



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E7L  
Title : Structure of a high-affinity mutant of the 2C TCR in complex with Ld/QL9  
Authors : Garcia, K.C.; Colf, L.A.  
Deposited on : 2007-01-11  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

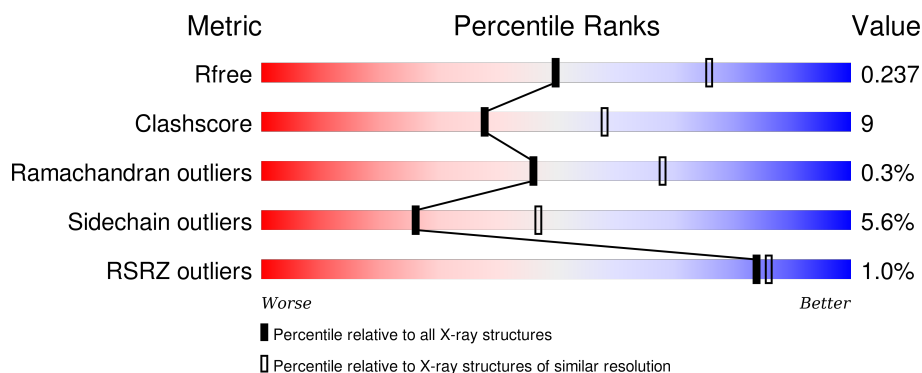
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	113	<div> <div>2%</div> <div>80%</div> <div>19%</div> <div>..</div> </div>
1	B	113	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	C	121	<div> <div>2%</div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
2	D	121	<div> <div>%</div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
3	E	181	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	181	<div><div><div>%</div><div><div></div></div></div><div><div></div><div>80%</div><div>15%</div><div></div><div></div></div></div>
4	P	9	<div><div><div></div><div>44%</div><div>22%</div><div>33%</div></div></div>
4	Q	9	<div><div><div></div><div>44%</div><div>22%</div><div>33%</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6682 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 Cytotoxic Tcell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			890	572	152	164	2			
1	B	110	Total	C	N	O	S	0	0	0
			869	558	149	160	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	PRO	LEU	ENGINEERED MUTATION	UNP A2NTU7
A	82	ARG	TRP	ENGINEERED MUTATION	UNP A2NTU7
A	99	HIS	GLY	ENGINEERED MUTATION	UNP A2NTU7
A	100	GLN	PHE	ENGINEERED MUTATION	UNP A2NTU7
A	101	GLY	ALA	ENGINEERED MUTATION	UNP A2NTU7
A	102	ARG	SER	ENGINEERED MUTATION	UNP A2NTU7
A	103	TYR	ALA	ENGINEERED MUTATION	UNP A2NTU7
A	118	ASN	-	SEE REMARK 999	UNP A2NTU7
B	43	PRO	LEU	ENGINEERED MUTATION	UNP A2NTU7
B	82	ARG	TRP	ENGINEERED MUTATION	UNP A2NTU7
B	99	HIS	GLY	ENGINEERED MUTATION	UNP A2NTU7
B	100	GLN	PHE	ENGINEERED MUTATION	UNP A2NTU7
B	101	GLY	ALA	ENGINEERED MUTATION	UNP A2NTU7
B	102	ARG	SER	ENGINEERED MUTATION	UNP A2NTU7
B	103	TYR	ALA	ENGINEERED MUTATION	UNP A2NTU7
B	118	ASN	-	SEE REMARK 999	UNP A2NTU7

