



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 02:22 PM EST

PDB ID : 3UTT
Title : 1E6-A*0201-ALWGPDPA AAA Complex, Triclinic
Authors : Rizkallah, P.J.; Cole, D.K.; Sewell, A.K.; Bulek, A.M.; Rossjohn, J.; Gras, S.
Deposited on : 2011-11-26
Resolution : 2.60 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 : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

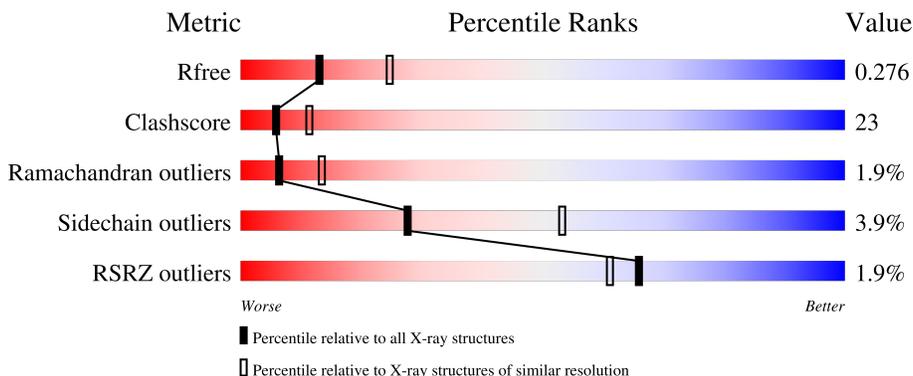
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	
1	F	275	
2	B	100	
2	G	100	
3	C	10	

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Mol	Chain	Length	Quality of chain
3	H	10	 40% 50% 10%
4	D	199	 4% 58% 37% 5%
4	I	199	 6% 58% 38% •
5	E	245	 2% 57% 39% •
5	J	245	 % 56% 41% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13562 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
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	1	0
			2257	1409	413	426	9			
1	F	275	Total	C	N	O	S	0	3	0
			2277	1420	418	430	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	Total	C	N	O	0	0	0
			69	45	11	13			
3	H	10	Total	C	N	O	0	0	0
			69	45	11	13			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

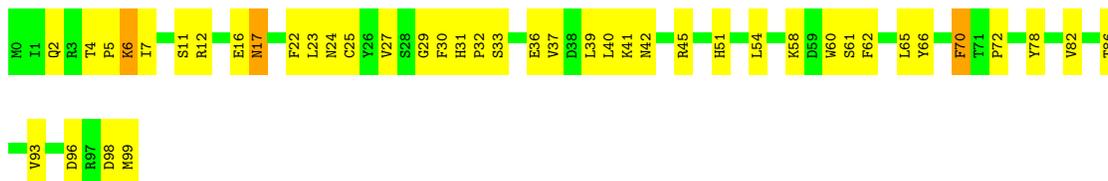
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1960	1242	339	369	10			
5	J	245	Total	C	N	O	S	0	0	0
			1965	1245	340	370	10			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	11	Total	O	0	0
			11	11		
6	D	10	Total	O	0	0
			10	10		
6	E	26	Total	O	0	0
			26	26		
6	F	28	Total	O	0	0
			28	28		
6	G	19	Total	O	0	0
			19	19		
6	H	1	Total	O	0	0
			1	1		
6	I	15	Total	O	0	0
			15	15		
6	J	18	Total	O	0	0
			18	18		



