



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:05 PM GMT

PDB ID : 3D3V  
Title : The complex between TCR A6 and human Class I MHC HLA-A2 with the modified HTLV-1 TAX (Y5(3,4-difluoroPhenylalanine))peptide  
Authors : Borbulevych, O.Y.; Clemens, J.R.; Baker, B.M.  
Deposited on : 2008-05-12  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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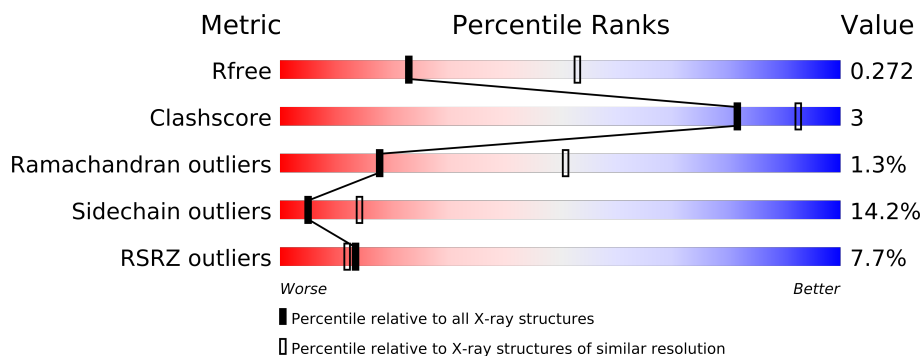
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	100	
3	C	9	
4	D	200	
5	E	245	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6732 atoms, of which 0 are hydrogen and 0 are deuterium.

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	3	0
			2265	1413	415	428	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	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called Modified HTLV-1 TAX (Y5(3,4-difluoro)F) peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	F	N	O	0	1	0
			87	63	4	9	11			

- 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
			1928	1209	339	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	B	1	Total	C	O	0	0
			6	3	3		
6	B	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		

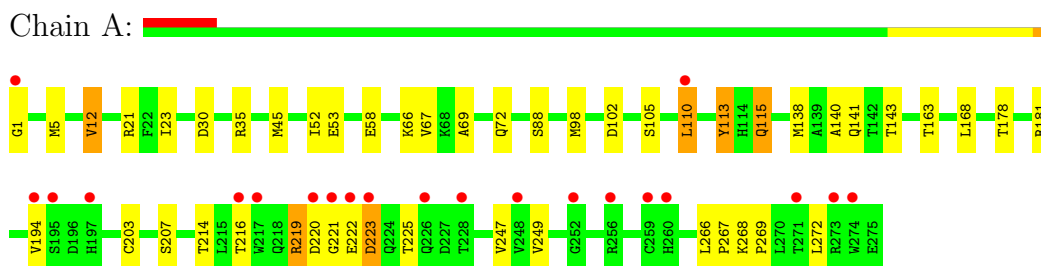
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	6	Total	O	0	0
			6	6		
7	D	2	Total	O	0	0
			2	2		
7	E	6	Total	O	0	0
			6	6		

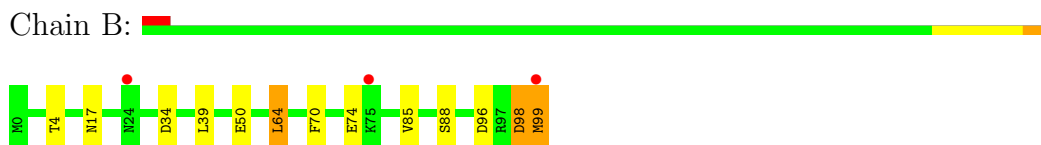
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 2: Beta-2-microglobulin

