wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:08 PM GMT

PDB ID	:	3T0E
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
http://wwpdb.org/validation/2016/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:

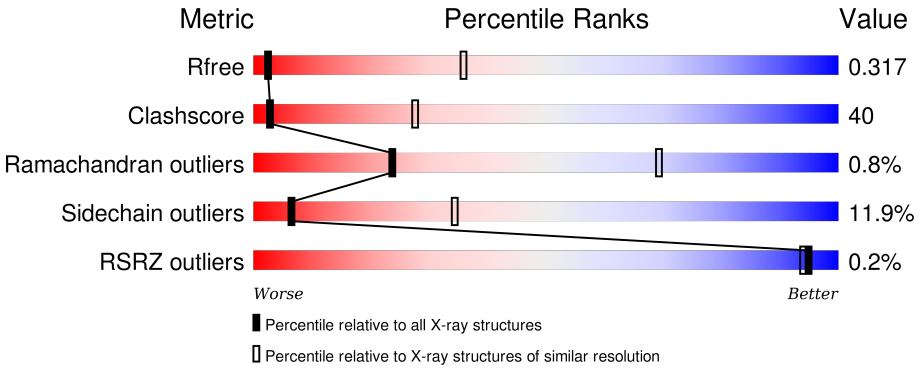
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 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	37% 55% 5% •
2	B	221	36% 47% 5% 12%
3	C	206	40% 47% 6% • 6%
4	D	245	49% 43% 7%
5	E	373	40% 46% 12% •

2 Entry composition (i)

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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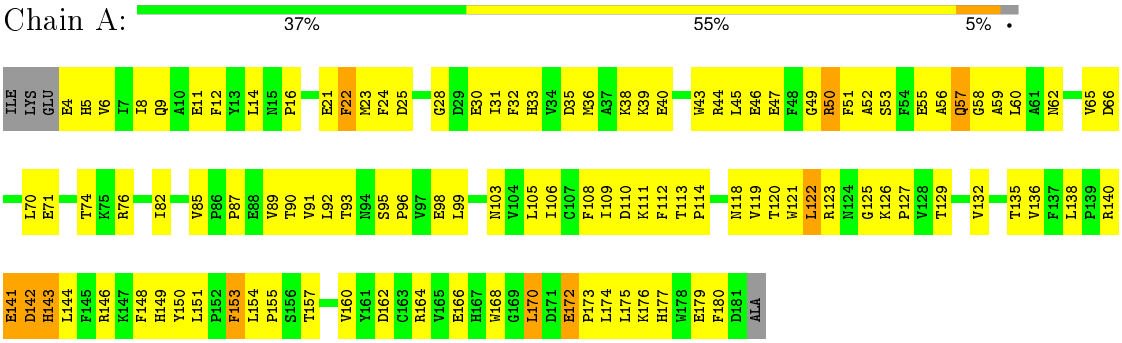
Chain	Residue	Modelled	Actual	Comment	Reference
E	373	LYS	-	EXPRESSION TAG	UNP P01730

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

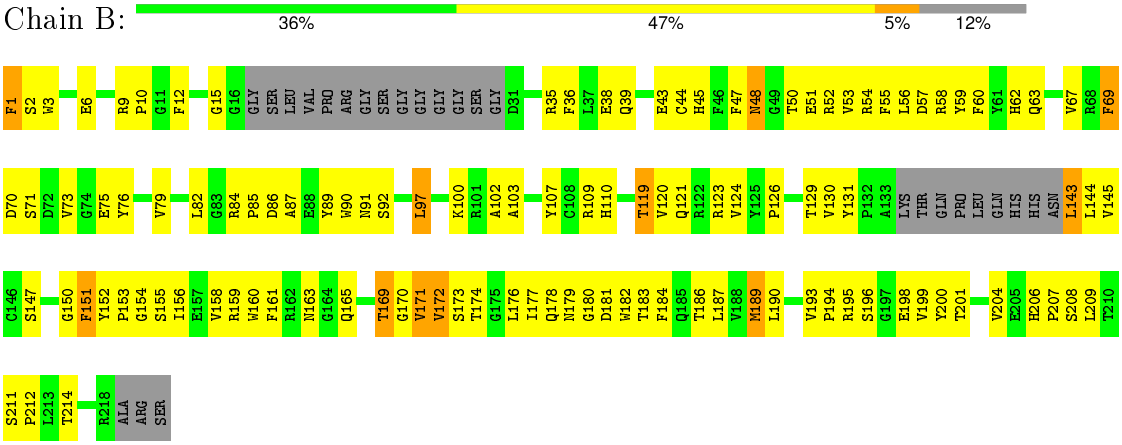
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



