



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:35 AM UTC

PDB ID : 3D39 / pdb_00003d39
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

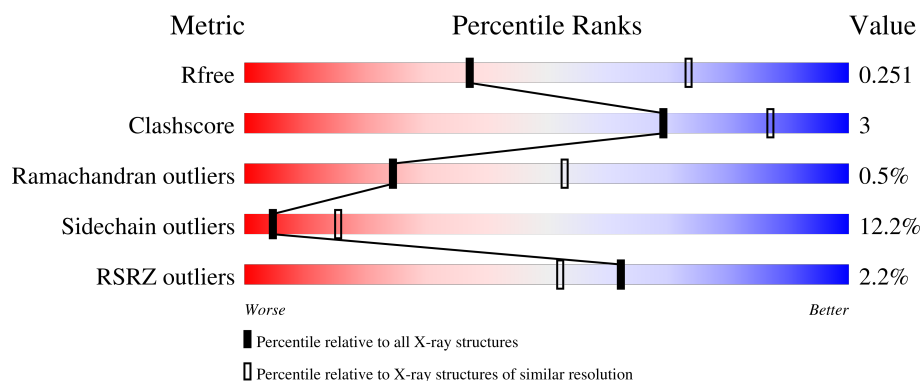
1 Overall quality at a glance

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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 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	275	4% 85% 14% .
2	B	100	% 88% 11% .
3	C	9	78% 22%
4	D	200	2% 74% 24% .
5	E	245	76% 21% .

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 (CCD ID: 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		

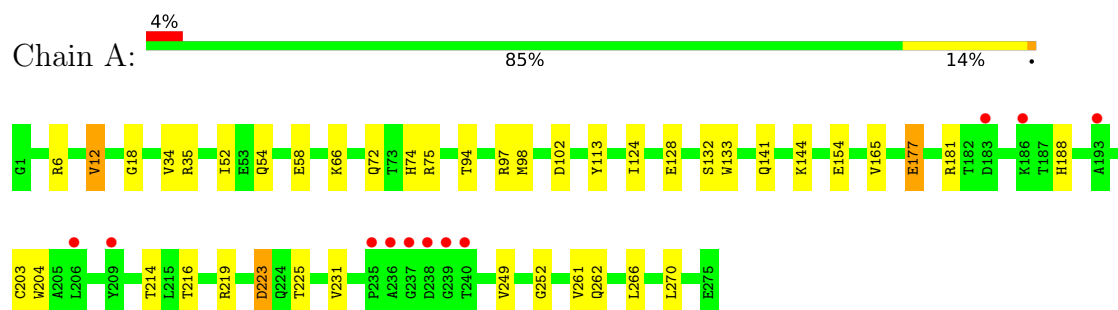
- Molecule 7 is water.

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		

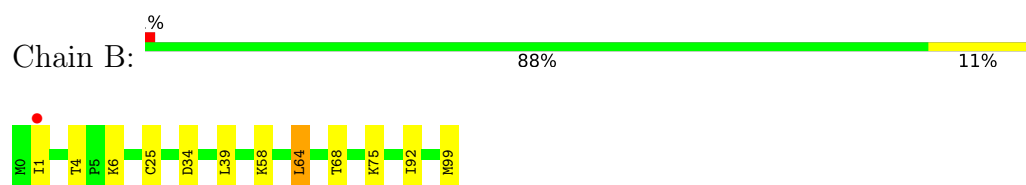
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

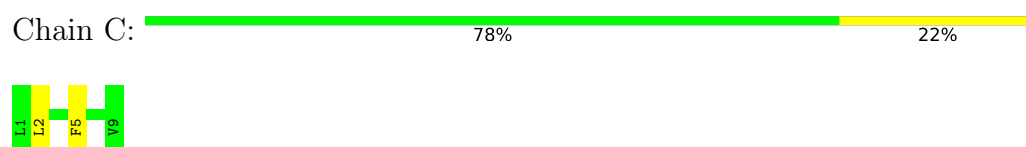
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



