



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 01:04 PM EDT

PDB ID : 7TMD  
Title : Crystal structure of Ornithine carbamoyltransferase from *Klebsiella pneumoniae*  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2022-01-19  
Resolution : 2.35 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)

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<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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

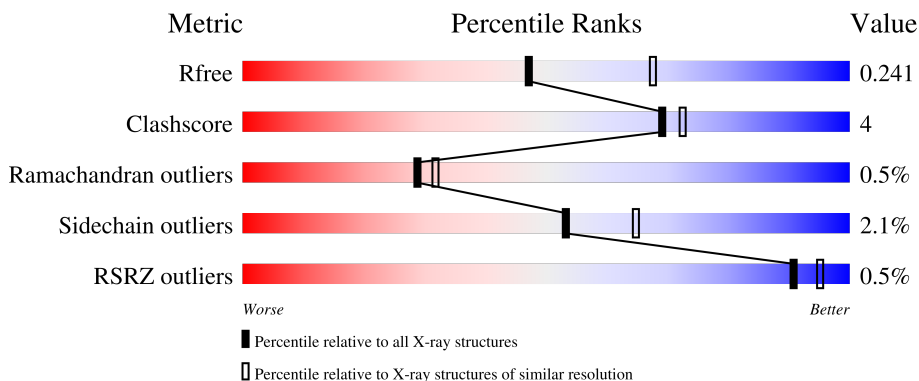
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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.



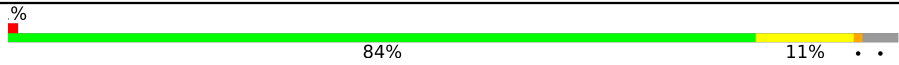
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	342	
1	B	342	
1	C	342	
1	D	342	
1	E	342	

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Mol	Chain	Length	Quality of chain
1	F	342	 <p>A horizontal bar chart showing the quality of chain. The bar is 84% green and 11% yellow. The percentage values are displayed below the bar. There is a small red square at the beginning of the bar and two dots at the end.</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BR	A	402[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15546 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 Ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2538	1605	437	482	14	0	0	0
1	B	328	2510	1589	432	474	15	0	0	0
1	C	333	2499	1584	426	474	15	0	0	0
1	D	329	2502	1585	426	476	15	0	0	0
1	E	329	2517	1594	432	476	15	0	0	0
1	F	327	2471	1564	423	470	14	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A0H3GHJ1
A	2	ALA	-	expression tag	UNP A0A0H3GHJ1
A	3	HIS	-	expression tag	UNP A0A0H3GHJ1
A	4	HIS	-	expression tag	UNP A0A0H3GHJ1
A	5	HIS	-	expression tag	UNP A0A0H3GHJ1
A	6	HIS	-	expression tag	UNP A0A0H3GHJ1
A	7	HIS	-	expression tag	UNP A0A0H3GHJ1
A	8	HIS	-	expression tag	UNP A0A0H3GHJ1
B	1	MET	-	expression tag	UNP A0A0H3GHJ1
B	2	ALA	-	expression tag	UNP A0A0H3GHJ1
B	3	HIS	-	expression tag	UNP A0A0H3GHJ1
B	4	HIS	-	expression tag	UNP A0A0H3GHJ1
B	5	HIS	-	expression tag	UNP A0A0H3GHJ1
B	6	HIS	-	expression tag	UNP A0A0H3GHJ1
B	7	HIS	-	expression tag	UNP A0A0H3GHJ1
B	8	HIS	-	expression tag	UNP A0A0H3GHJ1
C	1	MET	-	expression tag	UNP A0A0H3GHJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	expression tag	UNP A0A0H3GHJ1
C	3	HIS	-	expression tag	UNP A0A0H3GHJ1
C	4	HIS	-	expression tag	UNP A0A0H3GHJ1
C	5	HIS	-	expression tag	UNP A0A0H3GHJ1
C	6	HIS	-	expression tag	UNP A0A0H3GHJ1
C	7	HIS	-	expression tag	UNP A0A0H3GHJ1
C	8	HIS	-	expression tag	UNP A0A0H3GHJ1
D	1	MET	-	expression tag	UNP A0A0H3GHJ1
D	2	ALA	-	expression tag	UNP A0A0H3GHJ1
D	3	HIS	-	expression tag	UNP A0A0H3GHJ1
D	4	HIS	-	expression tag	UNP A0A0H3GHJ1
D	5	HIS	-	expression tag	UNP A0A0H3GHJ1
D	6	HIS	-	expression tag	UNP A0A0H3GHJ1
D	7	HIS	-	expression tag	UNP A0A0H3GHJ1
D	8	HIS	-	expression tag	UNP A0A0H3GHJ1
E	1	MET	-	expression tag	UNP A0A0H3GHJ1
E	2	ALA	-	expression tag	UNP A0A0H3GHJ1
E	3	HIS	-	expression tag	UNP A0A0H3GHJ1
E	4	HIS	-	expression tag	UNP A0A0H3GHJ1
E	5	HIS	-	expression tag	UNP A0A0H3GHJ1
E	6	HIS	-	expression tag	UNP A0A0H3GHJ1
E	7	HIS	-	expression tag	UNP A0A0H3GHJ1
E	8	HIS	-	expression tag	UNP A0A0H3GHJ1
F	1	MET	-	expression tag	UNP A0A0H3GHJ1
F	2	ALA	-	expression tag	UNP A0A0H3GHJ1
F	3	HIS	-	expression tag	UNP A0A0H3GHJ1
F	4	HIS	-	expression tag	UNP A0A0H3GHJ1
F	5	HIS	-	expression tag	UNP A0A0H3GHJ1
F	6	HIS	-	expression tag	UNP A0A0H3GHJ1
F	7	HIS	-	expression tag	UNP A0A0H3GHJ1
F	8	HIS	-	expression tag	UNP A0A0H3GHJ1

