



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 6RPA / pdb_00006rpa
Title : Crystal structure of the T-cell receptor NYE_S2 bound to HLA A2*01-SLLMWITQV
Authors : Coles, C.H.; Mulvaney, R.; Malla, S.; Lloyd, A.; Smith, K.; Chester, F.; Knox, A.; Stacey, A.R.; Dukes, J.; Baston, E.; Griffin, S.; Vuidepot, A.; Jakobsen, B.K.; Harper, S.
Deposited on : 2019-05-14
Resolution : 2.56 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
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

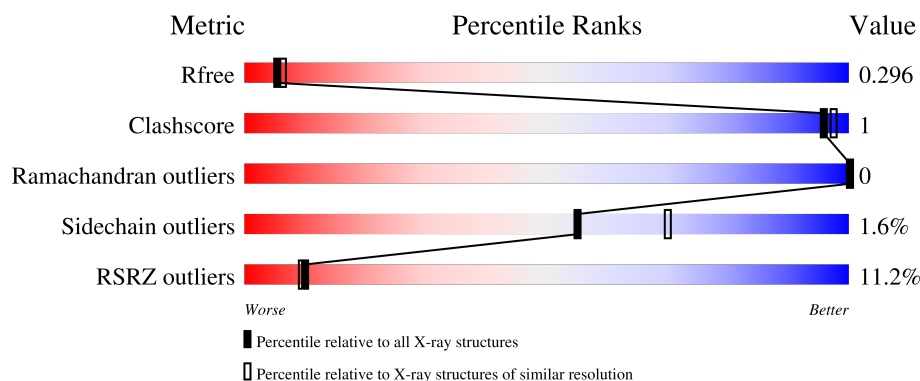
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	277	3% 95% .
2	B	100	7% 98% ..
3	C	9	89% 11%
4	D	212	17% 76% . 22%
5	E	246	15% 89% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6326 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	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Heteroclitic NY-ESO-1 157-165 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1292	823	209	256	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	235	Total	C	N	O	S	0	0	0
			1827	1148	310	361	8			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	8	Total	O	0	0
			8	8		
6	C	1	Total	O	0	0
			1	1		
6	D	3	Total	O	0	0
			3	3		
6	E	5	Total	O	0	0
			5	5		

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.

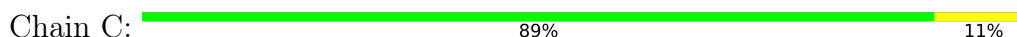
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



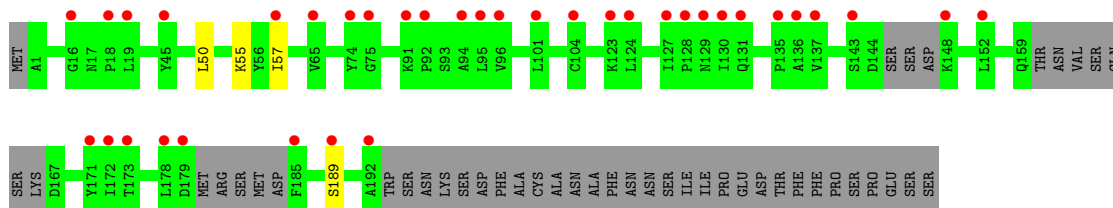
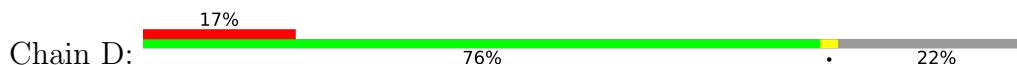
- Molecule 2: Beta-2-microglobulin



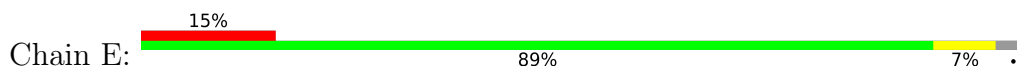
- Molecule 3: Heteroclitic NY-ESO-1 157-165 peptide