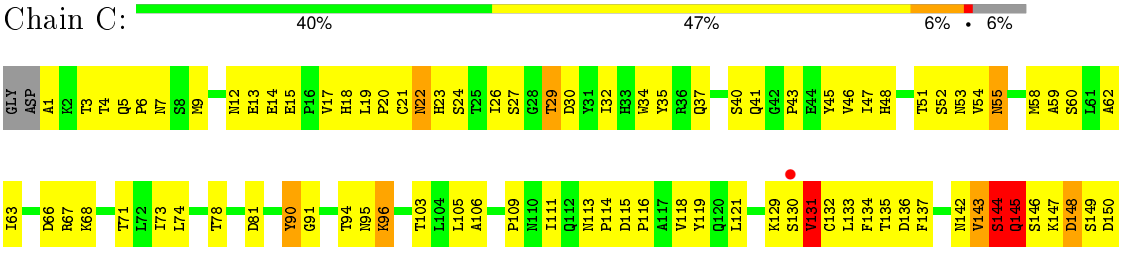
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain

Chain B:



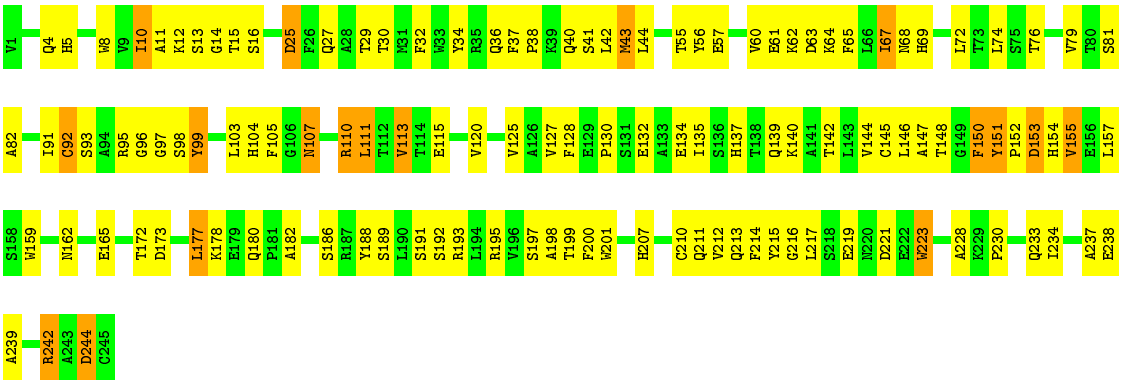
- Molecule 3: T-cell receptor alpha chain

Chain C:



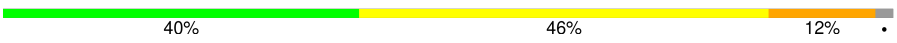
- Molecule 4: T-cell receptor beta chain

