



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 AM GMT

PDB ID : 3D39  
Title : The complex between TCR A6 and human Class I MHC HLA-A2 with the modified HTLV-1 TAX (Y5(4-fluoroPhenylalanine)) peptide  
Authors : Borbulevych, O.Y.; Clemens, J.R.; Baker, B.M.  
Deposited on : 2008-05-09  
Resolution : 2.81 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

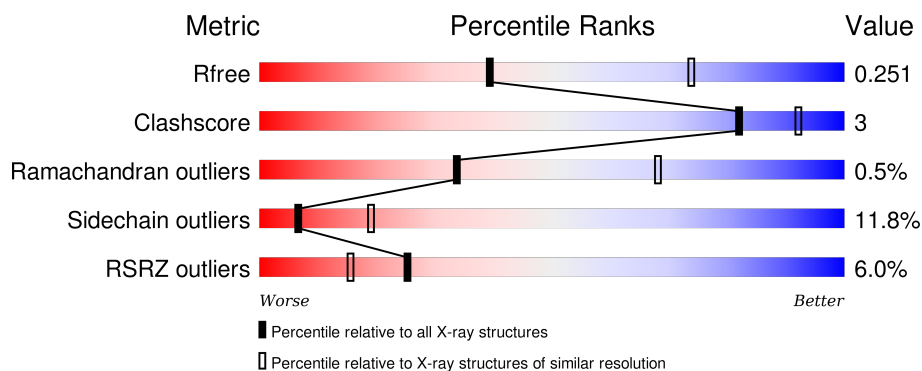
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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. 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	<div> <div>8%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	100	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>
4	D	200	<div> <div>9%</div> <div>78%</div> <div>21%</div> <div>..</div> </div>
5	E	245	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	E	250	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6718 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	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(4fluoro)F) peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	F	N	O	0	0	0
			77	56	1	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	D	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		
6	E	1	Total	C	O	0	0
			6	3	3		

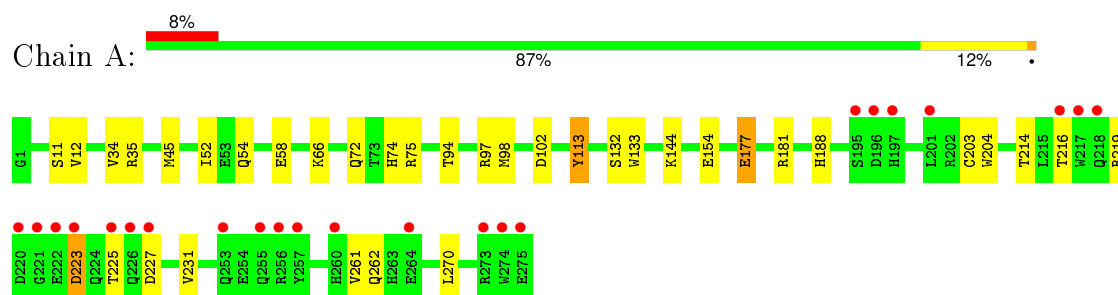
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total	O	0	0
			18	18		
7	B	13	Total	O	0	0
			13	13		
7	D	8	Total	O	0	0
			8	8		
7	E	14	Total	O	0	0
			14	14		

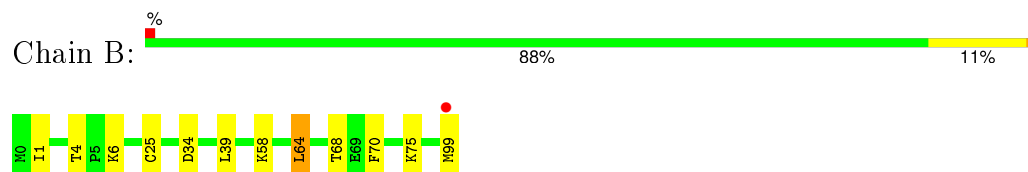
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

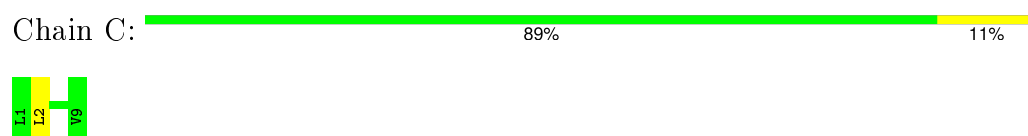
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