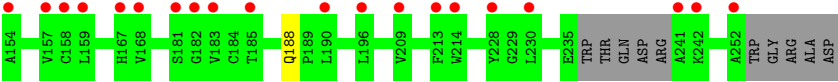
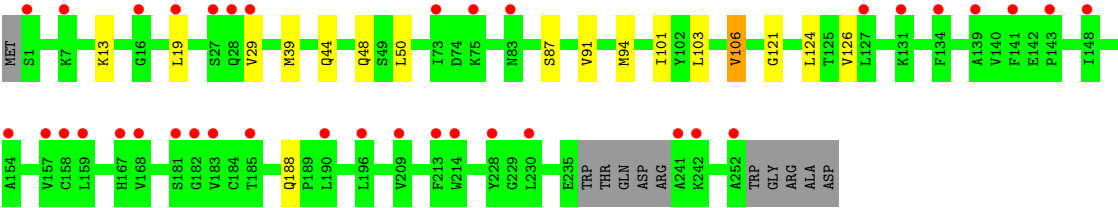


- Molecule 4: T-cell receptor alpha chain



- Molecule 5: T-cell receptor beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.16Å 84.25Å 111.51Å 90.00° 129.81° 90.00°	Depositor
Resolution (Å)	66.51 – 2.56 66.51 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.51-2.56) 99.3 (66.51-2.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.250 , 0.293 0.252 , 0.296	Depositor DCC
R_{free} test set	1945 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6326	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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 [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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/2319	0.80	0/3149
2	B	0.57	0/852	0.75	0/1152
3	C	0.48	0/77	0.80	0/103
4	D	0.58	0/1319	0.70	0/1788
5	E	0.60	0/1870	0.72	0/2546
All	All	0.59	0/6437	0.75	0/8738

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	2253	0	2103	5	0
2	B	829	0	794	0	0
3	C	76	0	83	1	0
4	D	1292	0	1242	2	0
5	E	1827	0	1759	8	0
6	A	32	0	0	0	0
6	B	8	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	5	0	0	0	0
All	All	6326	0	5981	14	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 1.

All (14) 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:13:LYS:HB2	5:E:94:MET:HE1	1.89	0.55
5:E:39:MET:SD	5:E:87:SER:HB3	2.50	0.52
1:A:70:HIS:CE1	3:C:6:ILE:HD11	2.46	0.49
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.49	0.48
5:E:29:VAL:HG11	5:E:106:VAL:CG1	2.44	0.47
5:E:29:VAL:HG11	5:E:106:VAL:HG13	1.97	0.46
5:E:94:MET:HE3	5:E:126:VAL:HG22	1.98	0.45
1:A:98:MET:HE1	1:A:113:TYR:CD1	2.51	0.45
1:A:187:THR:HG21	1:A:261:VAL:HG21	2.00	0.44
4:D:55:LYS:HE3	4:D:57:ILE:HD11	1.99	0.44
5:E:103:LEU:HD23	5:E:121:GLY:HA2	1.98	0.44
1:A:224:GLN:O	1:A:228:THR:HG21	2.17	0.44
4:D:50:LEU:HD11	5:E:50:LEU:HD11	2.02	0.41
5:E:19:LEU:CD2	5:E:124:LEU:HD13	2.51	0.41

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	274/277 (99%)	267 (97%)	7 (3%)	0	100	100
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	158/212 (74%)	153 (97%)	5 (3%)	0	100	100
5	E	231/246 (94%)	227 (98%)	4 (2%)	0	100	100
All	All	767/844 (91%)	746 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/233 (100%)	229 (99%)	3 (1%)	61	74
2	B	94/95 (99%)	93 (99%)	1 (1%)	65	77
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	145/188 (77%)	144 (99%)	1 (1%)	76	84
5	E	206/215 (96%)	200 (97%)	6 (3%)	37	53
All	All	686/740 (93%)	675 (98%)	11 (2%)	55	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	65	ARG
1	A	200	THR
2	B	33	SER
4	D	189	SER
5	E	44	GLN
5	E	48	GLN
5	E	91	VAL
5	E	101	ILE
5	E	106	VAL
5	E	188	GLN