- Molecule 2 is a protein called Beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	112	Total	C	N	O	S	0	0	0
			852	526	148	175	3			
2	D	112	Total	C	N	O	S	0	0	0
			852	526	148	175	3			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLU	GLY	ENGINEERED MUTATION	UNP A2NTY6
C	42	GLU	GLY	ENGINEERED MUTATION	UNP A2NTY6
C	47	TYR	HIS	ENGINEERED MUTATION	UNP A2NTY6
C	78	THR	ILE	ENGINEERED MUTATION	UNP A2NTY6
C	81	SER	LEU	ENGINEERED MUTATION	UNP A2NTY6
C	?	-	GLU	DELETION	UNP A2NTY6
C	?	-	LEU	DELETION	UNP A2NTY6
C	?	-	PHE	DELETION	UNP A2NTY6
C	?	-	ASN	DELETION	UNP A2NTY6
C	?	-	GLN	DELETION	UNP A2NTY6
C	97	GLY	ASP	ENGINEERED MUTATION	UNP A2NTY6
C	106	LEU	GLN	ENGINEERED MUTATION	UNP A2NTY6
C	110	ALA	PRO	ENGINEERED MUTATION	UNP A2NTY6
C	115	SER	LEU	ENGINEERED MUTATION	UNP A2NTY6
C	118	SER	-	SEE REMARK 999	UNP A2NTY6
C	119	SER	-	SEE REMARK 999	UNP A2NTY6
C	120	ALA	-	SEE REMARK 999	UNP A2NTY6
C	121	LEU	-	SEE REMARK 999	UNP A2NTY6
C	122	GLU	-	SEE REMARK 999	UNP A2NTY6
C	123	HIS	-	SEE REMARK 999	UNP A2NTY6
C	124	HIS	-	SEE REMARK 999	UNP A2NTY6
C	125	HIS	-	SEE REMARK 999	UNP A2NTY6
C	126	HIS	-	SEE REMARK 999	UNP A2NTY6
C	127	HIS	-	SEE REMARK 999	UNP A2NTY6
C	128	HIS	-	SEE REMARK 999	UNP A2NTY6
D	17	GLU	GLY	ENGINEERED MUTATION	UNP A2NTY6
D	42	GLU	GLY	ENGINEERED MUTATION	UNP A2NTY6
D	47	TYR	HIS	ENGINEERED MUTATION	UNP A2NTY6
D	78	THR	ILE	ENGINEERED MUTATION	UNP A2NTY6
D	81	SER	LEU	ENGINEERED MUTATION	UNP A2NTY6
D	?	-	GLU	DELETION	UNP A2NTY6
D	?	-	LEU	DELETION	UNP A2NTY6
D	?	-	PHE	DELETION	UNP A2NTY6
D	?	-	ASN	DELETION	UNP A2NTY6
D	?	-	GLN	DELETION	UNP A2NTY6
D	97	GLY	ASP	ENGINEERED MUTATION	UNP A2NTY6
D	106	LEU	GLN	ENGINEERED MUTATION	UNP A2NTY6
D	110	ALA	PRO	ENGINEERED MUTATION	UNP A2NTY6
D	115	SER	LEU	ENGINEERED MUTATION	UNP A2NTY6
D	118	SER	-	SEE REMARK 999	UNP A2NTY6
D	119	SER	-	SEE REMARK 999	UNP A2NTY6
D	120	ALA	-	SEE REMARK 999	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	121	LEU	-	SEE REMARK 999	UNP A2NTY6
D	122	GLU	-	SEE REMARK 999	UNP A2NTY6
D	123	HIS	-	SEE REMARK 999	UNP A2NTY6
D	124	HIS	-	SEE REMARK 999	UNP A2NTY6
D	125	HIS	-	SEE REMARK 999	UNP A2NTY6
D	126	HIS	-	SEE REMARK 999	UNP A2NTY6
D	127	HIS	-	SEE REMARK 999	UNP A2NTY6
D	128	HIS	-	SEE REMARK 999	UNP A2NTY6

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	175	Total	C	N	O	S	0	0	0
			1448	911	257	273	7			
3	F	175	Total	C	N	O	S	0	0	0
			1448	911	257	273	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	15	ARG	PRO	ENGINEERED MUTATION	UNP P01897
E	30	ASP	ASN	ENGINEERED MUTATION	UNP P01897
E	49	VAL	ALA	ENGINEERED MUTATION	UNP P01897
E	66	VAL	ILE	ENGINEERED MUTATION	UNP P01897
E	97	ARG	TRP	ENGINEERED MUTATION	UNP P01897
E	131	ARG	LYS	ENGINEERED MUTATION	UNP P01897
F	15	ARG	PRO	ENGINEERED MUTATION	UNP P01897
F	30	ASP	ASN	ENGINEERED MUTATION	UNP P01897
F	49	VAL	ALA	ENGINEERED MUTATION	UNP P01897
F	66	VAL	ILE	ENGINEERED MUTATION	UNP P01897
F	97	ARG	TRP	ENGINEERED MUTATION	UNP P01897
F	131	ARG	LYS	ENGINEERED MUTATION	UNP P01897

