



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:16 PM UTC

PDB ID : 3T0E / pdb_00003t0e
Title : Crystal structure of a complete ternary complex of T cell receptor, peptide-MHC and CD4
Authors : Yin, Y.; Mariuzza, R.A.
Deposited on : 2011-07-20
Resolution : 4.00 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
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

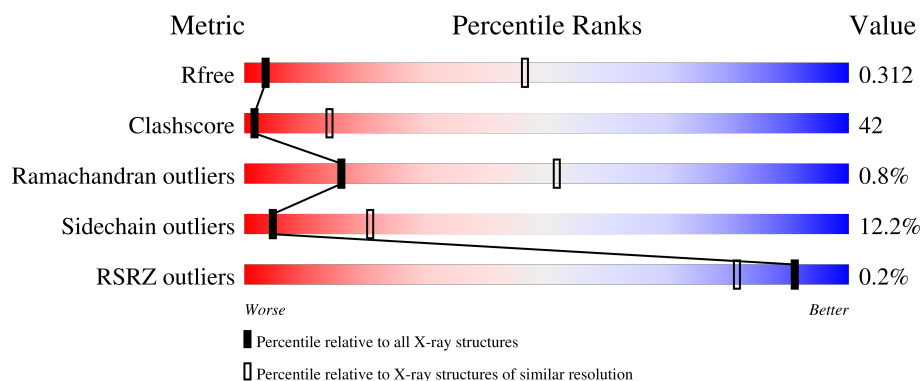
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	182	36%57%...
2	B	221	34%48%6%12%
3	C	206	38%46%8%6%
4	D	245	47%46%7%
5	E	373	39%47%12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9259 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1446	940	232	269	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1578	1001	271	301	5			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PHE	-	expression tag	UNP P13760
B	2	SER	-	expression tag	UNP P13760
B	3	TRP	-	expression tag	UNP P13760
B	4	GLY	-	expression tag	UNP P13760
B	5	ALA	-	expression tag	UNP P13760
B	6	GLU	-	expression tag	UNP P13760
B	7	GLY	-	expression tag	UNP P13760
B	8	GLN	-	expression tag	UNP P13760
B	9	ARG	-	expression tag	UNP P13760
B	10	PRO	-	expression tag	UNP P13760
B	11	GLY	-	expression tag	UNP P13760
B	12	PHE	-	expression tag	UNP P13760
B	13	GLY	-	expression tag	UNP P13760
B	14	SER	-	expression tag	UNP P13760
B	15	GLY	-	expression tag	UNP P13760
B	16	GLY	-	expression tag	UNP P13760
B	17	GLY	-	expression tag	UNP P13760
B	18	SER	-	expression tag	UNP P13760
B	19	LEU	-	expression tag	UNP P13760
B	20	VAL	-	expression tag	UNP P13760

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	PRO	-	expression tag	UNP P13760
B	22	ARG	-	expression tag	UNP P13760
B	23	GLY	-	expression tag	UNP P13760
B	24	SER	-	expression tag	UNP P13760
B	25	GLY	-	expression tag	UNP P13760
B	26	GLY	-	expression tag	UNP P13760
B	27	GLY	-	expression tag	UNP P13760
B	28	GLY	-	expression tag	UNP P13760
B	29	SER	-	expression tag	UNP P13760

- Molecule 3 is a protein called T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	193	Total	C	N	O	S	4	0	0
			1455	905	244	299	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1920	1210	327	375	8			

- Molecule 5 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	365	Total	C	N	O	S	0	0	0
			2860	1818	491	541	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	TYR	GLN	engineered mutation	UNP P01730
E	45	TRP	THR	engineered mutation	UNP P01730
E	364	ALA	-	expression tag	UNP P01730
E	365	ALA	-	expression tag	UNP P01730
E	366	ASP	-	expression tag	UNP P01730
E	367	TYR	-	expression tag	UNP P01730
E	368	LYS	-	expression tag	UNP P01730
E	369	ASP	-	expression tag	UNP P01730
E	370	ASP	-	expression tag	UNP P01730
E	371	ASP	-	expression tag	UNP P01730
E	372	ASP	-	expression tag	UNP P01730

