



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2016 – 11:14 AM EDT

PDB ID : 5K3H  
Title : Crystals structure of Acyl-CoA oxidase-1 in *Caenorhabditis elegans*, Apo form-II  
Authors : Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.  
Deposited on : 2016-05-19  
Resolution : 2.48 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

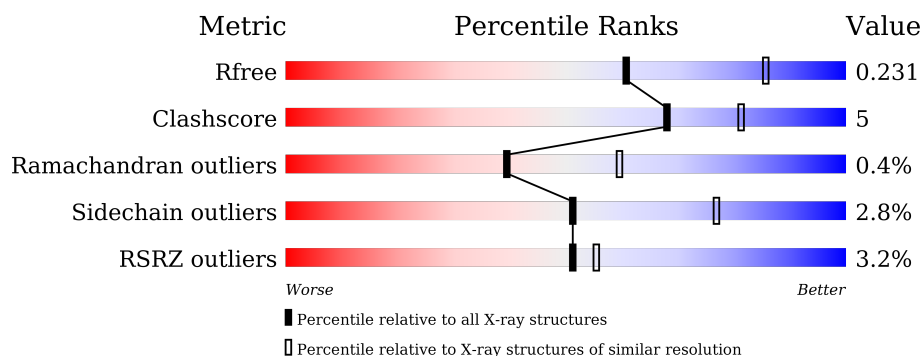
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	684	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div> </div>
1	B	684	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• 7%</div> </div> </div>
1	C	684	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	D	684	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>• 7%</div> </div> </div>
1	E	684	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	F	684	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	684	<div><div></div><div>3%</div><div>82%</div><div>11%</div><div>7%</div></div>
1	H	684	<div><div></div><div>2%</div><div>81%</div><div>10%</div><div>7%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41742 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 Acyl-coenzyme A oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5036	3199	885	928	24			
1	B	635	Total	C	N	O	S	0	0	0
			5039	3198	887	931	23			
1	C	633	Total	C	N	O	S	0	0	0
			5023	3190	885	925	23			
1	D	634	Total	C	N	O	S	0	0	0
			5035	3196	886	930	23			
1	E	635	Total	C	N	O	S	0	0	0
			5036	3197	887	929	23			
1	F	633	Total	C	N	O	S	0	0	0
			5030	3193	885	929	23			
1	G	634	Total	C	N	O	S	0	0	0
			5032	3195	886	928	23			
1	H	634	Total	C	N	O	S	0	0	0
			5035	3196	886	930	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	HIS	-	expression tag	UNP O62140
A	676	HIS	-	expression tag	UNP O62140
A	677	HIS	-	expression tag	UNP O62140
A	678	HIS	-	expression tag	UNP O62140
A	679	HIS	-	expression tag	UNP O62140
A	680	HIS	-	expression tag	UNP O62140
A	681	HIS	-	expression tag	UNP O62140
A	682	HIS	-	expression tag	UNP O62140
A	683	HIS	-	expression tag	UNP O62140
A	684	HIS	-	expression tag	UNP O62140
B	675	HIS	-	expression tag	UNP O62140
B	676	HIS	-	expression tag	UNP O62140
B	677	HIS	-	expression tag	UNP O62140

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Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	-	expression tag	UNP O62140
B	679	HIS	-	expression tag	UNP O62140
B	680	HIS	-	expression tag	UNP O62140
B	681	HIS	-	expression tag	UNP O62140
B	682	HIS	-	expression tag	UNP O62140
B	683	HIS	-	expression tag	UNP O62140
B	684	HIS	-	expression tag	UNP O62140
C	675	HIS	-	expression tag	UNP O62140
C	676	HIS	-	expression tag	UNP O62140
C	677	HIS	-	expression tag	UNP O62140
C	678	HIS	-	expression tag	UNP O62140
C	679	HIS	-	expression tag	UNP O62140
C	680	HIS	-	expression tag	UNP O62140
C	681	HIS	-	expression tag	UNP O62140
C	682	HIS	-	expression tag	UNP O62140
C	683	HIS	-	expression tag	UNP O62140
C	684	HIS	-	expression tag	UNP O62140
D	675	HIS	-	expression tag	UNP O62140
D	676	HIS	-	expression tag	UNP O62140
D	677	HIS	-	expression tag	UNP O62140
D	678	HIS	-	expression tag	UNP O62140
D	679	HIS	-	expression tag	UNP O62140
D	680	HIS	-	expression tag	UNP O62140
D	681	HIS	-	expression tag	UNP O62140
D	682	HIS	-	expression tag	UNP O62140
D	683	HIS	-	expression tag	UNP O62140
D	684	HIS	-	expression tag	UNP O62140
E	675	HIS	-	expression tag	UNP O62140
E	676	HIS	-	expression tag	UNP O62140
E	677	HIS	-	expression tag	UNP O62140
E	678	HIS	-	expression tag	UNP O62140
E	679	HIS	-	expression tag	UNP O62140
E	680	HIS	-	expression tag	UNP O62140
E	681	HIS	-	expression tag	UNP O62140
E	682	HIS	-	expression tag	UNP O62140
E	683	HIS	-	expression tag	UNP O62140
E	684	HIS	-	expression tag	UNP O62140
F	675	HIS	-	expression tag	UNP O62140
F	676	HIS	-	expression tag	UNP O62140
F	677	HIS	-	expression tag	UNP O62140
F	678	HIS	-	expression tag	UNP O62140
F	679	HIS	-	expression tag	UNP O62140