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total I 1 1	0	0

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Br	0	1
			2	2		
3	D	1	Total	Br	0	1
			2	2		

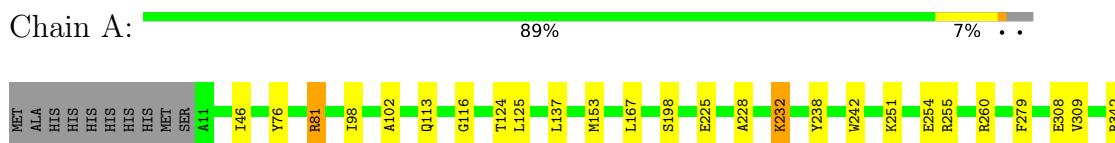
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	89	Total	O	0	0
			89	89		
4	C	72	Total	O	0	0
			72	72		
4	D	77	Total	O	0	0
			77	77		
4	E	98	Total	O	0	0
			98	98		
4	F	60	Total	O	0	0
			60	60		

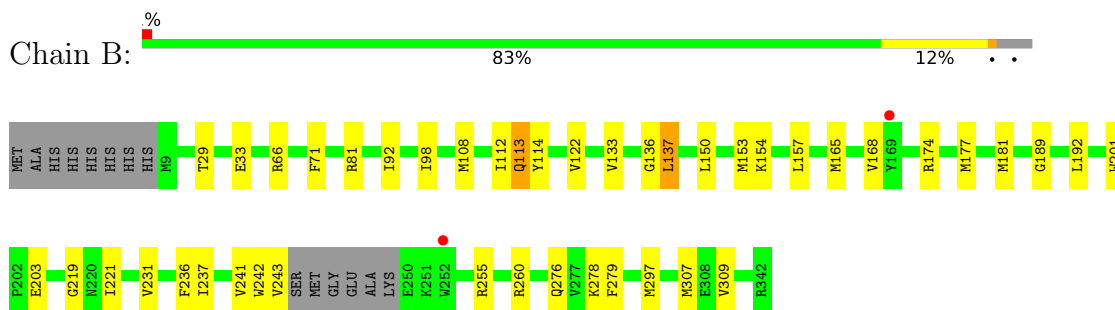
### 3 Residue-property plots [i](#)

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.