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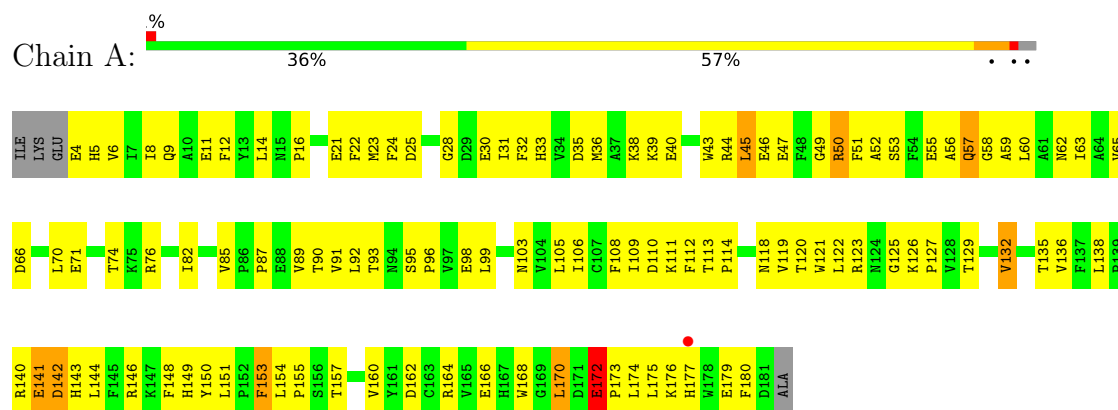
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Chain	Residue	Modelled	Actual	Comment	Reference
E	373	LYS	-	expression tag	UNP P01730

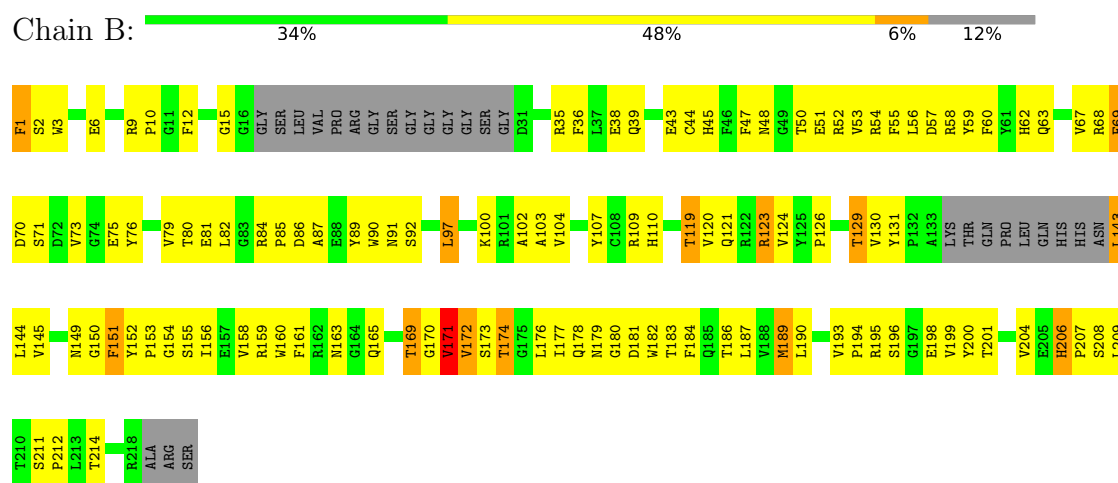
3 Residue-property plots [i](#)

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.

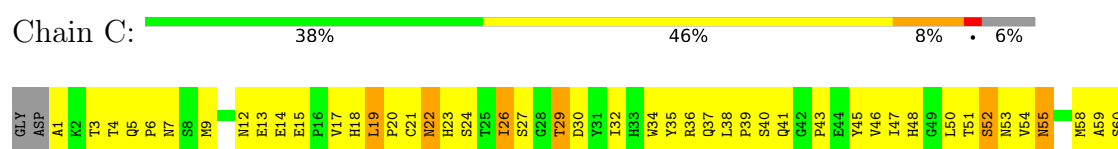
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