• Molecule 2: Beta-2-microglobulin



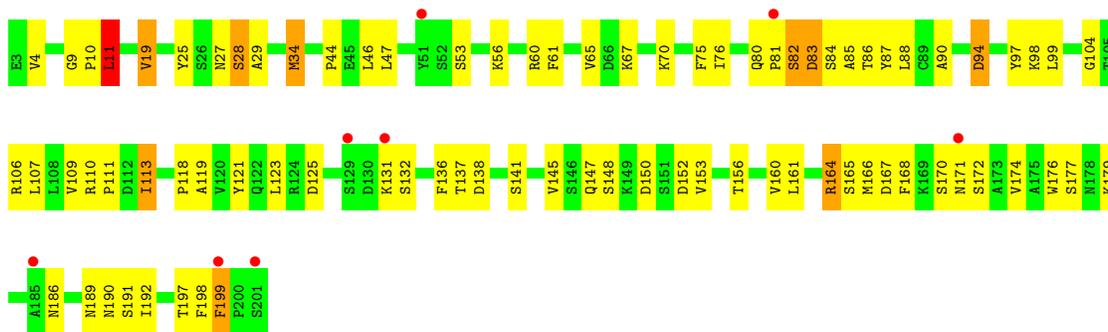
• Molecule 3: Insulin



• Molecule 3: Insulin

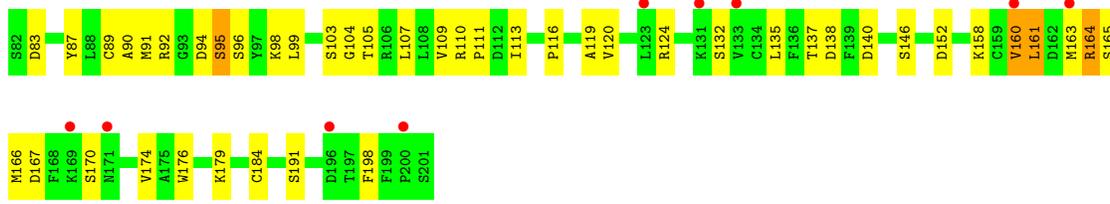


• Molecule 4: 1E6 TCR Alpha Chain

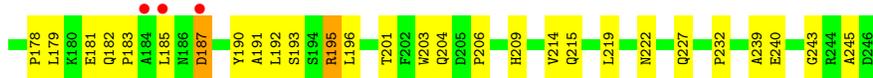


• Molecule 4: 1E6 TCR Alpha Chain

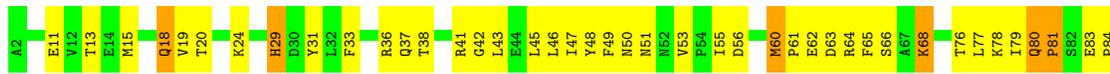




● Molecule 5: 1E6 TCR Beta Chain



● Molecule 5: 1E6 TCR Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.48Å 98.44Å 121.30Å 97.27° 98.16° 93.38°	Depositor
Resolution (Å)	29.34 – 2.60 29.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.34-2.60) 96.9 (29.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357, REFMAC	Depositor
R, R_{free}	0.195 , 0.274 0.200 , 0.276	Depositor DCC
R_{free} test set	2840 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13562	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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	0.24	0/2322	0.40	0/3151
1	F	0.23	0/2342	0.40	0/3177
2	B	0.26	0/860	0.40	0/1162
2	G	0.27	0/860	0.42	0/1162
3	C	0.20	0/72	0.58	0/99
3	H	0.18	0/72	0.68	0/99
4	D	0.24	0/1606	0.41	0/2174
4	I	0.25	0/1606	0.43	0/2174
5	E	0.25	0/2015	0.41	0/2741
5	J	0.25	0/2020	0.41	0/2748
All	All	0.24	0/13775	0.41	0/18687

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	2257	0	2108	102	0
1	F	2277	0	2125	123	0
2	B	837	0	803	26	0
2	G	837	0	803	39	0
3	C	69	0	64	15	0
3	H	69	0	64	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1570	0	1481	74	0
4	I	1570	0	1481	70	0
5	E	1960	0	1875	93	0
5	J	1965	0	1880	103	0
6	A	23	0	0	1	0
6	B	11	0	0	0	0
6	D	10	0	0	2	0
6	E	26	0	0	0	0
6	F	28	0	0	1	0
6	G	19	0	0	0	0
6	H	1	0	0	0	0
6	I	15	0	0	1	0
6	J	18	0	0	2	0
All	All	13562	0	12684	591	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 23.

