



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2025 – 06:07 PM EDT

PDB ID : 9YL4 / pdb\_00009yl4  
Title : Crystal structure of PprA S-F filament from *Deinococcus radiodurans*  
Authors : Szabla, R.; Junop, M.S.  
Deposited on : 2025-10-08  
Resolution : 3.70 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

<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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

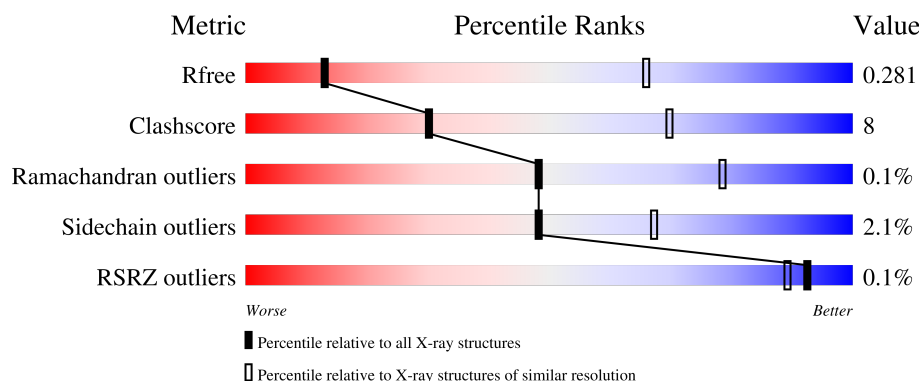
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 3.70 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	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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  $\geq 3$ , 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	276	
1	B	276	
1	C	276	
1	D	276	
1	E	276	

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Mol	Chain	Length	Quality of chain
1	F	276	 78% 21% .
1	G	276	 85% 14% .
1	H	276	 86% 14%
1	I	276	 81% 19%
1	J	276	 83% 16% .
1	K	276	 87% 11% .
1	L	276	 82% 17% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25066 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 DNA repair protein PprA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	B	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	C	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	D	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	E	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	F	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	G	275	Total	C	N	O	Se	0	0	0
			2085	1294	385	402	4			
1	H	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	I	275	Total	C	N	O	Se	0	0	0
			2085	1294	385	402	4			
1	J	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			
1	K	271	Total	C	N	O	Se	0	0	0
			2050	1274	378	394	4			
1	L	276	Total	C	N	O	Se	0	0	0
			2094	1299	387	404	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LYS	ASP	engineered mutation	UNP O32504
A	184	LYS	ASP	engineered mutation	UNP O32504
B	180	LYS	ASP	engineered mutation	UNP O32504
B	184	LYS	ASP	engineered mutation	UNP O32504
C	180	LYS	ASP	engineered mutation	UNP O32504

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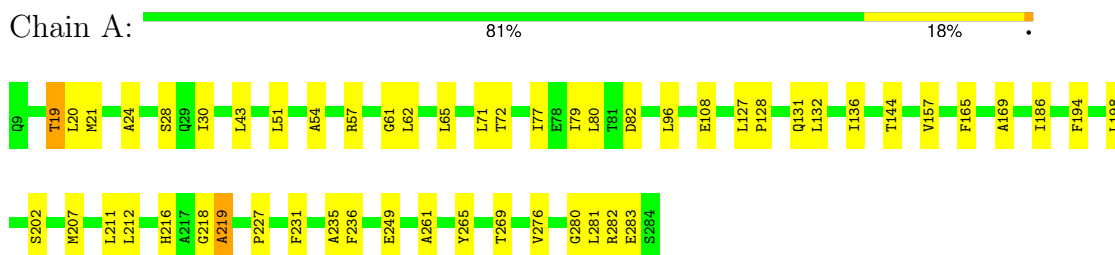
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Chain	Residue	Modelled	Actual	Comment	Reference
C	184	LYS	ASP	engineered mutation	UNP O32504
D	180	LYS	ASP	engineered mutation	UNP O32504
D	184	LYS	ASP	engineered mutation	UNP O32504
E	180	LYS	ASP	engineered mutation	UNP O32504
E	184	LYS	ASP	engineered mutation	UNP O32504
F	180	LYS	ASP	engineered mutation	UNP O32504
F	184	LYS	ASP	engineered mutation	UNP O32504
G	180	LYS	ASP	engineered mutation	UNP O32504
G	184	LYS	ASP	engineered mutation	UNP O32504
H	180	LYS	ASP	engineered mutation	UNP O32504
H	184	LYS	ASP	engineered mutation	UNP O32504
I	180	LYS	ASP	engineered mutation	UNP O32504
I	184	LYS	ASP	engineered mutation	UNP O32504
J	180	LYS	ASP	engineered mutation	UNP O32504
J	184	LYS	ASP	engineered mutation	UNP O32504
K	180	LYS	ASP	engineered mutation	UNP O32504
K	184	LYS	ASP	engineered mutation	UNP O32504
L	180	LYS	ASP	engineered mutation	UNP O32504
L	184	LYS	ASP	engineered mutation	UNP O32504