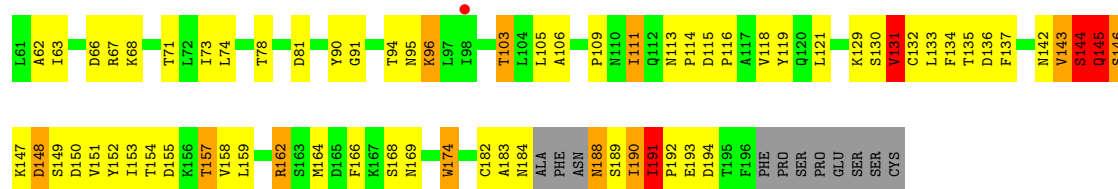


- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



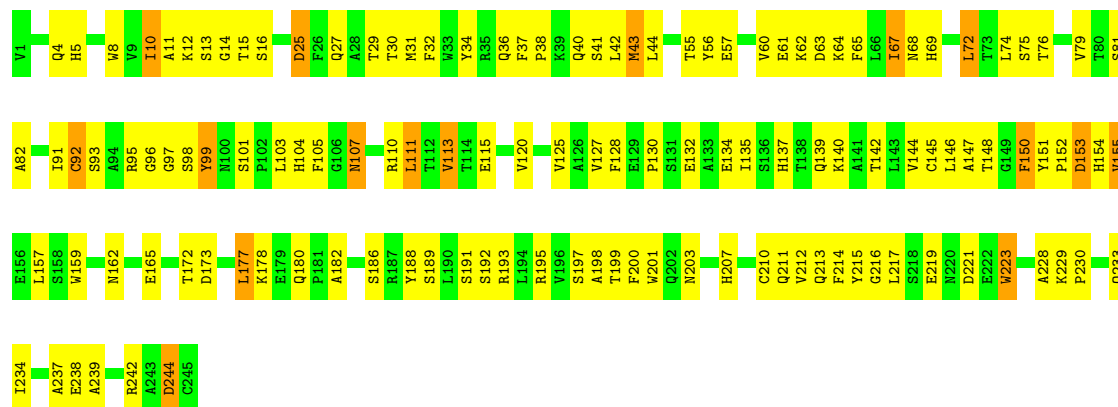
- Molecule 3: T-cell receptor alpha chain





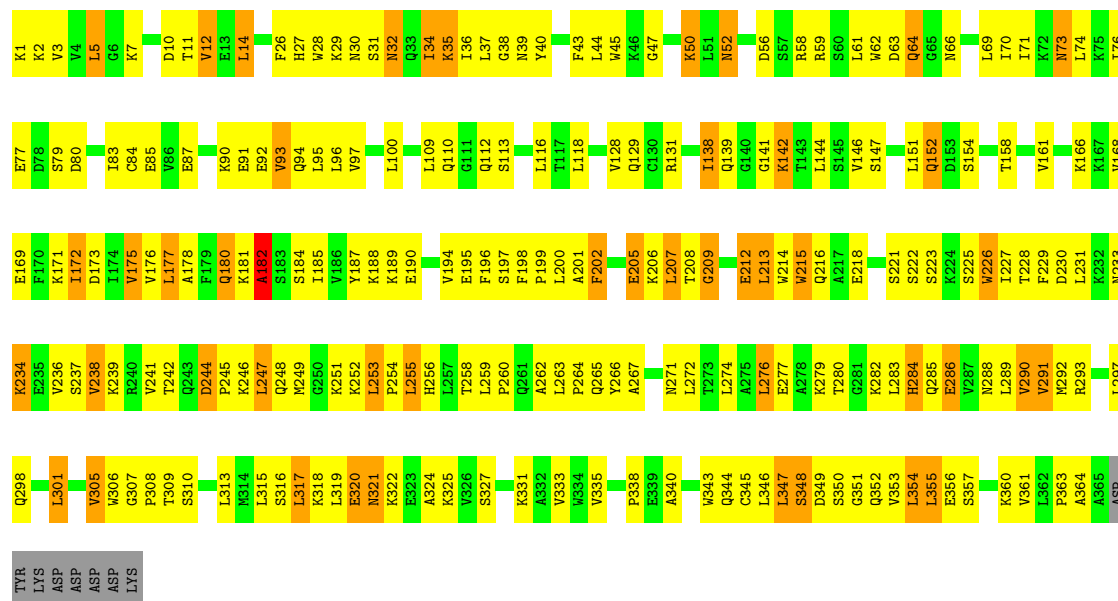
• Molecule 4: T-cell receptor beta chain