The worst 5 of 591 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:80:GLN:HB3	5:E:81:PRO:HD2	1.45	0.98
3:C:7:PRO:HA	3:C:8:ALA:HB3	1.45	0.97
1:A:274:TRP:HE3	1:A:275:GLU:H	1.08	0.96
1:A:191:HIS:HB2	1:A:275:GLU:HB3	1.51	0.92
4:D:34:MET:HB2	4:D:46:LEU:HD11	1.51	0.91

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	274/275 (100%)	251 (92%)	21 (8%)	2 (1%)	19	38
1	F	276/275 (100%)	259 (94%)	13 (5%)	4 (1%)	9	19
2	B	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	G	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	13	29
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
3	H	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
4	D	197/199 (99%)	160 (81%)	26 (13%)	11 (6%)	1	1
4	I	197/199 (99%)	165 (84%)	27 (14%)	5 (2%)	4	8
5	E	242/245 (99%)	217 (90%)	22 (9%)	3 (1%)	11	24
5	J	243/245 (99%)	220 (90%)	20 (8%)	3 (1%)	11	24
All	All	1641/1658 (99%)	1465 (89%)	145 (9%)	31 (2%)	6	13

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	11	LEU
4	D	82	SER
5	E	81	PRO
5	J	81	PRO
1	A	18	GLY

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	232/231 (100%)	224 (97%)	8 (3%)	32	58
1	F	234/231 (101%)	225 (96%)	9 (4%)	28	54
2	B	95/95 (100%)	93 (98%)	2 (2%)	48	73
2	G	95/95 (100%)	92 (97%)	3 (3%)	34	60
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	2
3	H	5/5 (100%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/180 (100%)	172 (96%)	8 (4%)	24	48
4	I	180/180 (100%)	173 (96%)	7 (4%)	27	53
5	E	215/215 (100%)	205 (95%)	10 (5%)	22	45
5	J	215/215 (100%)	206 (96%)	9 (4%)	25	50
All	All	1456/1452 (100%)	1399 (96%)	57 (4%)	27	53

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	201	THR
5	J	126	GLU
1	F	138	MET
5	J	100	LEU
5	J	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	155	GLN
4	I	142	GLN
4	I	122	GLN
5	J	29	HIS
5	E	10	HIS

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 [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	275/275 (100%)	-0.13	4 (1%) 71 67	18, 52, 97, 132	1 (0%)
1	F	275/275 (100%)	-0.43	0 100 100	13, 46, 82, 98	3 (1%)
2	B	100/100 (100%)	-0.30	1 (1%) 79 75	24, 51, 86, 102	0
2	G	100/100 (100%)	-0.42	0 100 100	19, 41, 76, 87	0
3	C	10/10 (100%)	0.21	1 (10%) 14 12	26, 42, 59, 60	0
3	H	10/10 (100%)	-0.34	0 100 100	25, 38, 40, 43	0
4	D	199/199 (100%)	0.28	8 (4%) 43 37	26, 75, 140, 184	0
4	I	199/199 (100%)	0.41	12 (6%) 29 23	25, 77, 144, 183	0
5	E	244/245 (99%)	-0.07	4 (1%) 70 65	21, 56, 111, 146	0
5	J	245/245 (100%)	-0.08	2 (0%) 82 79	24, 58, 112, 148	0
All	All	1657/1658 (99%)	-0.08	32 (1%) 66 61	13, 55, 120, 184	4 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	160	VAL	4.6
4	D	81	PRO	3.9
5	E	138	SER	3.6
4	I	169	LYS	3.2
4	D	129	SER	3.1

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 monosaccharides 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.