

Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2021 – 04:01 am BST

PDB ID : 6TRO

Title: Crystal structure of the T-cell receptor GVY01 bound to HLA A2*01-

GVYDGREHTV

Authors: Coles, C.H.; McMurran, C.; Lloyd, A.; Hibbert, L.; Lupardus, P.J.; Cole, D.K.;

Harper, S.

Deposited on : 2019-12-19

Resolution : 3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

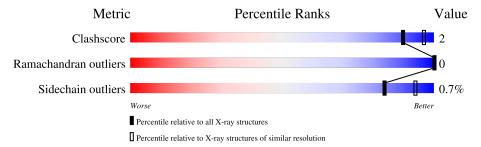
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	A	276	96%	
2	В	100	99%	
3	С	10	90%	10%
4	D	208	85% 6%	9%
5	Е	247	89%	9% •



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6595 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	273	Total 2233	C 1396	N 407	O 421	S 9	0	0	0

• Molecule 2 is a protein called Beta-2-microglobulin.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

• Molecule 3 is a protein called MAGE-A4 peptide (amino acids 230-239).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	10	Total 80	C 48	N 15	O 17	0	0	0

• Molecule 4 is a protein called T-cell receptor alpha chain.

Mo	l Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total 1465	C 915	N 245	O 297	S 8	0	0	0

• Molecule 5 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	Е	242	Total 1957	C 1239	N 332	O 376	S 10	0	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	В	3	Total O 3 3	0	0
6	С	1	Total O 1 1	0	0
6	D	9	Total O 9 9	0	0
6	Е	6	Total O 6 6	0	0

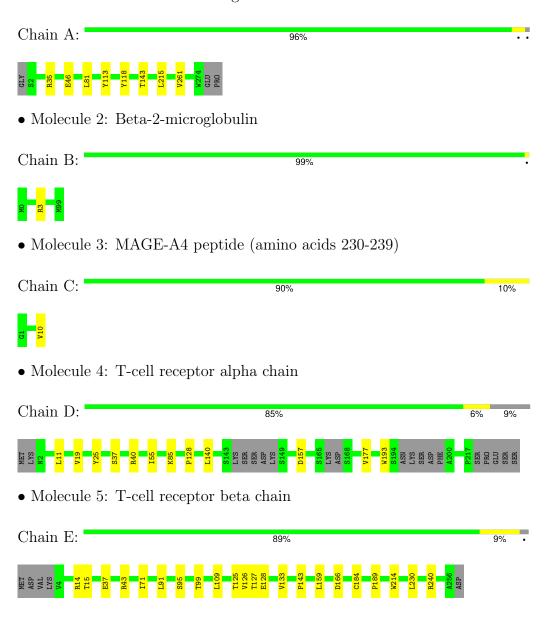


3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

• Molecule 1: MHC class I antigen





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 64 2 2	Depositor	
Cell constants	220.04Å 220.04Å 96.83Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	67.91 - 3.00	Depositor	
% Data completeness	98.5 (67.91-3.00)	Depositor	
(in resolution range)	, ,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC 5.8.0238	Depositor	
R, R_{free}	0.213 , 0.270	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6595	wwPDB-VP	
Average B, all atoms (Å ²)	111.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.63	0/2298	0.72	0/3120	
2	В	0.62	0/860	0.72	0/1162	
3	С	0.67	0/81	0.75	0/107	
4	D	0.64	0/1494	0.74	0/2030	
5	Е	0.62	0/2009	0.71	0/2726	
All	All	0.63	0/6742	0.72	0/9145	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2233	0	2084	4	0
2	В	837	0	803	0	0
3	С	80	0	72	1	0
4	D	1465	0	1396	7	0
5	Ε	1957	0	1867	13	0
6	A	4	0	0	0	0
6	В	3	0	0	0	0
6	С	1	0	0	0	0
6	D	9	0	0	0	0
6	Ε	6	0	0	0	0
All	All	6595	0	6222	23	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 2.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)	
5:E:37:GLU:HB2	5:E:109:LEU:HD13	1.76	0.67	
4:D:11:LEU:HD11	4:D:19:VAL:HG23	1.84	0.59	
4:D:40:ARG:NH2	4:D:55:ILE:HD12	2.20	0.57	
5:E:14:ARG:HA	5:E:127:THR:O	2.07	0.54	
5:E:133:VAL:HG11	5:E:230:LEU:HD13	1.91	0.52	
5:E:166:ASP:OD1	5:E:189:PRO:HG3	2.12	0.50	
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.48	0.49	
5:E:133:VAL:O	5:E:240:ARG:NH1	2.45	0.49	
1:A:143:THR:HG23	3:C:10:VAL:HA	1.95	0.48	
4:D:128:PRO:HD3	4:D:177:VAL:HG21	1.95	0.48	
5:E:43:ARG:HD3	5:E:71:ILE:HD12	1.96	0.47	
4:D:193:TRP:CD2	5:E:159:LEU:HD21	2.52	0.45	
4:D:140:LEU:N	4:D:140:LEU:HD12	2.31	0.45	
4:D:11:LEU:HD11	4:D:19:VAL:CG2	2.47	0.44	
4:D:25:TYR:CZ	4:D:85:LYS:HA	2.51	0.44	
5:E:143:PRO:HD2	5:E:214:TRP:CZ2	2.53	0.44	
5:E:37:GLU:CB	5:E:109:LEU:HD13	2.46	0.43	
1:A:35:ARG:NH1	1:A:46:GLU:OE1	2.51	0.43	
1:A:215:LEU:HD22	1:A:261:VAL:HG22	2.01	0.43	
5:E:15:THR:HG23	5:E:128:GLU:HA	2.01	0.42	
5:E:99:THR:HG23	5:E:125:THR:HA	2.01	0.42	
5:E:95:SER:N	5:E:126:VAL:HG11	2.34	0.41	
5:E:91:LEU:HD12	5:E:91:LEU:N	2.35	0.41	

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	Perce	ntiles
1	A	271/276 (98%)	256 (94%)	15 (6%)	0	100	100
2	В	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
3	С	8/10 (80%)	8 (100%)	0	0	100	100
4	D	181/208 (87%)	174 (96%)	7 (4%)	0	100	100
5	E	240/247 (97%)	233 (97%)	7 (3%)	0	100	100
All	All	798/841 (95%)	759 (95%)	39 (5%)	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 Percent		ntiles
1	A	230/232 (99%)	229 (100%)	1 (0%)	91	97
2	В	95/95 (100%)	94 (99%)	1 (1%)	73	90
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	171/190 (90%)	169 (99%)	2 (1%)	71	90
5	${f E}$	216/221 (98%)	215 (100%)	1 (0%)	88	96
All	All	720/746 (96%)	715 (99%)	5 (1%)	84	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
2	В	3	ARG
4	D	37	SER
4	D	157	ASP
5	Е	184	CYS

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



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

