



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 PM GMT

PDB ID : 4M23  
Title : Crystal structure of non-heme iron oxygenase OrfP  
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.  
Deposited on : 2013-08-05  
Resolution : 1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

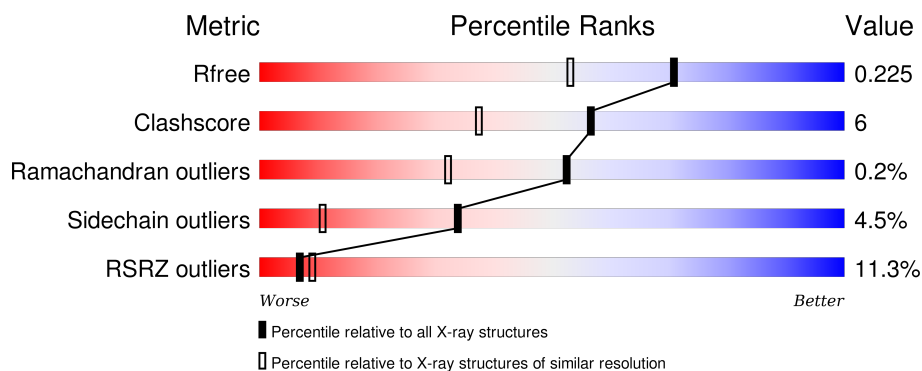
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	364	<div> <div>7%</div> <div>79% 10% • 9%</div> </div>
1	B	364	<div> <div>9%</div> <div>76% 8% • 14%</div> </div>
1	C	364	<div> <div>11%</div> <div>80% 7% • 12%</div> </div>
1	D	364	<div> <div>13%</div> <div>74% 12% • 13%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11527 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 L-arginine beta-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	6	0
			2720	1708	502	503	7			
1	B	314	Total	C	N	O	S	0	4	0
			2559	1615	466	472	6			
1	C	319	Total	C	N	O	S	0	3	0
			2592	1630	474	481	7			
1	D	316	Total	C	N	O	S	0	3	0
			2569	1619	467	477	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
A	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
A	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
A	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
A	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
A	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
A	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-19	MET	-	EXPRESSION TAG	UNP G9MBV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
B	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
B	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
B	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
B	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
B	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
C	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
C	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
C	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
C	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
C	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
C	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
D	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-17	SER	-	EXPRESSION TAG	UNP G9MBV2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
D	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
D	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
D	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
D	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
D	0	HIS	-	EXPRESSION TAG	UNP G9MBV2

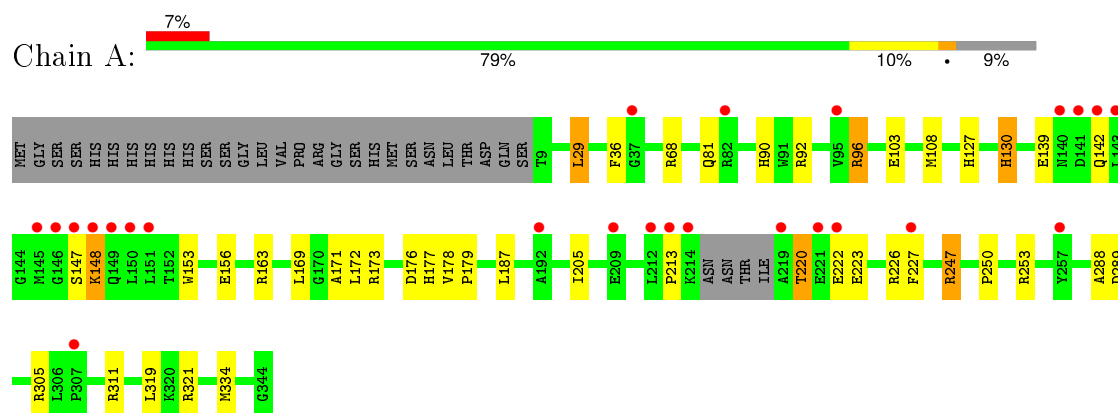
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	292	Total O 292 292	0	0
2	B	277	Total O 277 277	0	0
2	C	287	Total O 287 287	0	0
2	D	231	Total O 231 231	0	0