- Molecule 4 is a protein called Peptide (GLN)(LEU)(SER)(PRO)(PHE)(PRO)(PHE)(ASP)(LEU).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	9	Total	C	N	O	0	0	0
			75	52	10	13			
4	Q	9	Total	C	N	O	0	0	0
			75	52	10	13			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	21	Total 21	O 21	0	0
5	C	19	Total 19	O 19	0	0
5	D	13	Total 13	O 13	0	0
5	E	48	Total 48	O 48	0	0
5	F	42	Total 42	O 42	0	0
5	P	5	Total 5	O 5	0	0
5	Q	3	Total 3	O 3	0	0

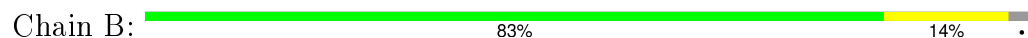
### 3 Residue-property plots [i](#)

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.

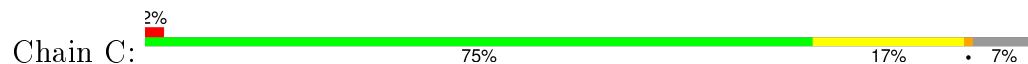
- Molecule 1: Cytotoxic Tcell receptor



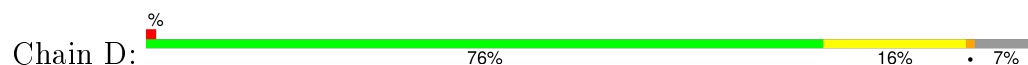
- Molecule 1: Cytotoxic Tcell receptor



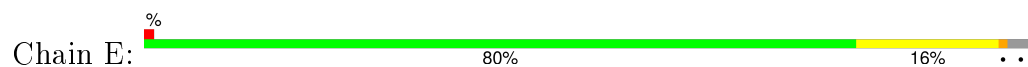
- Molecule 2: Beta-chain



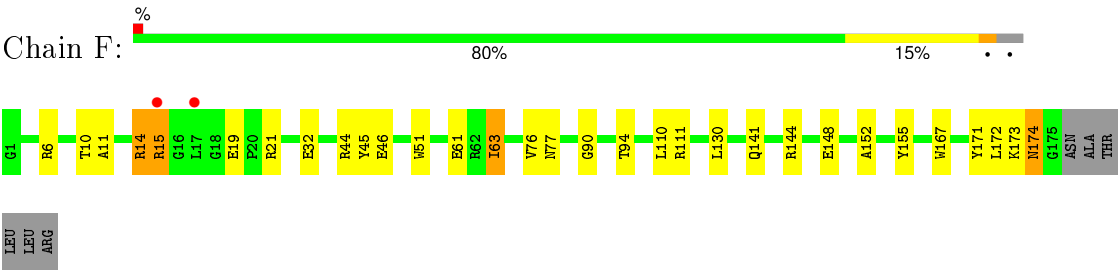
- Molecule 2: Beta-chain



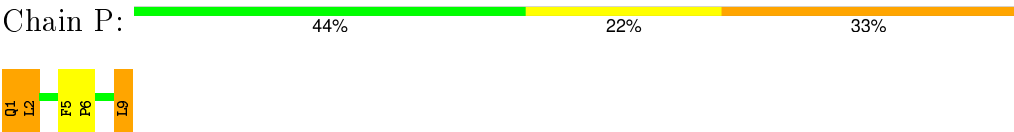
- Molecule 3: H-2 class I histocompatibility antigen, L-D alpha chain



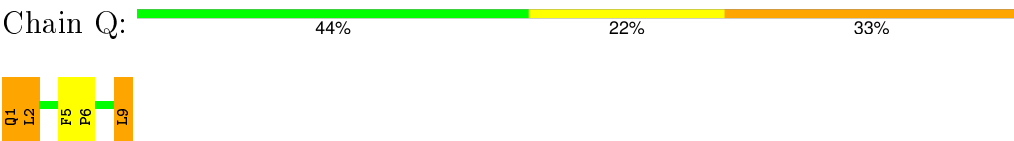
- Molecule 3: H-2 class I histocompatibility antigen, L-D alpha chain



- Molecule 4: Peptide (GLN)(LEU)(SER)(PRO)(PHE)(PRO)(PHE)(ASP)(LEU)