Chain D: 47% 46% 7%



• Molecule 5: T-cell surface glycoprotein CD4

Chain E: 39% 47% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.15Å 146.15Å 231.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 4.00 47.67 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.67-4.00) 99.8 (47.67-4.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.238 , 0.305 0.255 , 0.312	Depositor DCC
R_{free} test set	1066 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	179.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 216.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9259	wwPDB-VP
Average B, all atoms (Å ²)	218.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.39	0/1491	0.87	2/2036 (0.1%)
2	B	0.43	0/1622	0.88	5/2204 (0.2%)
3	C	0.46	1/1485 (0.1%)	0.96	7/2030 (0.3%)
4	D	0.35	0/1973	0.83	2/2690 (0.1%)
5	E	0.41	0/2912	0.91	9/3935 (0.2%)
All	All	0.41	1/9483 (0.0%)	0.89	25/12895 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
5	E	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	ALA	C-O	6.79	1.37	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	198	PHE	CA-C-N	10.32	130.42	120.31
5	E	198	PHE	C-N-CA	10.32	130.42	120.31
3	C	131	VAL	N-CA-C	8.72	127.47	109.34
5	E	202	PHE	N-CA-C	7.75	119.98	110.91
2	B	206	HIS	CA-C-N	-7.01	111.07	119.84

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	130	SER	Peptide
3	C	144	SER	Peptide
3	C	145	GLN	Peptide
5	E	182	ALA	Peptide

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	1446	0	1370	132	0
2	B	1578	0	1451	133	0
3	C	1455	0	1345	121	0
4	D	1920	0	1809	148	0
5	E	2860	0	2944	274	0
All	All	9259	0	8919	756	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 42.

The worst 5 of 756 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)
1:A:175:LEU:CD1	1:A:177:HIS:CE1	1.75	1.56
1:A:175:LEU:HD11	1:A:177:HIS:CE1	0.95	1.46
1:A:175:LEU:CD1	1:A:177:HIS:NE2	1.81	1.42
1:A:175:LEU:HD12	1:A:177:HIS:NE2	1.31	1.42
1:A:162:ASP:CG	1:A:177:HIS:ND1	2.02	1.18

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	176/182 (97%)	154 (88%)	22 (12%)	0	100	100
2	B	189/221 (86%)	158 (84%)	29 (15%)	2 (1%)	11	44
3	C	189/206 (92%)	163 (86%)	24 (13%)	2 (1%)	11	44
4	D	243/245 (99%)	213 (88%)	30 (12%)	0	100	100
5	E	363/373 (97%)	295 (81%)	63 (17%)	5 (1%)	9	39
All	All	1160/1227 (94%)	983 (85%)	168 (14%)	9 (1%)	16	52

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	182	ALA
5	E	286	GLU
5	E	352	GLN
3	C	144	SER
2	B	172	VAL

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	159/166 (96%)	147 (92%)	12 (8%)	12	36
2	B	167/189 (88%)	148 (89%)	19 (11%)	5	22
3	C	160/183 (87%)	137 (86%)	23 (14%)	3	17
4	D	212/216 (98%)	190 (90%)	22 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	324/332 (98%)	275 (85%)	49 (15%)	3	16
All	All	1022/1086 (94%)	897 (88%)	125 (12%)	5	21

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	43	MET
5	E	255	LEU
4	D	199	THR
5	E	253	LEU
5	E	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	110	GLN
5	E	139	GLN
5	E	180	GLN
3	C	113	ASN
3	C	108	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 [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	178/182 (97%)	-0.48	1 (0%) 85 71	99, 205, 259, 320	0
2	B	195/221 (88%)	-0.50	0 100 100	144, 185, 249, 292	0
3	C	193/206 (93%)	-0.34	1 (0%) 87 73	141, 207, 283, 424	1 (0%)
4	D	245/245 (100%)	-0.54	0 100 100	157, 220, 293, 346	0
5	E	365/373 (97%)	-0.47	0 100 100	160, 229, 319, 365	0
All	All	1176/1227 (95%)	-0.47	2 (0%) 91 81	99, 212, 295, 424	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	HIS	4.3
3	C	98	ILE	2.9

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.