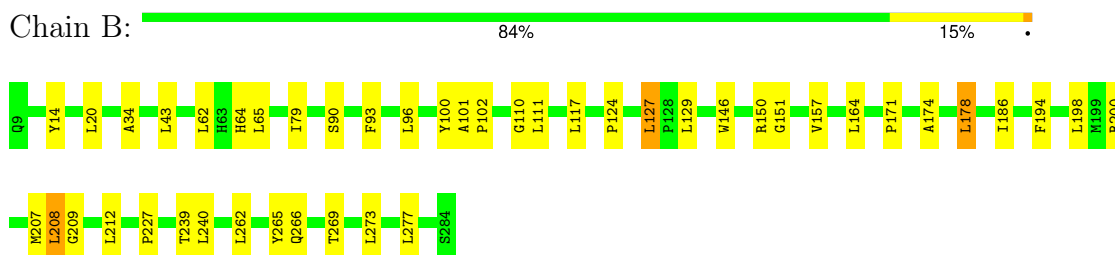
### 3 Residue-property plots

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.

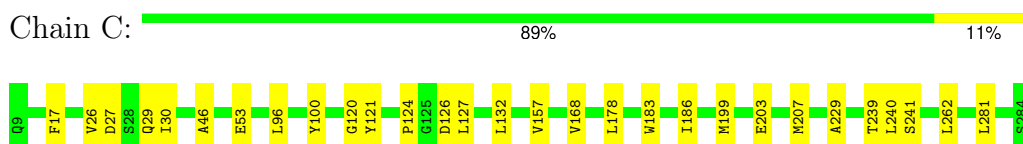
- Molecule 1: DNA repair protein PprA



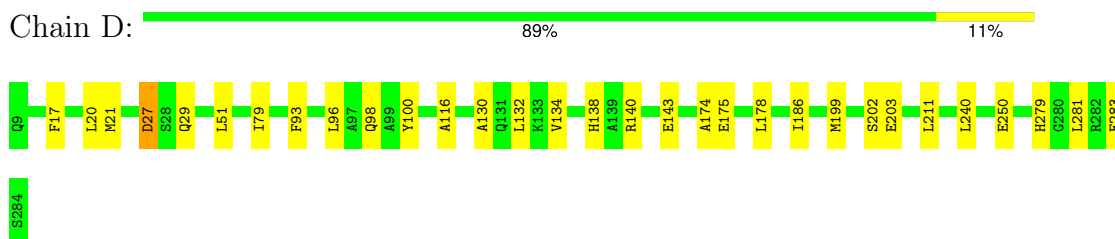
- Molecule 1: DNA repair protein PprA




- Molecule 1: DNA repair protein PprA

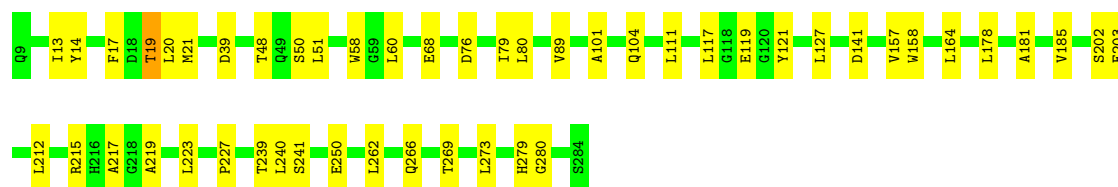


- Molecule 1: DNA repair protein PprA




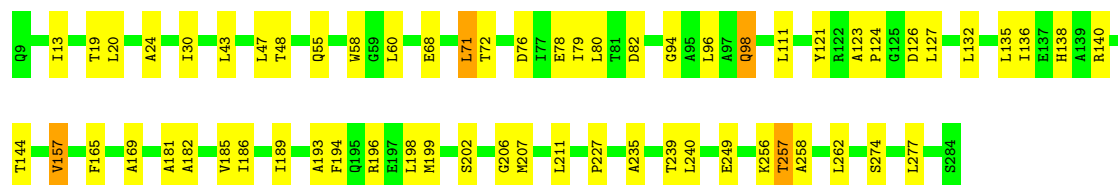
- Molecule 1: DNA repair protein PprA

Chain E:  82% 17%




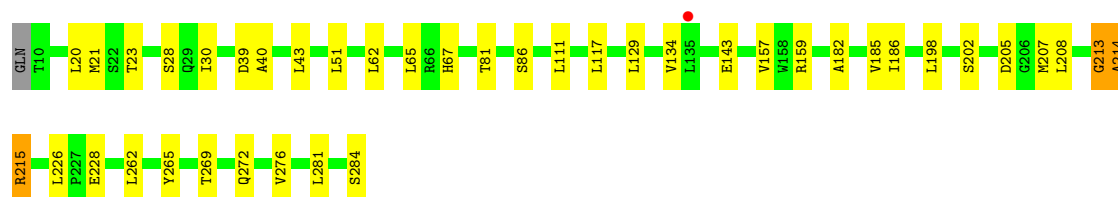
• Molecule 1: DNA repair protein PprA

Chain F:  78% 21%




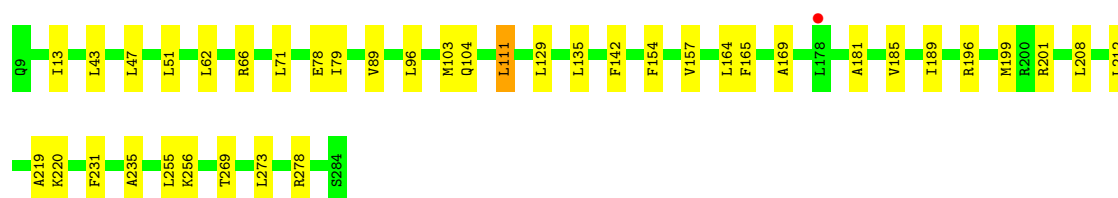
• Molecule 1: DNA repair protein PprA

Chain G:  85% 14%




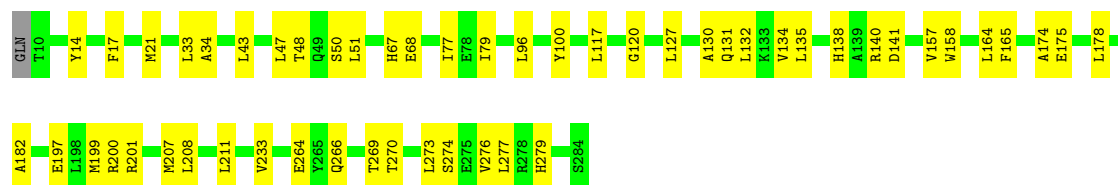
• Molecule 1: DNA repair protein PprA

Chain H:  86% 14%


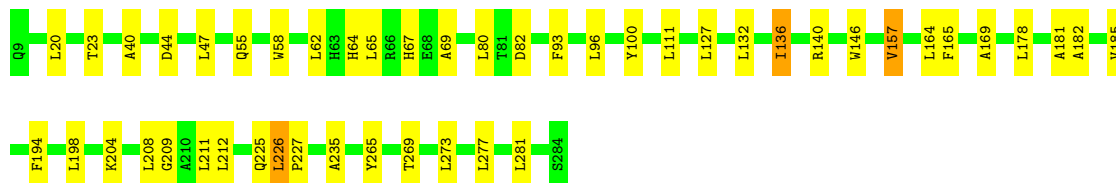


• Molecule 1: DNA repair protein PprA