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Chain	Residue	Modelled	Actual	Comment	Reference
F	680	HIS	-	expression tag	UNP O62140
F	681	HIS	-	expression tag	UNP O62140
F	682	HIS	-	expression tag	UNP O62140
F	683	HIS	-	expression tag	UNP O62140
F	684	HIS	-	expression tag	UNP O62140
G	675	HIS	-	expression tag	UNP O62140
G	676	HIS	-	expression tag	UNP O62140
G	677	HIS	-	expression tag	UNP O62140
G	678	HIS	-	expression tag	UNP O62140
G	679	HIS	-	expression tag	UNP O62140
G	680	HIS	-	expression tag	UNP O62140
G	681	HIS	-	expression tag	UNP O62140
G	682	HIS	-	expression tag	UNP O62140
G	683	HIS	-	expression tag	UNP O62140
G	684	HIS	-	expression tag	UNP O62140
H	675	HIS	-	expression tag	UNP O62140
H	676	HIS	-	expression tag	UNP O62140
H	677	HIS	-	expression tag	UNP O62140
H	678	HIS	-	expression tag	UNP O62140
H	679	HIS	-	expression tag	UNP O62140
H	680	HIS	-	expression tag	UNP O62140
H	681	HIS	-	expression tag	UNP O62140
H	682	HIS	-	expression tag	UNP O62140
H	683	HIS	-	expression tag	UNP O62140
H	684	HIS	-	expression tag	UNP O62140

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	150	Total O 150 150	0	0
2	B	180	Total O 180 180	0	0
2	C	199	Total O 199 199	0	0
2	D	215	Total O 215 215	0	0
2	E	188	Total O 188 188	0	0
2	F	156	Total O 156 156	0	0
2	G	203	Total O 203 203	0	0