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	155	GLN
1	A	191	HIS
1	A	224	GLN

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Mol	Chain	Res	Type
2	B	13	HIS
4	D	6	GLN
4	D	132	ASN
5	E	24	GLN
5	E	45	GLN
5	E	193	GLN
5	E	219	ASN
5	E	226	GLN

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](#)

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

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	276/277 (99%)	0.37	8 (2%) 53 55	40, 61, 94, 121	0
2	B	99/100 (99%)	0.69	7 (7%) 22 21	47, 66, 103, 127	0
3	C	9/9 (100%)	0.10	0 100 100	45, 50, 57, 59	0
4	D	166/212 (78%)	1.33	36 (21%) 2 2	49, 105, 140, 160	0
5	E	235/246 (95%)	1.27	37 (15%) 5 4	47, 103, 137, 151	0
All	All	785/844 (93%)	0.88	88 (11%) 10 9	40, 76, 132, 160	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	5.1
5	E	252	ALA	5.0
1	A	18	GLY	4.1
4	D	185	PHE	4.1
5	E	196	LEU	3.8
5	E	241	ALA	3.7
4	D	128	PRO	3.5
4	D	94	ALA	3.3
5	E	19	LEU	3.2
4	D	129	ASN	3.1
4	D	171	TYR	3.1
5	E	228	TYR	3.1
5	E	154	ALA	3.1
5	E	134	PHE	3.1
5	E	16	GLY	3.1
5	E	158	CYS	3.1
5	E	73	ILE	3.1
4	D	18	PRO	3.1
4	D	95	LEU	3.0
4	D	172	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	2.9
5	E	127	LEU	2.9
2	B	99	MET	2.9
5	E	143	PRO	2.8
5	E	141	PHE	2.8
4	D	135	PRO	2.8
2	B	18	GLY	2.7
5	E	183	VAL	2.7
4	D	152	LEU	2.7
5	E	185	THR	2.7
1	A	194	VAL	2.7
5	E	29	VAL	2.7
2	B	40	LEU	2.7
4	D	101	LEU	2.7
5	E	209	VAL	2.6
5	E	1	SER	2.6
5	E	181	SER	2.6
4	D	74	TYR	2.6
5	E	242	LYS	2.6
4	D	75	GLY	2.6
4	D	137	VAL	2.6
5	E	83	ASN	2.6
5	E	7	LYS	2.6
5	E	131	LYS	2.6
4	D	92	PRO	2.5
5	E	27	SER	2.5
1	A	274	TRP	2.5
4	D	136	ALA	2.5
5	E	167	HIS	2.4
5	E	159	LEU	2.4
5	E	214	TRP	2.4
2	B	15	ALA	2.4
4	D	45	TYR	2.3
1	A	249	VAL	2.3
4	D	65	VAL	2.3
4	D	127	ILE	2.3
5	E	190	LEU	2.3
2	B	75	LYS	2.3
4	D	123	LYS	2.3
5	E	28	GLN	2.3
4	D	143	SER	2.3
4	D	130	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	213	PHE	2.3
4	D	96	VAL	2.3
5	E	157	VAL	2.3
5	E	230	LEU	2.2
1	A	17	ARG	2.2
4	D	16	GLY	2.2
5	E	139	ALA	2.2
4	D	104	CYS	2.2
4	D	19	LEU	2.2
4	D	189	SER	2.2
4	D	179	ASP	2.2
4	D	192	ALA	2.2
1	A	16	GLY	2.2
4	D	124	LEU	2.2
4	D	91	LYS	2.2
5	E	148	ILE	2.1
5	E	75	LYS	2.1
2	B	97	ARG	2.1
4	D	131	GLN	2.1
1	A	131	ARG	2.1
4	D	173	THR	2.1
4	D	57	ILE	2.1
5	E	168	VAL	2.0
4	D	178	LEU	2.0
5	E	182	GLY	2.0
4	D	148	LYS	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.