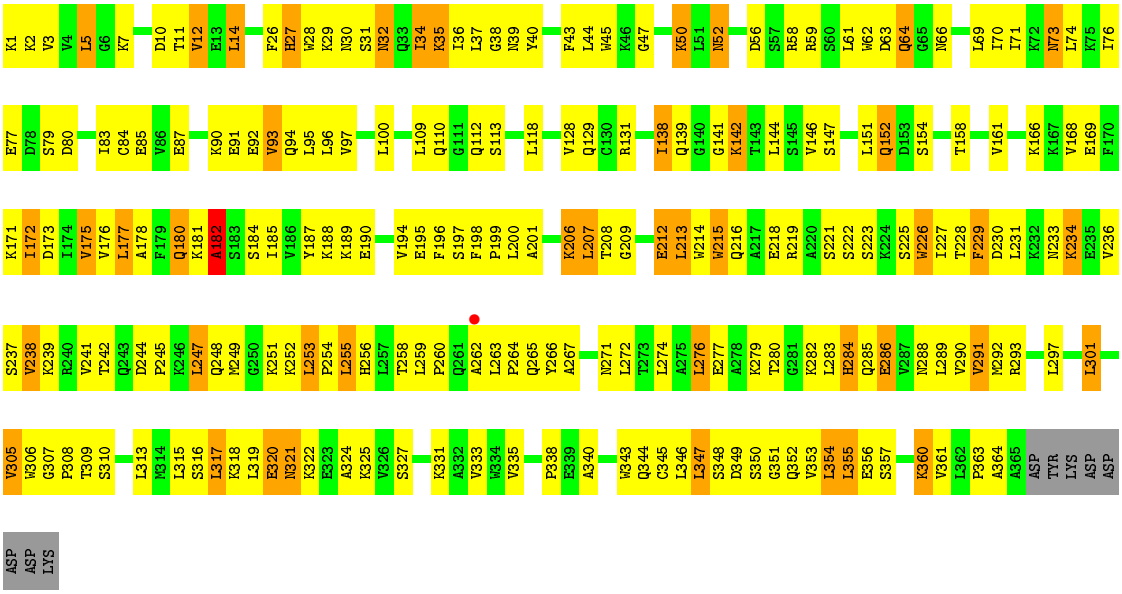
Chain D:



- Molecule 5: T-cell surface glycoprotein CD4

Chain E:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.65 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.238 , 0.305 0.248 , 0.317	Depositor DCC
R_{free} test set	1066 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	179.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 205.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 21831 reflections (0.005%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.31	0/1491	0.52	0/2036
2	B	0.33	0/1622	0.53	0/2204
3	C	0.37	1/1485 (0.1%)	0.61	2/2030 (0.1%)
4	D	0.27	0/1973	0.50	0/2690
5	E	0.30	0/2912	0.55	0/3935
All	All	0.31	1/9483 (0.0%)	0.54	2/12895 (0.0%)

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	7.25	1.37	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	131	VAL	N-CA-C	6.10	127.47	111.00
3	C	145	GLN	N-CA-C	5.19	125.02	111.00

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 (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	1446	0	1370	125	0
2	B	1578	0	1451	129	0
3	C	1455	0	1345	116	0
4	D	1920	0	1809	142	0
5	E	2860	0	2944	265	0
All	All	9259	0	8919	725	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 40.

The worst 5 of 725 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	1.13

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	176/182 (97%)	154 (88%)	22 (12%)	0	100	100
2	B	189/221 (86%)	158 (84%)	29 (15%)	2 (1%)	17	64
3	C	189/206 (92%)	163 (86%)	24 (13%)	2 (1%)	17	64
4	D	243/245 (99%)	213 (88%)	30 (12%)	0	100	100
5	E	363/373 (97%)	295 (81%)	63 (17%)	5 (1%)	14	59
All	All	1160/1227 (94%)	983 (85%)	168 (14%)	9 (1%)	24	69

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 (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	159/166 (96%)	146 (92%)	13 (8%)	14	51
2	B	167/189 (88%)	151 (90%)	16 (10%)	10	44
3	C	160/183 (87%)	142 (89%)	18 (11%)	7	37
4	D	212/216 (98%)	189 (89%)	23 (11%)	8	39
5	E	324/332 (98%)	272 (84%)	52 (16%)	3	23
All	All	1022/1086 (94%)	900 (88%)	122 (12%)	6	34

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	104	HIS

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Mol	Chain	Res	Type
4	D	242	ARG
5	E	301	LEU
4	D	107	ASN
4	D	151	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	27	GLN
4	D	107	ASN
5	E	152	GLN
4	D	100	ASN
4	D	137	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 carbohydrates 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, 95^{th} 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%)	-0.24	0 100 100	99, 205, 259, 320	0
2	B	195/221 (88%)	-0.19	0 100 100	144, 185, 249, 292	0
3	C	193/206 (93%)	-0.26	1 (0%) 91 88	146, 207, 283, 424	1 (0%)
4	D	245/245 (100%)	-0.33	0 100 100	157, 220, 293, 346	0
5	E	365/373 (97%)	-0.27	1 (0%) 94 92	160, 229, 319, 365	0
All	All	1176/1227 (95%)	-0.26	2 (0%) 95 94	99, 212, 295, 424	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	262	ALA	2.5
3	C	130	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.