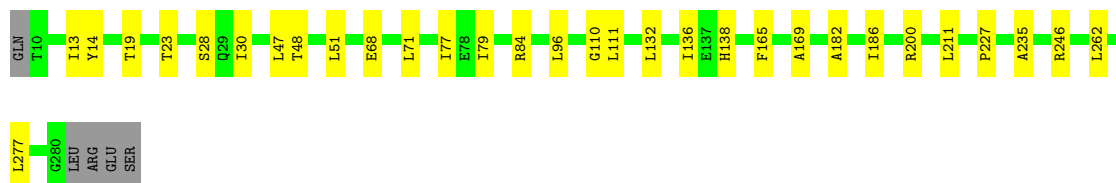
Chain I:  81% 19%




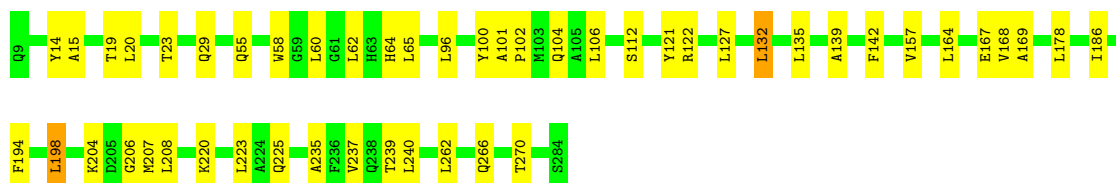
## ● Molecule 1: DNA repair protein PprA

Chain J:  83% 16%

## ● Molecule 1: DNA repair protein PprA

Chain K:  87% 11%

## ● Molecule 1: DNA repair protein PprA

Chain L:  82% 17%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.84Å 111.34Å 402.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.57 – 3.70 40.57 – 3.70	Depositor EDS
% Data completeness (in resolution range)	73.1 (40.57-3.70) 73.0 (40.57-3.70)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 3.66Å)	Xtriage
Refinement program	PHENIX 2.0_5824	Depositor
R, $R_{free}$	0.226 , 0.283 0.226 , 0.281	Depositor DCC
$R_{free}$ test set	1591 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	134.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.18	0/2125	0.33	0/2866
1	B	0.17	0/2125	0.31	0/2866
1	C	0.16	0/2125	0.34	0/2866
1	D	0.19	0/2125	0.38	0/2866
1	E	0.18	0/2125	0.34	0/2866
1	F	0.20	0/2125	0.38	0/2866
1	G	0.24	0/2116	0.45	1/2854 (0.0%)
1	H	0.16	0/2125	0.32	0/2866
1	I	0.16	0/2116	0.35	0/2854
1	J	0.18	0/2125	0.34	0/2866
1	K	0.19	0/2081	0.34	0/2809
1	L	0.21	0/2125	0.36	0/2866
All	All	0.19	0/25438	0.36	1/34311 (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
1	G	0	1
1	K	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	213	GLY	N-CA-C	-5.63	106.78	113.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	215	ARG	Sidechain
1	K	200	ARG	Sidechain

## 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	2094	0	2053	37	0
1	B	2094	0	2053	36	0
1	C	2094	0	2053	26	0
1	D	2094	0	2053	24	0
1	E	2094	0	2053	40	0
1	F	2094	0	2053	50	0
1	G	2085	0	2045	29	0
1	H	2094	0	2053	28	0
1	I	2085	0	2045	51	0
1	J	2094	0	2053	45	0
1	K	2050	0	2010	26	0
1	L	2094	0	2053	44	0
All	All	25066	0	24577	414	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 8.