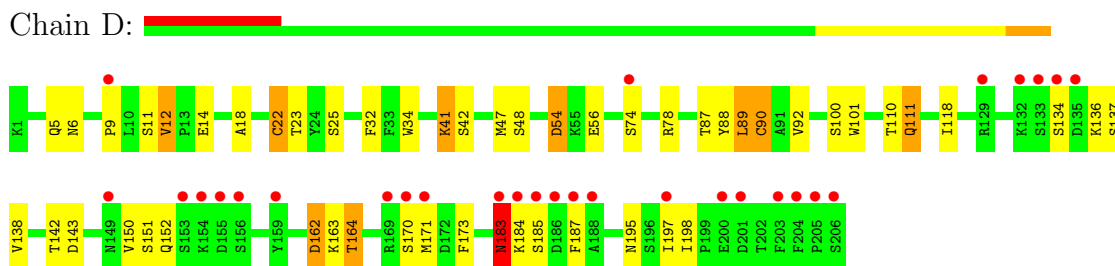


- Molecule 3: Modified HTLV-1 TAX (Y5(3,4-difluoro)F) peptide

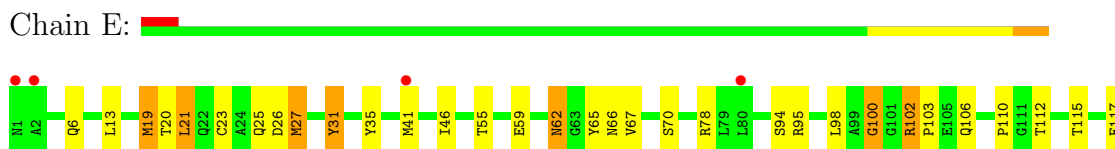


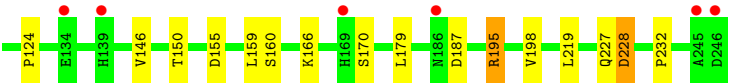
There are no outlier residues recorded for this chain.

- 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, $\alpha$ , $\beta$ , $\gamma$	224.45Å 48.54Å 93.79Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.80) 98.6 (19.18-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.278 0.219 , 0.272	Depositor DCC
$R_{free}$ test set	1277 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.5	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 24962 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, F2F

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	0.82	3/2342 (0.1%)	0.81	0/3176
2	B	0.71	0/860	0.84	0/1162
3	C	0.95	0/66	0.92	0/86
4	D	0.66	3/1585 (0.2%)	0.79	1/2150 (0.0%)
5	E	0.92	7/1981 (0.4%)	0.90	3/2699 (0.1%)
All	All	0.80	13/6834 (0.2%)	0.84	4/9273 (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
5	E	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	65	TYR	CG-CD2	14.36	1.57	1.39
1	A	222	GLU	CD-OE1	12.87	1.39	1.25
1	A	222	GLU	CG-CD	12.74	1.71	1.51
5	E	117	GLU	CD-OE2	10.10	1.36	1.25
5	E	117	GLU	CD-OE1	10.09	1.36	1.25
5	E	65	TYR	CE2-CZ	7.10	1.47	1.38
4	D	163	LYS	CE-NZ	6.50	1.65	1.49
1	A	222	GLU	CD-OE2	6.26	1.32	1.25
5	E	117	GLU	CG-CD	5.63	1.60	1.51
4	D	22	CYS	CB-SG	-5.63	1.72	1.81
5	E	23	CYS	CB-SG	-5.41	1.73	1.81
5	E	62	ASN	N-CA	5.17	1.56	1.46
4	D	90	CYS	CB-SG	-5.15	1.73	1.81