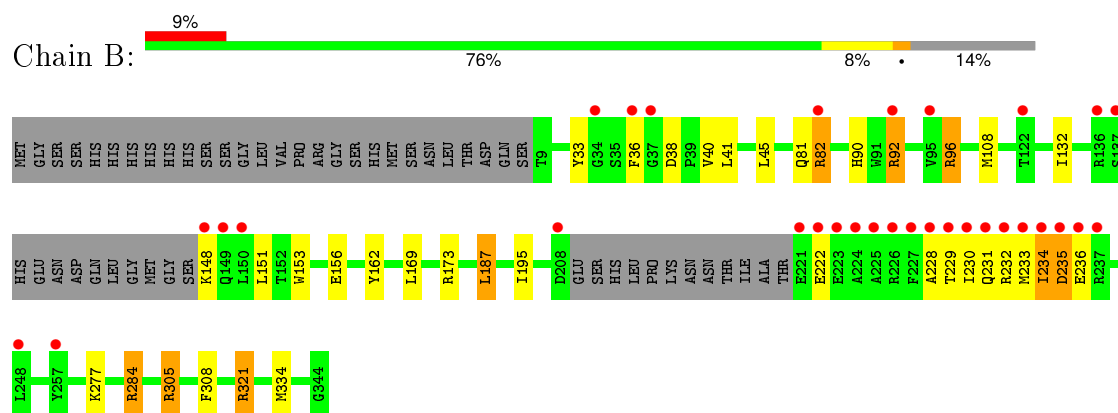
### 3 Residue-property plots [i](#)

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.

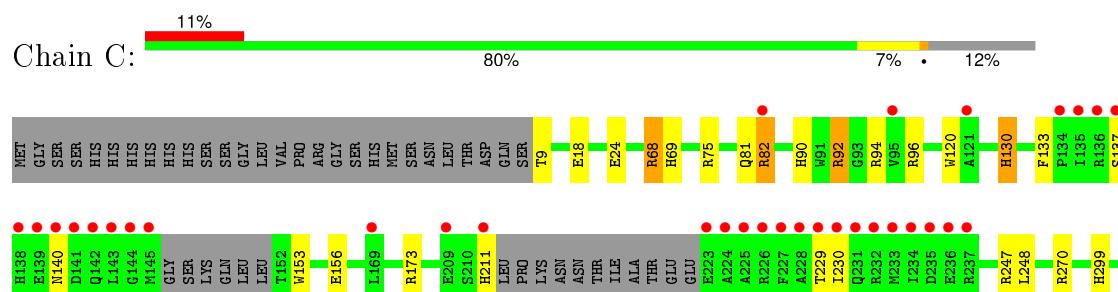
#### • Molecule 1: L-arginine beta-hydroxylase