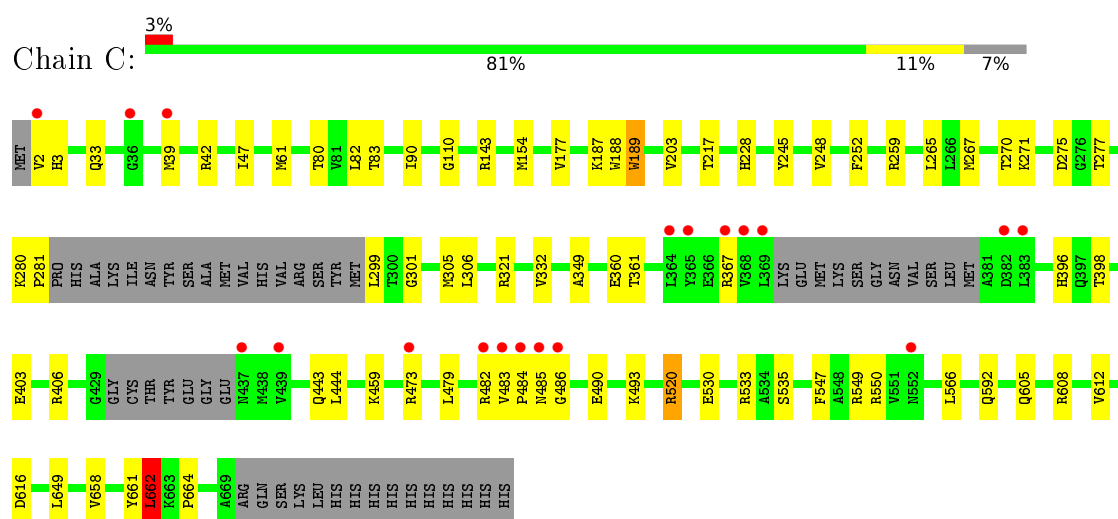
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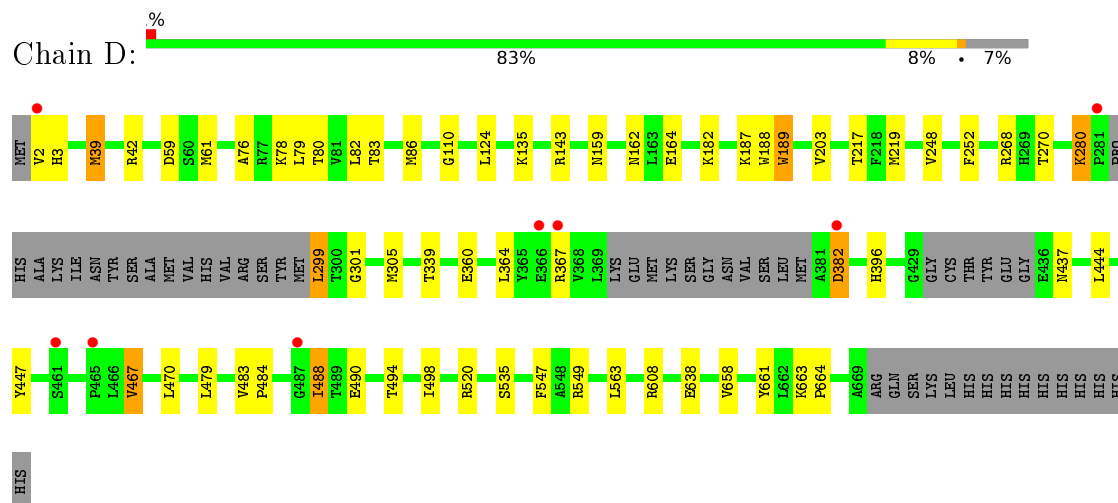
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	185	Total 185	O 185	0	0



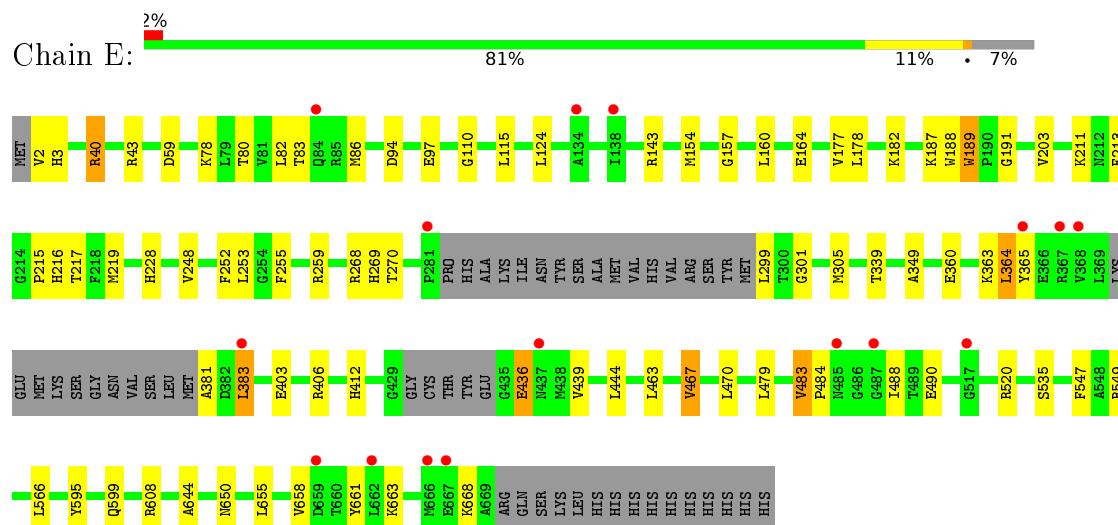




- Molecule 1: Acyl-coenzyme A oxidase



- Molecule 1: Acyl-coenzyme A oxidase



- Molecule 1: Acyl-coenzyme A oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.07Å 140.79Å 154.93Å 90.00° 117.20° 90.00°	Depositor
Resolution (Å)	49.24 – 2.48 49.24 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-2.48) 99.7 (49.24-2.48)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.191 , 0.232 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	10069 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.074 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1995e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