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	65	TYR	CZ-CE2-CD2	-6.70	113.77	119.80
5	E	62	ASN	CB-CG-ND2	-5.93	102.46	116.70
5	E	35	TYR	CB-CA-C	-5.76	98.88	110.40
4	D	89	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	100	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2265	0	2114	14	0
2	B	837	0	803	5	0
3	C	87	0	82	0	0
4	D	1552	0	1461	13	0
5	E	1928	0	1832	13	0
6	A	12	0	16	0	0
6	B	12	0	16	0	0
6	E	12	0	16	0	0
7	A	13	0	0	0	0
7	B	6	0	0	0	0
7	D	2	0	0	0	0
7	E	6	0	0	0	0
All	All	6732	0	6340	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:228:ASP:N	5:E:228:ASP:OD2	2.29	0.63
2:B:98:ASP:OD1	2:B:98:ASP:N	2.33	0.62
4:D:142:THR:OG1	4:D:143:ASP:N	2.31	0.61
4:D:164:THR:OG1	5:E:195:ARG:NH2	2.34	0.59
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.68	0.59
5:E:95:ARG:HG3	5:E:106:GLN:HB2	1.85	0.57
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.19	0.57
4:D:183:ASN:N	4:D:183:ASN:OD1	2.35	0.57
5:E:155:ASP:N	5:E:155:ASP:OD1	2.37	0.56
4:D:54:ASP:N	4:D:54:ASP:OD2	2.40	0.55
4:D:171:MET:HB3	4:D:173:PHE:HB2	1.88	0.54
4:D:9:PRO:HB3	4:D:111:GLN:HG2	1.93	0.51
5:E:6:GLN:HG2	5:E:110:PRO:HD2	1.94	0.49
1:A:12:VAL:HG13	1:A:21:ARG:HB3	1.95	0.49
1:A:140:ALA:O	1:A:143:THR:HB	2.13	0.49
5:E:124:PRO:HD3	5:E:232:PRO:HB3	1.96	0.48
5:E:21:LEU:HD22	5:E:112:THR:HG21	1.97	0.47
1:A:115:GLN:H	1:A:115:GLN:HG2	1.59	0.47
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.98	0.46
2:B:64:LEU:HA	2:B:64:LEU:HD12	1.73	0.46
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.97	0.46
4:D:5:GLN:NE2	4:D:88:TYR:O	2.49	0.45
1:A:69:ALA:HB1	5:E:98:LEU:HD11	1.98	0.44
5:E:31:TYR:HB3	5:E:95:ARG:HB3	1.99	0.44
5:E:219:LEU:HD22	5:E:232:PRO:HD2	1.98	0.44
1:A:219:ARG:O	1:A:221:GLY:N	2.48	0.44
2:B:39:LEU:HA	2:B:39:LEU:HD23	1.75	0.43
2:B:17:ASN:HD21	2:B:74:GLU:HG3	1.84	0.43
1:A:266:LEU:HA	1:A:267:PRO:HD3	1.79	0.43
4:D:162:ASP:N	4:D:162:ASP:OD1	2.51	0.43
1:A:110:LEU:HA	1:A:110:LEU:HD12	1.74	0.42
4:D:32:PHE:HD1	4:D:92:VAL:HG22	1.84	0.42
1:A:266:LEU:HA	1:A:266:LEU:HD23	1.84	0.42
4:D:12:VAL:HG21	4:D:18:ALA:HB2	2.01	0.42
4:D:138:VAL:HG11	5:E:146:VAL:HG21	2.02	0.41
1:A:268:LYS:HA	1:A:269:PRO:HD3	1.91	0.41
5:E:13:LEU:HD11	5:E:19:MET:HB3	2.02	0.41
1:A:1:GLY:HA2	1:A:105:SER:HB3	2.01	0.41
4:D:41:LYS:HB2	4:D:42:SER:H	1.68	0.41
1:A:223:ASP:N	1:A:223:ASP:OD1	2.38	0.41
5:E:27:MET:H	5:E:27:MET:HG2	1.51	0.41
4:D:34:TRP:HB2	4:D:47:MET:HB2	2.03	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	276/275 (100%)	252 (91%)	22 (8%)	2 (1%)	30	69
2	B	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	22	60
3	C	6/9 (67%)	5 (83%)	1 (17%)	0	100	100
4	D	198/200 (99%)	175 (88%)	20 (10%)	3 (2%)	15	46
5	E	243/245 (99%)	222 (91%)	16 (7%)	5 (2%)	11	33
All	All	821/829 (99%)	748 (91%)	62 (8%)	11 (1%)	18	51

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	6	ASN
5	E	27	MET
2	B	34	ASP
5	E	62	ASN
4	D	183	ASN
4	D	184	LYS
1	A	220	ASP
5	E	102	ARG
1	A	194	VAL
5	E	103	PRO
5	E	100	GLY