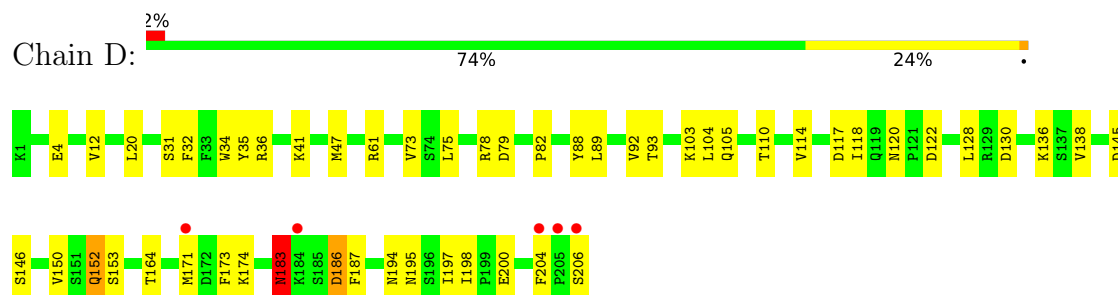
- Molecule 2: Beta-2-microglobulin



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



- Molecule 4: A6 TCR alpha chain

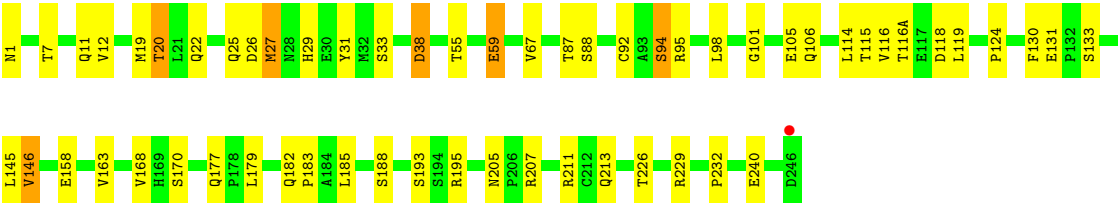


- Molecule 5: A6 TCR beta chain

Chain E:

76%

21%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.25Å 48.32Å 93.22Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	20.00 – 2.81 20.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.81) 90.7 (20.00-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1166 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6718	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 5.25% 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, 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	0.74	1/2312 (0.0%)	1.09	5/3137 (0.2%)
2	B	0.71	0/860	1.07	0/1162
3	C	0.78	0/66	1.08	0/86
4	D	0.73	0/1585	1.16	6/2150 (0.3%)
5	E	0.72	0/1981	1.12	7/2699 (0.3%)
All	All	0.73	1/6804 (0.0%)	1.11	18/9234 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	VAL	CA-CB	7.60	1.64	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	204	PHE	CA-C-N	7.98	127.93	120.03
4	D	204	PHE	C-N-CA	7.98	127.93	120.03
5	E	38	ASP	CA-C-N	7.61	129.35	119.84
5	E	38	ASP	C-N-CA	7.61	129.35	119.84
1	A	18	GLY	N-CA-C	6.74	118.92	110.29
4	D	122	ASP	CA-C-N	6.46	126.41	119.76
4	D	122	ASP	C-N-CA	6.46	126.41	119.76
5	E	168	VAL	N-CA-C	5.94	117.15	108.53
5	E	131	GLU	CA-C-N	5.57	126.80	119.84
5	E	131	GLU	C-N-CA	5.57	126.80	119.84
1	A	252	GLY	N-CA-C	-5.56	107.36	114.37
1	A	266	LEU	CA-C-N	5.38	124.56	118.97
1	A	266	LEU	C-N-CA	5.38	124.56	118.97
5	E	188	SER	N-CA-C	5.32	118.06	110.24
1	A	128	GLU	N-CA-C	5.31	117.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	153	SER	O-C-N	5.24	124.71	120.83
5	E	229	ARG	N-CA-C	-5.12	103.64	110.55
4	D	103	LYS	N-CA-C	5.10	117.49	110.35

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	11	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	18	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	45	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 (45) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:223:ASP:N	2.34	0.51
4:D:183:ASN:OD1	4:D:183:ASN:N	2.42	0.51
5:E:11:GLN:HB3	5:E:114:LEU:HD13	1.92	0.51
4:D:104:LEU:O	6:D:207:GOL:O3	2.24	0.50
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
5:E:38:ASP:OD2	5:E:88:SER:OG	2.29	0.46
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:27:MET:HE2	5:E:27:MET:HB3	1.73	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:98:MET:HE1	1:A:113:TYR:CE1	2.51	0.45
1:A:177:GLU:H	1:A:177:GLU:HG2	1.46	0.45
4:D:82:PRO:HA	4:D:114:VAL:HB	1.98	0.44
1:A:6:ARG:HD3	1:A:98:MET:HE3	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
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:HD12	2:B:64:LEU:HA	1.81	0.42
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.41
4:D:152:GLN:HE21	4:D:152:GLN:HB3	1.66	0.41
5:E:95:ARG:HG3	5:E:106:GLN:HB2	2.02	0.41
4:D:36:ARG:HG3	4:D:88:TYR:CE2	2.55	0.41
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.28	0.41
1:A:133:TRP:HB2	1:A:144:LYS:HG3	2.03	0.40
1:A:261:VAL:HB	1:A:270:LEU:HB2	2.04	0.40
4:D:20:LEU:HD12	4:D:75:LEU:HD23	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
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.40	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%)	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%)	12	36
5	E	243/245 (99%)	233 (96%)	8 (3%)	2 (1%)	16	41
All	All	818/829 (99%)	774 (95%)	40 (5%)	4 (0%)	24	53