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	0.44	0/5137	0.61	0/6943
1	B	0.45	0/5140	0.62	0/6949
1	C	0.46	0/5124	0.60	0/6928
1	D	0.48	0/5136	0.62	0/6944
1	E	0.45	0/5137	0.64	0/6945
1	F	0.44	0/5131	0.60	0/6937
1	G	0.47	0/5133	0.62	0/6940
1	H	0.46	0/5136	0.62	0/6944
All	All	0.45	0/41074	0.62	0/55530

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	5036	0	5056	57	0
1	B	5039	0	5058	45	0
1	C	5023	0	5047	44	0
1	D	5035	0	5055	37	0
1	E	5036	0	5056	49	0
1	F	5030	0	5050	73	0
1	G	5032	0	5053	46	0
1	H	5035	0	5055	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	150	0	0	5	0
2	B	180	0	0	2	0
2	C	199	0	0	3	0
2	D	215	0	0	2	0
2	E	188	0	0	1	0
2	F	156	0	0	2	0
2	G	203	0	0	1	0
2	H	185	0	0	6	0
All	All	41742	0	40430	376	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 5.

The worst 5 of 376 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:658:VAL:HA	1:A:662:LEU:HB2	1.30	1.13
1:G:661:TYR:O	1:G:664:PRO:HD2	1.56	1.04
1:H:658:VAL:HA	1:H:662:LEU:HB2	1.36	1.03
1:F:658:VAL:HG22	1:F:662:LEU:HD12	1.44	0.99
1:F:658:VAL:HA	1:F:662:LEU:HB2	1.44	0.97

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	624/684 (91%)	610 (98%)	13 (2%)	1 (0%)	52 73
1	B	627/684 (92%)	613 (98%)	12 (2%)	2 (0%)	46 66
1	C	625/684 (91%)	609 (97%)	14 (2%)	2 (0%)	46 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	626/684 (92%)	613 (98%)	10 (2%)	3 (0%)	34	53
1	E	627/684 (92%)	614 (98%)	11 (2%)	2 (0%)	46	66
1	F	625/684 (91%)	607 (97%)	15 (2%)	3 (0%)	34	53
1	G	626/684 (92%)	617 (99%)	7 (1%)	2 (0%)	46	66
1	H	626/684 (92%)	609 (97%)	14 (2%)	3 (0%)	34	53
All	All	5006/5472 (92%)	4892 (98%)	96 (2%)	18 (0%)	39	59

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	B	189	TRP
1	C	189	TRP
1	D	189	TRP
1	D	488	ILE

### 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	534/579 (92%)	516 (97%)	18 (3%)	44	70
1	B	534/579 (92%)	521 (98%)	13 (2%)	57	81
1	C	532/579 (92%)	518 (97%)	14 (3%)	54	79
1	D	534/579 (92%)	518 (97%)	16 (3%)	48	74
1	E	533/579 (92%)	520 (98%)	13 (2%)	57	81
1	F	534/579 (92%)	519 (97%)	15 (3%)	51	77
1	G	533/579 (92%)	517 (97%)	16 (3%)	48	74
1	H	534/579 (92%)	520 (97%)	14 (3%)	54	79
All	All	4268/4632 (92%)	4149 (97%)	119 (3%)	51	77

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	367	ARG
1	E	365	TYR
1	H	339	THR
1	D	467	VAL
1	D	638	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	ASN
1	H	269	HIS
1	F	322	GLN
1	D	159	ASN
1	G	443	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 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<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	634/684 (92%)	0.22	26 (4%)	41	45	18, 30, 55, 71	0
1	B	635/684 (92%)	0.06	15 (2%)	62	65	15, 26, 46, 67	0
1	C	633/684 (92%)	0.09	19 (3%)	54	58	15, 26, 43, 63	0
1	D	634/684 (92%)	-0.04	8 (1%)	79	82	12, 22, 41, 64	0
1	E	635/684 (92%)	0.09	16 (2%)	61	64	14, 26, 46, 65	0
1	F	633/684 (92%)	0.33	41 (6%)	22	24	18, 30, 58, 71	0
1	G	634/684 (92%)	0.02	20 (3%)	51	55	13, 23, 44, 69	0
1	H	634/684 (92%)	0.07	16 (2%)	61	64	15, 27, 45, 81	0
All	All	5072/5472 (92%)	0.10	161 (3%)	51	55	12, 26, 48, 81	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	7.6
1	F	486	GLY	7.5
1	F	485	ASN	6.0
1	B	435	GLY	6.0
1	H	368	VAL	5.5

### 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.