- Molecule 4: Peptide (GLN)(LEU)(SER)(PRO)(PHE)(PRO)(PHE)(ASP)(LEU)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.54Å 113.54Å 177.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.50) 99.9 (48.82-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.246 0.215 , 0.237	Depositor DCC
$R_{free}$ test set	2057 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41065 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/916	0.57	0/1244
1	B	0.50	0/894	0.59	0/1214
2	C	0.51	0/870	0.59	0/1180
2	D	0.52	0/870	0.61	0/1180
3	E	0.60	0/1488	0.62	0/2014
3	F	0.54	0/1488	0.60	0/2014
4	P	0.65	0/78	0.82	0/106
4	Q	0.58	0/78	0.79	0/106
All	All	0.54	0/6682	0.61	0/9058

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	SER	Mainchain

### 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	890	0	863	14	0
1	B	869	0	843	15	0
2	C	852	0	804	12	0
2	D	852	0	804	20	0
3	E	1448	0	1343	23	0
3	F	1448	0	1343	31	0
4	P	75	0	73	14	0
4	Q	75	0	73	16	0
5	A	22	0	0	0	0
5	B	21	0	0	0	0
5	C	19	0	0	2	0
5	D	13	0	0	0	0
5	E	48	0	0	0	0
5	F	42	0	0	4	0
5	P	5	0	0	0	0
5	Q	3	0	0	0	0
All	All	6682	0	6146	116	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 116 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)
4:P:1:GLN:CA	4:P:1:GLN:HE21	1.80	0.94
4:P:1:GLN:NE2	4:P:1:GLN:HA	1.87	0.89
3:F:77:ASN:HD22	4:P:9:LEU:HB2	1.45	0.81
4:P:1:GLN:HA	4:P:1:GLN:HE21	1.44	0.81
3:E:77:ASN:HD22	4:Q:9:LEU:HB2	1.49	0.76

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	110/113 (97%)	102 (93%)	7 (6%)	1 (1%)	21	37
1	B	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
2	C	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
2	D	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
3	E	173/181 (96%)	165 (95%)	8 (5%)	0	100	100
3	F	173/181 (96%)	166 (96%)	6 (4%)	1 (1%)	30	50
4	P	7/9 (78%)	7 (100%)	0	0	100	100
4	Q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	798/848 (94%)	762 (96%)	34 (4%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	172	LEU
1	A	28	ALA

### 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	97/98 (99%)	93 (96%)	4 (4%)	37	63
1	B	95/98 (97%)	93 (98%)	2 (2%)	61	85
2	C	92/100 (92%)	88 (96%)	4 (4%)	35	61
2	D	92/100 (92%)	89 (97%)	3 (3%)	45	73
3	E	144/149 (97%)	135 (94%)	9 (6%)	22	40
3	F	144/149 (97%)	134 (93%)	10 (7%)	19	35
4	P	9/9 (100%)	6 (67%)	3 (33%)	0	0
4	Q	9/9 (100%)	6 (67%)	3 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	682/712 (96%)	644 (94%)	38 (6%)	26	47

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	61	GLU
3	E	170	ARG
4	Q	1	GLN
3	E	80	THR
3	F	6	ARG

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

Mol	Chain	Res	Type
2	D	6	GLN
2	D	86	GLN
3	F	174	ASN
2	D	37	GLN
3	E	42	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	112/113 (99%)	-0.14	2 (1%) 71 75	20, 33, 48, 61	0
1	B	110/113 (97%)	-0.17	0 100 100	16, 31, 44, 51	0
2	C	112/121 (92%)	-0.33	2 (1%) 71 75	17, 28, 43, 51	0
2	D	112/121 (92%)	-0.20	1 (0%) 85 88	21, 36, 45, 61	0
3	E	175/181 (96%)	-0.16	1 (0%) 90 91	20, 30, 48, 56	0
3	F	175/181 (96%)	-0.18	2 (1%) 82 84	16, 27, 43, 50	0
4	P	9/9 (100%)	-0.14	0 100 100	17, 20, 25, 30	0
4	Q	9/9 (100%)	-0.11	0 100 100	23, 26, 30, 35	0
All	All	814/848 (95%)	-0.19	8 (0%) 84 86	16, 30, 46, 61	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	ALA	3.4
3	E	89	ALA	2.5
1	A	117	TYR	2.4
3	F	15	ARG	2.3
3	F	17	LEU	2.3

### 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

There are no such residues in this entry.