



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 04:32 PM UTC

PDB ID : 6D7G / pdb_00006d7g
Title : Structure of 5F3 TCR in complex with HLA-A2/MART-1
Authors : Roy, S.; Adams, E.J.
Deposited on : 2018-04-24
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

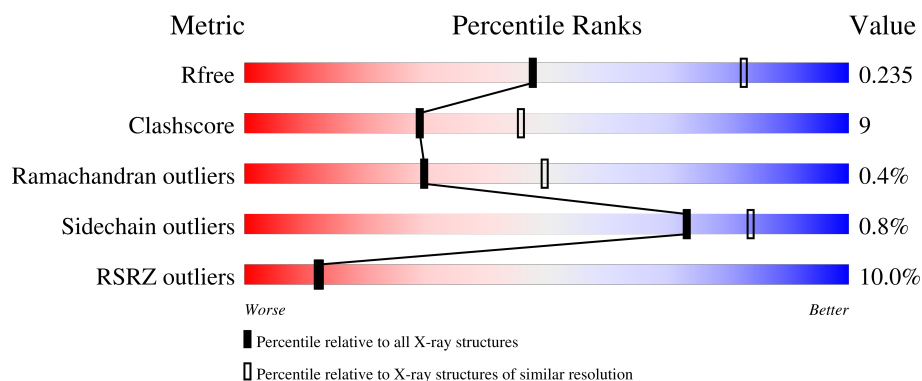
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	427	4% 76% 14% 10%
2	D	229	7% 67% 19% 14%
3	E	258	17% 59% 21% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6022 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 MART1 PEPTIDE-BETA-2-MICROGLOBULIN-HLA-A*02 CHIMERA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3023	1907	535	571	10			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLY	-	linker	PDB ?
A	87	GLY	-	linker	PDB ?
A	88	GLY	-	linker	PDB ?
A	89	GLY	-	linker	PDB ?
A	90	SER	-	linker	PDB ?
A	91	GLY	-	linker	PDB ?
A	92	GLY	-	linker	PDB ?
A	93	GLY	-	linker	PDB ?
A	94	GLY	-	linker	PDB ?
A	95	SER	-	linker	PDB ?
A	96	GLY	-	linker	PDB ?
A	97	GLY	-	linker	PDB ?
A	98	GLY	-	linker	PDB ?
A	99	GLY	-	linker	PDB ?
A	100	SER	-	linker	PDB ?
A	981	GLY	-	linker	UNP P61769
A	982	GLY	-	linker	UNP P61769
A	983	GLY	-	linker	UNP P61769
A	984	GLY	-	linker	UNP P61769
A	985	SER	-	linker	UNP P61769
A	986	GLY	-	linker	UNP P61769
A	987	GLY	-	linker	UNP P61769
A	988	GLY	-	linker	UNP P61769
A	989	GLY	-	linker	UNP P61769
A	990	SER	-	linker	UNP P61769
A	991	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
A	992	GLY	-	linker	UNP P61769
A	993	GLY	-	linker	UNP P61769
A	994	GLY	-	linker	UNP P61769
A	995	SER	-	linker	UNP P61769
A	996	GLY	-	linker	UNP P61769
A	997	GLY	-	linker	UNP P61769
A	998	GLY	-	linker	UNP P61769
A	999	GLY	-	linker	UNP P61769
A	1000	SER	-	linker	UNP P61769
A	1276	HIS	-	expression tag	UNP P01892
A	1277	HIS	-	expression tag	UNP P01892
A	1278	HIS	-	expression tag	UNP P01892
A	1279	HIS	-	expression tag	UNP P01892
A	1280	HIS	-	expression tag	UNP P01892
A	1281	HIS	-	expression tag	UNP P01892
A	1282	HIS	-	expression tag	UNP P01892
A	1283	HIS	-	expression tag	UNP P01892

- Molecule 2 is a protein called TRA@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	198	Total	C	N	O	S	0	0	0
			1489	949	252	281	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP Q6PJ56
D	-1	ASP	-	expression tag	UNP Q6PJ56
D	0	PRO	-	expression tag	UNP Q6PJ56
D	96	LEU	-	linker	UNP Q6PJ56
D	97	GLY	-	linker	UNP Q6PJ56
D	98	TRP	-	linker	UNP Q6PJ56
D	99	ASP	-	linker	UNP Q6PJ56

