
5	E	100	GLY	N-CA-C	5.08	125.81	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	25	GLN	Peptide
5	E	99	ALA	Peptide

## 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	2247	0	2096	13	0
2	B	843	0	811	6	0
3	C	75	0	72	0	0
4	D	1552	0	1461	13	0
5	E	1927	0	1830	14	0
6	A	30	0	40	0	0
6	E	12	0	16	1	0
7	B	5	0	0	0	0
8	A	19	0	0	0	0
8	B	16	0	0	0	0
8	D	7	0	0	0	0
8	E	24	0	0	0	0
All	All	6757	0	6326	44	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 (44) 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)
4:D:162:ASP:OD2	4:D:162:ASP:N	2.30	0.63
5:E:95:ARG:HG2	5:E:106:GLN:HB2	1.84	0.59
1:A:25:VAL:HG13	1:A:32:GLN:HE21	1.68	0.57
1:A:188:HIS:HB3	1:A:204:TRP:HB2	1.88	0.55
4:D:118:ILE:HD11	4:D:145:ASP:HA	1.90	0.53
5:E:124:PRO:HD3	5:E:232:PRO:HB3	1.93	0.50
4:D:183:ASN:N	4:D:183:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.45	0.49
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.94	0.49
5:E:57:GLN:HB2	5:E:61:PRO:HB3	1.95	0.48
1:A:72:GLN:HG2	1:A:75:ARG:HH21	1.78	0.48
5:E:36:ARG:NH1	5:E:65:TYR:OH	2.45	0.48
1:A:154:GLU:OE1	5:E:102:ARG:NH1	2.47	0.48
5:E:38:ASP:HA	5:E:39:PRO:HD2	1.65	0.48
1:A:268:LYS:HA	1:A:269:PRO:HD2	1.69	0.47
2:B:55:SER:OG	2:B:56:PHE:N	2.48	0.47
4:D:186:ASP:N	4:D:186:ASP:OD1	2.48	0.46
2:B:48:LYS:O	2:B:68:THR:OG1	2.31	0.46
4:D:82:PRO:HA	4:D:114:VAL:HB	1.98	0.46
4:D:138:VAL:HG11	5:E:146:VAL:HG21	1.98	0.45
1:A:223:ASP:OD1	1:A:223:ASP:N	2.35	0.45
2:B:64:LEU:HA	2:B:64:LEU:HD12	1.80	0.45
5:E:209:HIS:ND1	6:E:248:GOL:H31	2.33	0.44
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.98	0.44
5:E:177:GLN:HE21	5:E:177:GLN:HB2	1.56	0.44
4:D:171:MET:HB3	4:D:173:PHE:HB2	1.99	0.44
4:D:120:ASN:HA	4:D:121:PRO:HD2	1.53	0.44
4:D:32:PHE:HD1	4:D:92:VAL:HG22	1.83	0.44
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.77	0.43
1:A:47:PRO:O	1:A:48:ARG:NH1	2.45	0.43
1:A:195:SER:O	1:A:197:HIS:N	2.51	0.43
1:A:196:ASP:N	1:A:196:ASP:OD1	2.50	0.43
4:D:6:ASN:HA	4:D:6:ASN:HD22	1.64	0.42
4:D:153:SER:OG	4:D:158:VAL:O	2.37	0.42
5:E:29:HIS:ND1	5:E:94:SER:OG	2.48	0.42
4:D:201:ASP:OD2	4:D:201:ASP:N	2.53	0.41
4:D:154:LYS:HE3	4:D:154:LYS:HB3	1.89	0.41
2:B:1:ILE:HA	2:B:1:ILE:HD12	1.61	0.41
5:E:231:LYS:HA	5:E:232:PRO:HD3	1.87	0.41
5:E:148:LEU:HA	5:E:148:LEU:HD23	1.80	0.41
1:A:48:ARG:HA	1:A:48:ARG:HD3	1.82	0.40
5:E:59:GLU:H	5:E:59:GLU:HG3	1.69	0.40
2:B:71:THR:HA	2:B:72:PRO:HD2	1.88	0.40
5:E:27:MET:HE3	5:E:27:MET:HB3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	273/275 (99%)	265 (97%)	6 (2%)	2 (1%)	24	50
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	182 (92%)	15 (8%)	1 (0%)	31	58
5	E	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	21	47
All	All	820/829 (99%)	781 (95%)	34 (4%)	5 (1%)	27	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
4	D	6	ASN
5	E	39	PRO
5	E	183	PRO
1	A	269	PRO