### 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	234/231 (101%)	202 (86%)	32 (14%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/95 (100%)	87 (92%)	8 (8%)	16	41
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	178/178 (100%)	143 (80%)	35 (20%)	2	6
5	E	209/209 (100%)	181 (87%)	28 (13%)	6	16
All	All	723/720 (100%)	620 (86%)	103 (14%)	5	14

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	30[A]	ASP
1	A	30[B]	ASP
1	A	35	ARG
1	A	45	MET
1	A	52	ILE
1	A	53	GLU
1	A	58	GLU
1	A	66	LYS
1	A	67	VAL
1	A	72	GLN
1	A	88	SER
1	A	98	MET
1	A	110	LEU
1	A	113	TYR
1	A	115	GLN
1	A	138	MET
1	A	141	GLN
1	A	163	THR
1	A	178	THR
1	A	181	ARG
1	A	187	THR
1	A	203	CYS
1	A	207	SER
1	A	214	THR
1	A	216	THR
1	A	219	ARG
1	A	223	ASP
1	A	225	THR
1	A	247	VAL
1	A	249	VAL
1	A	272	LEU

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Mol	Chain	Res	Type
2	B	4	THR
2	B	50	GLU
2	B	64	LEU
2	B	70	PHE
2	B	85	VAL
2	B	88	SER
2	B	98	ASP
2	B	99	MET
4	D	11	SER
4	D	12	VAL
4	D	14	GLU
4	D	22	CYS
4	D	23	THR
4	D	25	SER
4	D	41	LYS
4	D	48	SER
4	D	54	ASP
4	D	56	GLU
4	D	74	SER
4	D	78	ARG
4	D	87	THR
4	D	89	LEU
4	D	90	CYS
4	D	100	SER
4	D	101	TRP
4	D	110	THR
4	D	111	GLN
4	D	118	ILE
4	D	134	SER
4	D	136	LYS
4	D	137	SER
4	D	150	VAL
4	D	151	SER
4	D	152	GLN
4	D	162	ASP
4	D	164	THR
4	D	170	SER
4	D	183	ASN
4	D	185	SER
4	D	187	PHE
4	D	195	ASN
4	D	197	ILE

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Mol	Chain	Res	Type
4	D	198	ILE
5	E	19	MET
5	E	20	THR
5	E	21	LEU
5	E	25	GLN
5	E	26	ASP
5	E	31	TYR
5	E	41	MET
5	E	46	ILE
5	E	55	THR
5	E	59	GLU
5	E	66	ASN
5	E	67	VAL
5	E	70	SER
5	E	78	ARG
5	E	94	SER
5	E	102	ARG
5	E	115	THR
5	E	150	THR
5	E	159	LEU
5	E	160	SER
5	E	166	LYS
5	E	170	SER
5	E	179	LEU
5	E	187	ASP
5	E	195	ARG
5	E	198	VAL
5	E	227	GLN
5	E	228	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	72	GLN
1	A	115	GLN
1	A	226	GLN
4	D	30	GLN
4	D	37	GLN
4	D	111	GLN
4	D	152	GLN
4	D	176	ASN

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Mol	Chain	Res	Type
5	E	28	ASN
5	E	57	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	F2F	C	5[A]	-	9,9,14	1.02	1 (11%)	12,12,19	2.08	2 (16%)
3	F2F	C	5[B]	-	9,9,14	0.96	1 (11%)	12,12,19	1.99	3 (25%)