- Molecule 3 is a protein called T-CELL RECEPTOR GAMMA VARIABLE 8,T-CELL RECEPTOR GAMMA-2 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	208	Total	C	N	O	S	0	0	0
			1493	952	254	281	6			

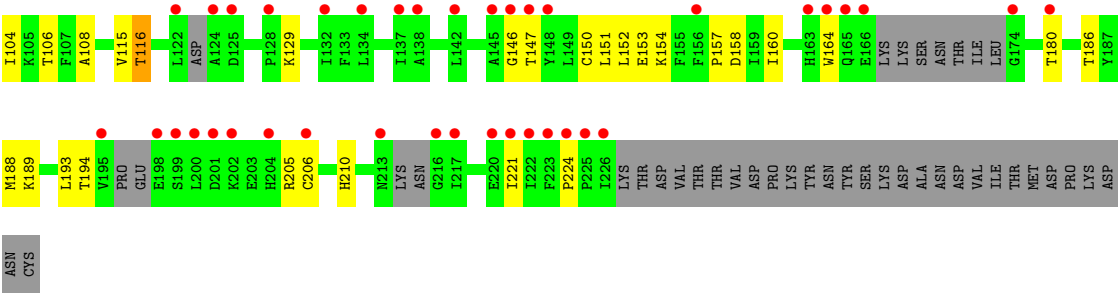
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	123.95Å 123.95Å 154.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 2.75 48.30 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.30-2.75) 99.9 (48.30-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.211 , 0.237 0.213 , 0.235	Depositor DCC
R_{free} test set	1806 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6022	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 3.13% 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: NAG

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	0.56	0/3109	0.63	0/4242
2	D	0.66	0/1522	1.08	4/2072 (0.2%)
3	E	0.49	0/1527	0.64	0/2092
All	All	0.57	0/6158	0.77	4/8406 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	107	LYS	N-CA-C	-7.88	99.91	110.55
2	D	113	VAL	CA-C-N	6.12	138.35	120.97
2	D	113	VAL	C-N-CA	6.12	138.35	120.97
2	D	137	LEU	CA-CB-CG	5.40	135.20	116.30

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	3023	0	2741	39	0
2	D	1489	0	1414	28	0
3	E	1493	0	1287	38	0
4	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	6022	0	5455	100	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 9.

The worst 5 of 100 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)
3:E:147:THR:HA	3:E:193:LEU:O	1.72	0.90
2:D:42:SER:OG	2:D:44:GLU:OE1	1.98	0.81
3:E:25:LEU:HB2	3:E:108:ALA:HB2	1.65	0.79
3:E:71:TYR:HE2	3:E:81:ILE:HD11	1.50	0.77
1:A:1219:ARG:NH2	1:A:1257:TYR:OH	2.17	0.77

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	380/427 (89%)	370 (97%)	9 (2%)	1 (0%)	36	56
2	D	194/229 (85%)	181 (93%)	12 (6%)	1 (0%)	24	43
3	E	196/258 (76%)	178 (91%)	17 (9%)	1 (0%)	24	43
All	All	770/914 (84%)	729 (95%)	38 (5%)	3 (0%)	30	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
3	E	224	PRO
2	D	140	GLU

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	Percentiles	
1	A	301/347 (87%)	300 (100%)	1 (0%)	86	93
2	D	155/206 (75%)	154 (99%)	1 (1%)	78	88
3	E	136/235 (58%)	133 (98%)	3 (2%)	45	67
All	All	592/788 (75%)	587 (99%)	5 (1%)	73	84

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

Mol	Chain	Res	Type
1	A	134	ASP
2	D	77	THR
3	E	46	ARG
3	E	90	SER
3	E	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	82	GLN
2	D	190	GLN
3	E	38	HIS
3	E	54	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
4	NAG	D	301	2	14,14,15	0.20	0	17,19,21	0.56	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
4	NAG	D	301	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	386/427 (90%)	0.06	18 (4%)	36 36	31, 56, 93, 121	0
2	D	198/229 (86%)	0.40	17 (8%)	16 16	41, 57, 127, 154	0
3	E	208/258 (80%)	0.94	44 (21%)	2 2	39, 81, 155, 175	0
All	All	792/914 (86%)	0.38	79 (9%)	12 12	31, 59, 131, 175	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ASP	4.9
3	E	29	ASN	4.9
3	E	195	VAL	4.7
2	D	1	ALA	4.7
3	E	199	SER	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	D	301	14/15	0.59	0.23	53,74,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.