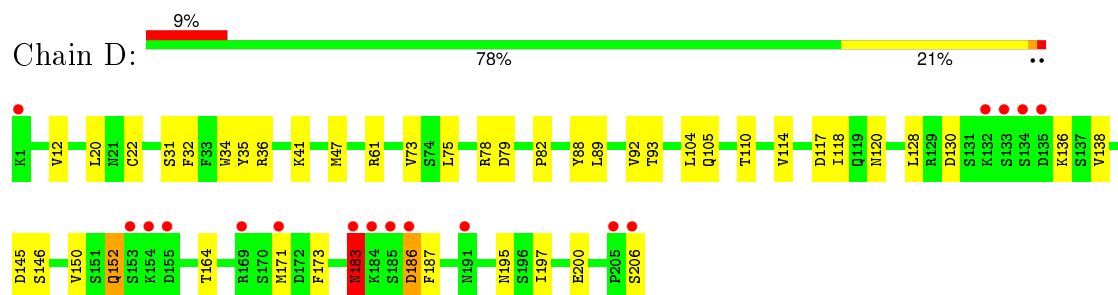
- Molecule 2: Beta-2-microglobulin



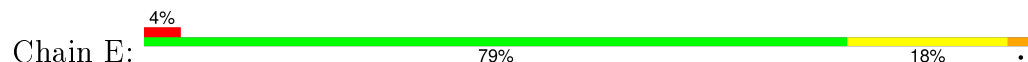
- Molecule 3: Modified HTLV-1 TAX (Y5(4fluoro)F) peptide

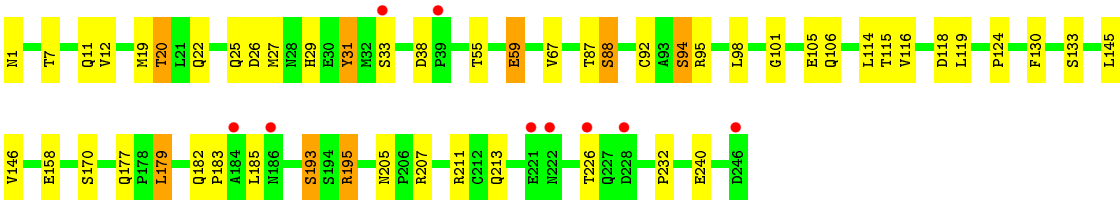


- Molecule 4: A6 TCR alpha chain



- 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, $\alpha$ , $\beta$ , $\gamma$	224.25Å 48.32Å 93.22Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	20.00 – 2.81 19.94 – 2.81	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.81) 90.7 (19.94-2.81)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.269 0.195 , 0.251	Depositor DCC
$R_{free}$ test set	1165 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.3	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22591 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PFF

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	0.59	0/2312	0.74	0/3137
2	B	0.60	0/860	0.75	0/1162
3	C	0.73	0/66	0.90	0/86
4	D	0.57	1/1585 (0.1%)	0.75	1/2150 (0.0%)
5	E	0.59	0/1981	0.80	1/2699 (0.0%)
All	All	0.59	1/6804 (0.0%)	0.76	2/9234 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	22	CYS	CB-SG	-5.92	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	179	LEU	CA-CB-CG	6.62	130.53	115.30
4	D	128	LEU	CA-CB-CG	5.02	126.84	115.30