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%)	208 (90%)	23 (10%)	7	23
2	B	95/95 (100%)	85 (90%)	10 (10%)	6	21
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	178/178 (100%)	152 (85%)	26 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	209/209 (100%)	180 (86%)	29 (14%)	3	11
All	All	720/720 (100%)	632 (88%)	88 (12%)	5	15

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	34	VAL
1	A	35	ARG
1	A	52	ILE
1	A	54	GLN
1	A	58	GLU
1	A	72	GLN
1	A	75	ARG
1	A	94	THR
1	A	124	ILE
1	A	132	SER
1	A	141	GLN
1	A	154	GLU
1	A	165	VAL
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	231	VAL
1	A	249	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	75	LYS
2	B	92	ILE
2	B	99	MET
4	D	4	GLU
4	D	12	VAL
4	D	31	SER

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Mol	Chain	Res	Type
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	128	LEU
4	D	136	LYS
4	D	146	SER
4	D	150	VAL
4	D	152	GLN
4	D	164	THR
4	D	174	LYS
4	D	183	ASN
4	D	186	ASP
4	D	187	PHE
4	D	194	ASN
4	D	195	ASN
4	D	197	ILE
4	D	198	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	33	SER
5	E	55	THR
5	E	59	GLU
5	E	67	VAL
5	E	92	CYS
5	E	94	SER
5	E	98	LEU
5	E	105	GLU
5	E	116	VAL
5	E	116(A)	THR
5	E	118	ASP
5	E	119	LEU

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Mol	Chain	Res	Type
5	E	133	SER
5	E	145	LEU
5	E	146	VAL
5	E	163	VAL
5	E	170	SER
5	E	177	GLN
5	E	179	LEU
5	E	182	GLN
5	E	185	LEU
5	E	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	115	GLN
1	A	224	GLN
4	D	37	GLN
4	D	81	GLN
4	D	105	GLN
4	D	111	GLN
4	D	119	GLN
4	D	152	GLN
5	E	1	ASN
5	E	17	GLN
5	E	22	GLN
5	E	37	GLN
5	E	57	GLN
5	E	106	GLN
5	E	177	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	0.84	0	10,15,17	1.29	1 (10%)

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	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	5	PFF	CD2-CG-CD1	2.39	121.78	118.23

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 oligosaccharides 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	E	250	-	5,5,5	0.29	0	5,5,5	0.34	0
6	GOL	E	248	-	5,5,5	0.48	0	5,5,5	0.66	0
6	GOL	E	249	-	5,5,5	0.41	0	5,5,5	0.34	0
6	GOL	D	207	-	5,5,5	0.39	0	5,5,5	0.37	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	E	250	-	-	2/4/4/4	-
6	GOL	E	248	-	-	0/4/4/4	-
6	GOL	E	249	-	-	4/4/4/4	-
6	GOL	D	207	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	249	GOL	O1-C1-C2-C3
6	E	249	GOL	C1-C2-C3-O3
6	E	250	GOL	C1-C2-C3-O3
6	E	249	GOL	O1-C1-C2-O2
6	E	250	GOL	O2-C2-C3-O3
6	E	249	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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, 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	275/275 (100%)	0.18	11 (4%) 42 33	53, 66, 80, 85	0
2	B	100/100 (100%)	-0.26	1 (1%) 79 72	47, 64, 75, 87	0
3	C	8/9 (88%)	-0.52	0 100 100	58, 64, 65, 67	0
4	D	200/200 (100%)	0.19	5 (2%) 58 48	57, 67, 78, 83	0
5	E	245/245 (100%)	-0.14	1 (0%) 88 84	54, 65, 78, 83	0
All	All	828/829 (99%)	0.03	18 (2%) 62 52	47, 66, 78, 87	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	5.0
1	A	236	ALA	3.5
4	D	205	PRO	3.0
5	E	246	ASP	2.9
4	D	206	SER	2.8
1	A	235	PRO	2.7
1	A	209	TYR	2.5
1	A	239	GLY	2.3
4	D	184	LYS	2.3
1	A	186	LYS	2.3
1	A	193	ALA	2.2
1	A	206	LEU	2.2
1	A	238	ASP	2.2
4	D	171	MET	2.1
1	A	240	THR	2.1
1	A	183	ASP	2.1
2	B	1	ILE	2.1
4	D	204	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	PFF	C	5	12/13	0.95	0.07	59,60,63,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
6	GOL	E	249	6/6	0.69	0.15	72,73,73,73	0
6	GOL	E	248	6/6	0.82	0.26	50,52,52,52	6
6	GOL	E	250	6/6	0.84	0.18	59,61,62,62	0
6	GOL	D	207	6/6	0.87	0.13	69,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.