The worst 5 of 414 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:L:127:LEU:HD23	1:L:132:LEU:HD12	1.52	0.90
1:I:17:PHE:CE2	1:I:47:LEU:HD23	2.05	0.89
1:F:48:THR:HG23	1:F:68:GLU:HA	1.58	0.84
1:I:266:GLN:O	1:I:270:THR:HG23	1.78	0.83
1:H:181:ALA:O	1:H:185:VAL:HG23	1.79	0.81

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	274/276 (99%)	262 (96%)	11 (4%)	1 (0%)	30	62
1	B	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	C	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	D	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	E	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	F	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
1	G	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	30	62
1	H	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	I	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	J	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	K	269/276 (98%)	264 (98%)	5 (2%)	0	100	100
1	L	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
All	All	3281/3312 (99%)	3178 (97%)	101 (3%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	214	ALA
1	A	219	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	200/196 (102%)	195 (98%)	5 (2%)	42	62
1	B	200/196 (102%)	194 (97%)	6 (3%)	36	58
1	C	200/196 (102%)	199 (100%)	1 (0%)	86	92
1	D	200/196 (102%)	196 (98%)	4 (2%)	50	68
1	E	200/196 (102%)	196 (98%)	4 (2%)	50	68
1	F	200/196 (102%)	192 (96%)	8 (4%)	27	52
1	G	199/196 (102%)	193 (97%)	6 (3%)	36	58
1	H	200/196 (102%)	195 (98%)	5 (2%)	42	62
1	I	199/196 (102%)	197 (99%)	2 (1%)	73	82
1	J	200/196 (102%)	196 (98%)	4 (2%)	50	68
1	K	195/196 (100%)	193 (99%)	2 (1%)	73	82
1	L	200/196 (102%)	196 (98%)	4 (2%)	50	68
All	All	2393/2352 (102%)	2342 (98%)	51 (2%)	48	67

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	86	SER
1	H	111	LEU
1	L	186	ILE
1	G	111	LEU
1	G	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	230	HIS
1	I	230	HIS
1	L	104	GLN
1	K	49	GLN
1	K	230	HIS

### 5.3.3 RNA ⓘ

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, 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	272/276 (98%)	-0.66	0	100	100	67, 110, 170, 218	0
1	B	272/276 (98%)	-0.67	0	100	100	67, 125, 186, 236	0
1	C	272/276 (98%)	-0.54	0	100	100	79, 160, 226, 248	0
1	D	272/276 (98%)	-0.44	0	100	100	118, 199, 266, 285	0
1	E	272/276 (98%)	-0.56	0	100	100	82, 148, 204, 233	0
1	F	272/276 (98%)	-0.63	0	100	100	70, 130, 181, 203	0
1	G	271/276 (98%)	-0.64	1 (0%)	89	76	66, 108, 158, 205	0
1	H	272/276 (98%)	-0.67	1 (0%)	89	76	84, 147, 207, 244	0
1	I	271/276 (98%)	-0.62	0	100	100	109, 189, 228, 253	0
1	J	272/276 (98%)	-0.55	0	100	100	110, 161, 227, 279	0
1	K	267/276 (96%)	-0.68	0	100	100	77, 114, 152, 200	0
1	L	272/276 (98%)	-0.59	0	100	100	68, 125, 204, 236	0
All	All	3257/3312 (98%)	-0.60	2 (0%)	92	89	66, 141, 222, 285	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	178	LEU	3.2
1	G	135	LEU	2.6

### 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.