### 5.3.2 Protein sidechains

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	231/231 (100%)	211 (91%)	20 (9%)	11	26
2	B	96/95 (101%)	82 (85%)	14 (15%)	3	8
3	C	7/7 (100%)	4 (57%)	3 (43%)	0	0
4	D	178/178 (100%)	149 (84%)	29 (16%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	209/209 (100%)	178 (85%)	31 (15%)	3	8
All	All	721/720 (100%)	624 (86%)	97 (14%)	4	10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	12	VAL
1	A	32	GLN
1	A	35	ARG
1	A	45	MET
1	A	52	ILE
1	A	66	LYS
1	A	72	GLN
1	A	89	GLU
1	A	98	MET
1	A	113	TYR
1	A	115	GLN
1	A	182	THR
1	A	223	ASP
1	A	227	ASP
1	A	247	VAL
1	A	249	VAL
1	A	256	ARG
1	A	262	GLN
1	A	272	LEU
2	B	0	MET
2	B	1	ILE
2	B	6	LYS
2	B	34	ASP
2	B	44	GLU
2	B	50	GLU
2	B	64	LEU
2	B	68	THR
2	B	70	PHE
2	B	75	LYS
2	B	85	VAL
2	B	91	LYS
2	B	98	ASP
2	B	99	MET
3	C	1	LEU
3	C	6	VAL

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Mol	Chain	Res	Type
3	C	7	ASN
4	D	1	LYS
4	D	6	ASN
4	D	23	THR
4	D	31	SER
4	D	39	SER
4	D	41	LYS
4	D	51	SER
4	D	63	THR
4	D	76	LEU
4	D	87	THR
4	D	90	CYS
4	D	100	SER
4	D	103	LYS
4	D	110	THR
4	D	120	ASN
4	D	127	GLN
4	D	128	LEU
4	D	130	ASP
4	D	135	ASP
4	D	137	SER
4	D	145	ASP
4	D	151	SER
4	D	158	VAL
4	D	162	ASP
4	D	170	SER
4	D	183	ASN
4	D	186	ASP
4	D	195	ASN
4	D	197	ILE
5	E	7	THR
5	E	25	GLN
5	E	27	MET
5	E	31	TYR
5	E	55	THR
5	E	59	GLU
5	E	67	VAL
5	E	70	SER
5	E	72	THR
5	E	81	SER
5	E	88	SER
5	E	105	GLU

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Mol	Chain	Res	Type
5	E	113	ARG
5	E	119	LEU
5	E	120	LYS
5	E	133	SER
5	E	137	ILE
5	E	138	SER
5	E	145	LEU
5	E	146	VAL
5	E	163	VAL
5	E	166	LYS
5	E	170	SER
5	E	172	VAL
5	E	177	GLN
5	E	187	ASP
5	E	192	LEU
5	E	195	ARG
5	E	211	ARG
5	E	226	THR
5	E	246	ASP

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	32	GLN
4	D	5	GLN
4	D	6	ASN
4	D	105	GLN
4	D	111	GLN
4	D	119	GLN
4	D	127	GLN
5	E	177	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	A	276	-	5,5,5	0.60	0	5,5,5	0.65	0
6	GOL	A	277	-	5,5,5	0.49	0	5,5,5	0.72	0
6	GOL	A	278	-	5,5,5	0.45	0	5,5,5	0.96	0
6	GOL	A	279	-	5,5,5	0.38	0	5,5,5	0.43	0
6	GOL	A	280	-	5,5,5	0.43	0	5,5,5	0.48	0
7	SO4	B	100	-	4,4,4	0.54	0	6,6,6	0.32	0
6	GOL	E	247	-	5,5,5	0.35	0	5,5,5	0.89	0
6	GOL	E	248	-	5,5,5	0.47	0	5,5,5	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
6	GOL	A	276	-	-	0/4/4/4	0/0/0/0
6	GOL	A	277	-	-	0/4/4/4	0/0/0/0
6	GOL	A	278	-	-	0/4/4/4	0/0/0/0
6	GOL	A	279	-	-	0/4/4/4	0/0/0/0
6	GOL	A	280	-	-	0/4/4/4	0/0/0/0
7	SO4	B	100	-	-	0/0/0/0	0/0/0/0
6	GOL	E	247	-	-	0/4/4/4	0/0/0/0
6	GOL	E	248	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	248	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](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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