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	2247	0	2096	9	0
2	B	837	0	803	2	0
3	C	77	0	77	1	0
4	D	1552	0	1461	16	0
5	E	1928	0	1832	17	0
6	D	6	0	8	2	0
6	E	18	0	24	2	0
7	A	18	0	0	0	0
7	B	13	0	0	0	0
7	D	8	0	0	0	0
7	E	14	0	0	1	0
All	All	6718	0	6301	42	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 (42) 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)
5:E:1:ASN:N	7:E:254:HOH:O	2.25	0.69
4:D:93:THR:HB	4:D:104:LEU:HD12	1.84	0.59
5:E:29:HIS:ND1	5:E:94:SER:OG	2.31	0.59
4:D:171:MET:HB3	4:D:173:PHE:HB2	1.86	0.58
5:E:193:SER:OG	5:E:195:ARG:NH1	2.40	0.55
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.90	0.52
1:A:223:ASP:OD1	1:A:223:ASP:N	2.34	0.51
5:E:11:GLN:HB3	5:E:114:LEU:HD13	1.92	0.51
4:D:183:ASN:N	4:D:183:ASN:OD1	2.42	0.51
4:D:104:LEU:O	6:D:207:GOL:O3	2.24	0.51
4:D:130:ASP:HA	5:E:130:PHE:HA	1.94	0.49
1:A:188:HIS:HB3	1:A:204:TRP:HB2	1.95	0.49
4:D:138:VAL:HG11	5:E:146:VAL:HG21	1.95	0.48
4:D:118:ILE:HD11	4:D:145:ASP:HA	1.97	0.47
4:D:35:TYR:HB2	4:D:89:LEU:HB2	1.97	0.46
5:E:124:PRO:HD3	5:E:232:PRO:HB3	1.96	0.46
5:E:87:THR:HG23	5:E:115:THR:HA	1.98	0.46
5:E:240:GLU:HG2	6:E:248:GOL:H31	1.98	0.46
1:A:66:LYS:NZ	3:C:2:LEU:O	2.48	0.45
1:A:177:GLU:HG2	1:A:177:GLU:H	1.46	0.45
4:D:82:PRO:HA	4:D:114:VAL:HB	1.98	0.44
4:D:61:ARG:NH1	4:D:79:ASP:O	2.51	0.44
5:E:31:TYR:HB3	5:E:95:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.28	0.44
4:D:34:TRP:HB2	4:D:47:MET:HB2	2.00	0.42
5:E:205:ASN:HD21	5:E:207:ARG:HH11	1.67	0.42
4:D:20:LEU:HB2	4:D:75:LEU:HB3	2.00	0.42
4:D:32:PHE:HD1	4:D:92:VAL:HG22	1.83	0.42
5:E:211:ARG:NH2	5:E:213:GLN:OE1	2.52	0.42
6:D:207:GOL:O2	5:E:59:GLU:OE1	2.37	0.42
2:B:64:LEU:HA	2:B:64:LEU:HD12	1.81	0.42
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.41
5:E:95:ARG:HG3	5:E:106:GLN:HB2	2.02	0.41
4:D:152:GLN:HB3	4:D:152:GLN:HE21	1.66	0.41
4:D:36:ARG:HG3	4:D:88:TYR:CE2	2.55	0.41
1:A:133:TRP:HB2	1:A:144:LYS:HG3	2.03	0.40
4:D:20:LEU:HD12	4:D:75:LEU:HD23	2.04	0.40
1:A:261:VAL:HB	1:A:270:LEU:HB2	2.04	0.40
5:E:20:THR:OG1	5:E:22:GLN:NE2	2.55	0.40
5:E:158:GLU:HA	6:E:250:GOL:H11	2.02	0.40
5:E:38:ASP:OD2	5:E:88:SER:OG	2.29	0.40
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.40	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	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	6/9 (67%)	5 (83%)	1 (17%)	0	100	100
4	D	198/200 (99%)	175 (88%)	21 (11%)	2 (1%)	19	51
5	E	243/245 (99%)	233 (96%)	8 (3%)	2 (1%)	24	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	818/829 (99%)	774 (95%)	40 (5%)	4 (0%)	34 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	101	GLY
4	D	183	ASN
4	D	186	ASP
5	E	183	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%)	207 (90%)	24 (10%)	9 25
2	B	95/95 (100%)	85 (90%)	10 (10%)	8 24
3	C	7/7 (100%)	7 (100%)	0	100 100
4	D	178/178 (100%)	157 (88%)	21 (12%)	6 19
5	E	209/209 (100%)	179 (86%)	30 (14%)	4 11
All	All	720/720 (100%)	635 (88%)	85 (12%)	6 19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	12	VAL
1	A	34	VAL
1	A	35	ARG
1	A	45	MET
1	A	52	ILE
1	A	54	GLN
1	A	58	GLU
1	A	72	GLN
1	A	75	ARG

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Mol	Chain	Res	Type
1	A	94	THR
1	A	98	MET
1	A	113	TYR
1	A	132	SER
1	A	154	GLU
1	A	177	GLU
1	A	181	ARG
1	A	203	CYS
1	A	216	THR
1	A	219	ARG
1	A	223	ASP
1	A	225	THR
1	A	227	ASP
1	A	231	VAL
2	B	1	ILE
2	B	4	THR
2	B	6	LYS
2	B	34	ASP
2	B	58	LYS
2	B	64	LEU
2	B	68	THR
2	B	70	PHE
2	B	75	LYS
2	B	99	MET
4	D	12	VAL
4	D	31	SER
4	D	41	LYS
4	D	73	VAL
4	D	78	ARG
4	D	105	GLN
4	D	110	THR
4	D	117	ASP
4	D	120	ASN
4	D	136	LYS
4	D	146	SER
4	D	150	VAL
4	D	152	GLN
4	D	164	THR
4	D	183	ASN
4	D	186	ASP
4	D	187	PHE
4	D	195	ASN