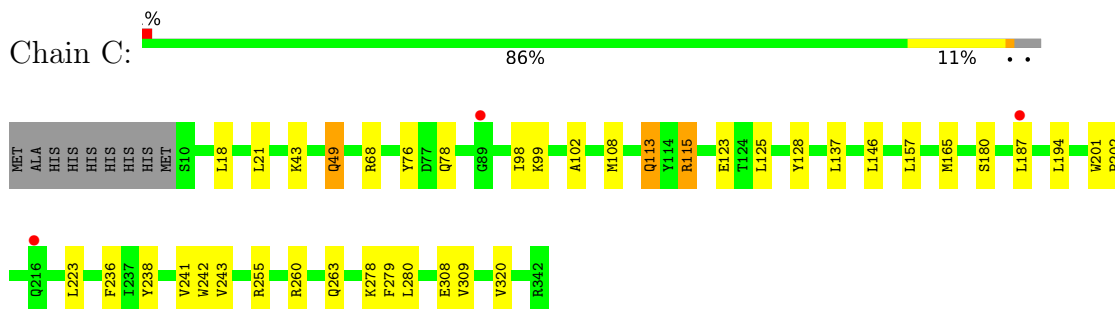
- Molecule 1: Ornithine carbamoyltransferase



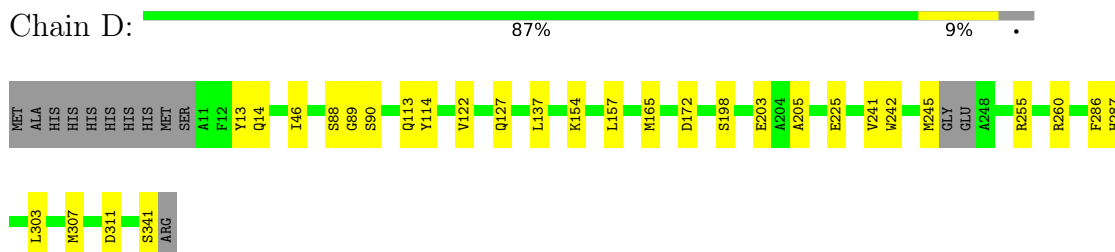
- Molecule 1: Ornithine carbamoyltransferase




- Molecule 1: Ornithine carbamoyltransferase

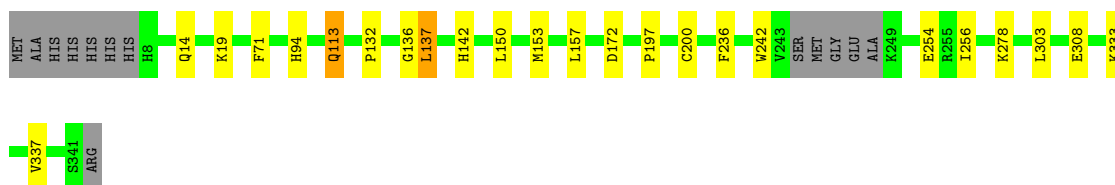


- Molecule 1: Ornithine carbamoyltransferase




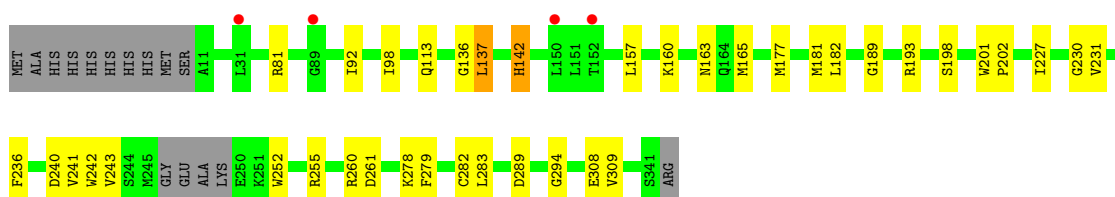
- Molecule 1: Ornithine carbamoyltransferase

Chain E:  89% 6% . .



- Molecule 1: Ornithine carbamoyltransferase

Chain F:  84% 11% . .





## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.09Å 154.71Å 150.56Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	47.54 – 2.35 48.79 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.54-2.35) 98.0 (48.79-2.35)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20_4474	Depositor
R, $R_{free}$	0.171 , 0.240 0.178 , 0.241	Depositor DCC
$R_{free}$ test set	4419 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.005 for -h,l,k 0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, BR

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	0.41	0/2585	0.60	0/3501
1	B	0.39	0/2556	0.59	0/3461
1	C	0.40	0/2545	0.59	0/3453
1	D	0.39	0/2548	0.59	0/3455
1	E	0.40	0/2564	0.60	0/3474
1	F	0.38	0/2517	0.57	0/3419
All	All	0.40	0/15315	0.59	0/20763

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	2538	0	2514	15	0
1	B	2510	0	2489	28	0
1	C	2499	0	2451	23	0
1	D	2502	0	2465	13	0
1	E	2517	0	2489	12	0
1	F	2471	0	2410	21	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	2	0
3	D	2	0	0	0	0
4	A	108	0	0	1	0
4	B	89	0	0	1	0
4	C	72	0	0	2	0
4	D	77	0	0	1	0
4	E	98	0	0	0	0
4	F	60	0	0	0	0
All	All	15546	0	14818	111	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 4.

The worst 5 of 111 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:153:MET:CE	1:A:167:LEU:HD13	2.25	0.67
1:C:242:TRP:O	1:C:255:ARG:NH1	2.26	0.67
1:B:243:VAL:HG23	1:B:255:ARG:NH1	2.10	0.65
1:C:157:LEU:HD23	1:C:165:MET:HG2	1.81	0.63
1:B:174:ARG:NH2	1:B:203:GLU:OE2	2.27	0.63

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	330/342 (96%)	321 (97%)	7 (2%)	2 (1%)	25 27
1	B	324/342 (95%)	311 (96%)	12 (4%)	1 (0%)	41 47
1	C	331/342 (97%)	318 (96%)	12 (4%)	1 (0%)	41 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	325/342 (95%)	309 (95%)	13 (4%)	3 (1%)	17	17
1	E	325/342 (95%)	312 (96%)	12 (4%)	1 (0%)	41	47
1	F	323/342 (94%)	305 (94%)	17 (5%)	1 (0%)	41	47
All	All	1958/2052 (95%)	1876 (96%)	73 (4%)	9 (0%)	29	32

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	B	137	LEU
1	D	137	LEU
1	E	137	LEU
1	F	137	LEU

### 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	260/272 (96%)	253 (97%)	7 (3%)	44	55
1	B	258/272 (95%)	253 (98%)	5 (2%)	57	68
1	C	251/272 (92%)	244 (97%)	7 (3%)	43	53
1	D	256/272 (94%)	252 (98%)	4 (2%)	62	75
1	E	259/272 (95%)	255 (98%)	4 (2%)	65	76
1	F	250/272 (92%)	245 (98%)	5 (2%)	55	66
All	All	1534/1632 (94%)	1502 (98%)	32 (2%)	53	65

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	113	GLN
1	F	142	HIS
1	C	43	LYS
1	B	276	GLN

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Mol	Chain	Res	Type
1	F	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	216	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	332/342 (97%)	-0.36	0 <a href="#">100</a>   <a href="#">100</a>	19, 28, 44, 62	0
1	B	328/342 (95%)	-0.19	2 (0%) <a href="#">89</a>   <a href="#">93</a>	20, 35, 52, 68	0
1	C	333/342 (97%)	-0.12	3 (0%) <a href="#">84</a>   <a href="#">90</a>	22, 35, 60, 76	0
1	D	329/342 (96%)	-0.22	0 <a href="#">100</a>   <a href="#">100</a>	20, 31, 52, 74	0
1	E	329/342 (96%)	-0.30	0 <a href="#">100</a>   <a href="#">100</a>	19, 29, 53, 78	0
1	F	327/342 (95%)	0.17	4 (1%) <a href="#">79</a>   <a href="#">86</a>	21, 42, 56, 74	0
All	All	1978/2052 (96%)	-0.17	9 (0%) <a href="#">91</a>   <a href="#">95</a>	19, 33, 54, 78	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	LEU	3.0
1	F	89	GLY	3.0
1	F	150	LEU	2.3
1	B	169	TYR	2.2
1	F	152	THR	2.1

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BR	A	402[A]	1/1	0.97	0.19	31,31,31,31	1
3	BR	A	402[B]	1/1	0.97	0.19	38,38,38,38	1
3	BR	D	401[A]	1/1	0.97	0.18	33,33,33,33	1
3	BR	D	401[B]	1/1	0.97	0.18	28,28,28,28	1
2	IOD	A	401	1/1	0.99	0.13	33,33,33,33	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.