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	F2F	C	5[A]	-	-	0/0/0/8	0/1/1/1
3	F2F	C	5[B]	-	-	0/0/0/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5[A]	F2F	CB-CG	2.27	1.51	1.40
3	C	5[B]	F2F	CB-CG	2.16	1.50	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5[B]	F2F	CD1-CG-CD2	5.04	120.47	114.14
3	C	5[A]	F2F	CD1-CG-CD2	4.77	120.13	114.14
3	C	5[A]	F2F	CB-CG-CD2	-4.44	118.42	122.94
3	C	5[B]	F2F	CB-CG-CD1	-3.40	119.48	122.94
3	C	5[B]	F2F	CB-CG-CD2	-2.88	120.01	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	0.41	0	5,5,5	0.17	0
6	GOL	A	277	-	5,5,5	0.28	0	5,5,5	0.40	0
6	GOL	B	100	-	5,5,5	0.27	0	5,5,5	0.48	0
6	GOL	B	101	-	5,5,5	0.38	0	5,5,5	0.12	0
6	GOL	E	247	-	5,5,5	0.47	0	5,5,5	0.64	0
6	GOL	E	248	-	5,5,5	0.27	0	5,5,5	0.27	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	277	-	-	0/4/4/4	0/0/0/0
6	GOL	B	100	-	-	0/4/4/4	0/0/0/0
6	GOL	B	101	-	-	0/4/4/4	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	0.28	22 (8%) 12 11	38, 63, 76, 85	0
2	B	100/100 (100%)	0.10	3 (3%) 48 49	53, 65, 73, 90	0
3	C	8/9 (88%)	-0.36	0 100 100	57, 61, 64, 65	0
4	D	200/200 (100%)	0.65	29 (14%) 3 3	53, 67, 77, 81	0
5	E	245/245 (100%)	0.06	10 (4%) 35 36	28, 61, 71, 77	0
All	All	828/829 (99%)	0.28	64 (7%) 13 12	28, 64, 75, 90	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	153	SER	9.3
4	D	184	LYS	8.5
4	D	171	MET	8.0
4	D	133	SER	7.7
5	E	1	ASN	6.3
4	D	205	PRO	5.8
1	A	1	GLY	5.2
4	D	154	LYS	5.0
1	A	260	HIS	4.9
1	A	221	GLY	4.5
4	D	206	SER	4.5
1	A	223	ASP	4.4
4	D	186	ASP	4.3
1	A	226	GLN	4.2
5	E	245	ALA	4.1
5	E	186	ASN	4.1
4	D	183	ASN	4.0
4	D	156	SER	4.0
1	A	195	SER	4.0
1	A	194	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	169	ARG	3.8
5	E	169	HIS	3.6
5	E	41	MET	3.6
4	D	185	SER	3.6
5	E	2	ALA	3.6
4	D	132	LYS	3.4
4	D	159	TYR	3.4
1	A	256	ARG	3.3
1	A	220	ASP	3.3
1	A	259	CYS	3.2
1	A	197	HIS	3.2
1	A	248	VAL	3.2
1	A	222	GLU	3.1
5	E	80	LEU	2.9
4	D	201	ASP	2.8
1	A	252	GLY	2.8
4	D	135	ASP	2.8
1	A	273	ARG	2.7
2	B	75	LYS	2.7
4	D	200	GLU	2.7
1	A	216	THR	2.6
5	E	139	HIS	2.6
4	D	149	ASN	2.6
4	D	188	ALA	2.6
4	D	155	ASP	2.6
5	E	134	GLU	2.5
5	E	246	ASP	2.5
4	D	129	ARG	2.5
4	D	134	SER	2.5
1	A	191	HIS	2.5
4	D	203	PHE	2.4
4	D	74	SER	2.3
4	D	204	PHE	2.3
4	D	197	ILE	2.3
2	B	24	ASN	2.2
2	B	99	MET	2.2
1	A	271	THR	2.2
4	D	187	PHE	2.2
1	A	228	THR	2.1
1	A	274	TRP	2.1
1	A	110	LEU	2.1
4	D	9	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	217	TRP	2.0
4	D	170	SER	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	F2F	C	5[B]	9/14	0.15	-	66,66,66,66	9
3	F2F	C	5[A]	9/14	0.15	-	65,66,66,66	9

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	276	6/6	0.17	-	65,66,66,66	0
6	GOL	E	248	6/6	0.34	-	64,64,64,64	6
6	GOL	E	247	6/6	0.25	-	67,68,69,69	0
6	GOL	B	100	6/6	0.34	-	56,57,57,57	6
6	GOL	A	277	6/6	0.30	-	68,68,68,68	6
6	GOL	B	101	6/6	0.26	-	68,70,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.