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Mol	Chain	Res	Type
4	D	197	ILE
4	D	200	GLU
4	D	206	SER
5	E	7	THR
5	E	12	VAL
5	E	19	MET
5	E	20	THR
5	E	25	GLN
5	E	26	ASP
5	E	27	MET
5	E	31	TYR
5	E	33	SER
5	E	55	THR
5	E	59	GLU
5	E	67	VAL
5	E	88	SER
5	E	92	CYS
5	E	94	SER
5	E	98	LEU
5	E	105	GLU
5	E	116	VAL
5	E	118	ASP
5	E	119	LEU
5	E	133	SER
5	E	145	LEU
5	E	170	SER
5	E	177	GLN
5	E	179	LEU
5	E	182	GLN
5	E	185	LEU
5	E	193	SER
5	E	195	ARG
5	E	226	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	224	GLN
2	B	2	GLN
4	D	37	GLN
4	D	105	GLN

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Mol	Chain	Res	Type
4	D	111	GLN
4	D	152	GLN
5	E	1	ASN
5	E	22	GLN
5	E	37	GLN
5	E	57	GLN
5	E	227	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PFF	C	5	3	11,12,13	0.85	0	12,15,17	2.09	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	PFF	C	5	3	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	PFF	CG-CB-CA	-5.62	101.52	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	PFF	O-C-CA	-2.32	119.45	125.49
3	C	5	PFF	CD2-CG-CD1	2.28	121.78	118.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	D	207	-	5,5,5	0.34	0	5,5,5	0.35	0
6	GOL	E	248	-	5,5,5	0.45	0	5,5,5	0.64	0
6	GOL	E	249	-	5,5,5	0.34	0	5,5,5	0.33	0
6	GOL	E	250	-	5,5,5	0.23	0	5,5,5	0.33	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	D	207	-	-	0/4/4/4	0/0/0/0
6	GOL	E	248	-	-	0/4/4/4	0/0/0/0
6	GOL	E	249	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	250	-	-	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	207	GOL	2	0
6	E	248	GOL	1	0
6	E	250	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

### 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%)	0.29	23 (8%) 14 6	53, 66, 80, 85	0
2	B	100/100 (100%)	-0.11	1 (1%) 84 77	47, 64, 75, 87	0
3	C	8/9 (88%)	-0.48	0 100 100	58, 64, 65, 67	0
4	D	200/200 (100%)	0.40	17 (8%) 13 6	57, 67, 78, 83	0
5	E	245/245 (100%)	0.06	9 (3%) 45 33	54, 65, 78, 83	0
All	All	828/829 (99%)	0.19	50 (6%) 25 15	47, 66, 78, 87	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ASP	5.7
1	A	220	ASP	5.5
1	A	273	ARG	5.3
4	D	171	MET	5.3
1	A	253	GLN	5.2
4	D	184	LYS	4.8
4	D	183	ASN	4.8
4	D	133	SER	4.8
4	D	134	SER	4.6
4	D	206	SER	4.5
1	A	257	TYR	4.4
1	A	222	GLU	4.1
4	D	155	ASP	4.0
1	A	221	GLY	3.9
4	D	185	SER	3.8
5	E	246	ASP	3.7
1	A	197	HIS	3.7
4	D	205	PRO	3.6
1	A	260	HIS	3.6
2	B	99	MET	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	135	ASP	3.5
4	D	154	LYS	3.4
5	E	221	GLU	3.3
4	D	186	ASP	3.3
5	E	184	ALA	3.2
4	D	132	LYS	3.1
1	A	227	ASP	3.1
4	D	169	ARG	3.1
1	A	218	GLN	3.0
5	E	39	PRO	2.9
5	E	33	SER	2.8
4	D	1	LYS	2.8
1	A	226	GLN	2.7
4	D	153	SER	2.7
5	E	228	ASP	2.6
1	A	256	ARG	2.6
1	A	225	THR	2.4
1	A	196	ASP	2.4
1	A	201	LEU	2.3
1	A	216	THR	2.3
1	A	274	TRP	2.3
5	E	226	THR	2.2
4	D	191	ASN	2.2
1	A	217	TRP	2.2
1	A	275	GLU	2.1
5	E	186	ASN	2.1
1	A	255	GLN	2.1
5	E	222	ASN	2.1
1	A	195	SER	2.1
1	A	264	GLU	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PFF	C	5	12/13	0.97	0.12	-	59,60,63,64	0

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	E	250	6/6	0.83	0.42	3.87	59,61,62,62	0
6	GOL	D	207	6/6	0.83	0.26	1.61	69,71,71,71	0
6	GOL	E	248	6/6	0.87	0.44	-	50,52,52,52	6
6	GOL	E	249	6/6	0.88	0.44	-	72,73,73,73	0

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

There are no such residues in this entry.