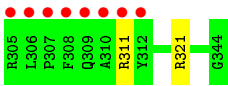


#### • Molecule 1: L-arginine beta-hydroxylase

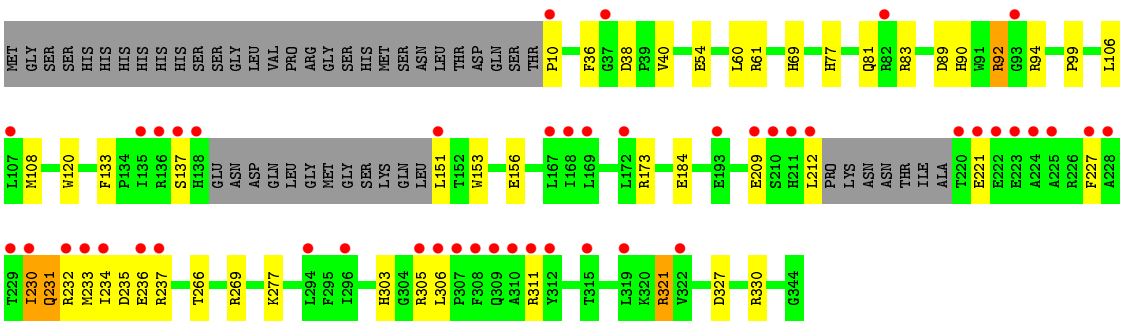


#### • Molecule 1: L-arginine beta-hydroxylase





● Molecule 1: L-arginine beta-hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.31Å 117.17Å 96.60Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	30.00 – 1.76 28.62 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.76) 99.8 (28.62-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.190 , 0.227 0.190 , 0.225	Depositor DCC
$R_{free}$ test set	7526 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.8	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 150084 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	0.67	1/2789 (0.0%)	0.77	2/3786 (0.1%)
1	B	0.65	1/2624 (0.0%)	0.76	0/3565
1	C	0.69	4/2659 (0.2%)	0.78	0/3612
1	D	0.63	2/2636 (0.1%)	0.72	0/3582
All	All	0.66	8/10708 (0.1%)	0.76	2/14545 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	TRP	CD2-CE2	6.23	1.48	1.41
1	C	247[A]	ARG	CA-CB	6.07	1.67	1.53
1	C	247[B]	ARG	CA-CB	6.07	1.67	1.53
1	B	153	TRP	CD2-CE2	5.80	1.48	1.41
1	A	153	TRP	CD2-CE2	5.53	1.48	1.41
1	C	120	TRP	CD2-CE2	5.48	1.48	1.41
1	D	120	TRP	CD2-CE2	5.38	1.47	1.41
1	D	153	TRP	CD2-CE2	5.20	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CB-CG-CD1	6.01	121.22	111.00
1	A	288	ALA	N-CA-C	-5.63	95.81	111.00

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	2720	0	2639	38	1
1	B	2559	0	2487	36	0
1	C	2592	0	2497	19	0
1	D	2569	0	2478	32	0
2	A	292	0	0	10	0
2	B	277	0	0	9	1
2	C	287	0	0	12	0
2	D	231	0	0	13	0
All	All	11527	0	10101	125	1

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 6.

All (125) 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:B:321[A]:ARG:HH11	1:B:321[A]:ARG:HG2	1.04	1.14
1:A:334:MET:CE	2:A:619:HOH:O	1.99	1.09
1:A:92[B]:ARG:NH1	2:A:591:HOH:O	1.85	1.01
1:A:334:MET:HE2	2:A:619:HOH:O	1.59	1.00
1:A:156:GLU:OE2	1:A:321:ARG:NH2	1.96	0.98
1:B:234:ILE:HG12	1:B:334:MET:HE2	1.47	0.96
1:B:234:ILE:HG12	1:B:334:MET:CE	1.95	0.95
1:B:82:ARG:NH1	2:B:589:HOH:O	1.90	0.94
1:C:96:ARG:NH1	2:C:610:HOH:O	2.02	0.90
1:B:321[A]:ARG:HH11	1:B:321[A]:ARG:CG	1.90	0.85
1:B:321[A]:ARG:NH1	1:B:321[A]:ARG:HG2	1.76	0.84
1:B:277:LYS:HE3	2:B:601:HOH:O	1.79	0.83
1:B:90:HIS:CD2	1:B:92:ARG:H	1.97	0.82
1:C:299:HIS:HD2	2:C:622:HOH:O	1.63	0.81
1:B:90:HIS:HD2	1:B:92:ARG:H	1.27	0.80
1:B:38:ASP:OD1	1:B:40[B]:VAL:HG12	1.84	0.78
1:C:299:HIS:CD2	2:C:622:HOH:O	2.36	0.77
1:C:75:ARG:NE	2:C:597:HOH:O	2.06	0.76
1:D:184:GLU:OE2	2:D:547:HOH:O	2.04	0.75
1:A:247[B]:ARG:HG3	1:A:247[B]:ARG:HH11	1.51	0.74
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.21	0.73
1:A:334:MET:HE3	2:A:619:HOH:O	1.76	0.71
1:C:9:THR:N	2:C:675:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:OE2	1:B:321[A]:ARG:NH2	2.23	0.70
1:B:305:ARG:NH1	2:B:639:HOH:O	2.10	0.70
1:C:18:GLU:OE2	2:C:565:HOH:O	2.10	0.70
1:D:90:HIS:CD2	1:D:92:ARG:HG3	2.27	0.70
1:A:96:ARG:NE	2:A:600:HOH:O	2.24	0.69
1:C:156:GLU:OE2	1:C:321:ARG:NH2	2.28	0.67
1:B:234:ILE:HG12	1:B:334:MET:HE1	1.77	0.67
1:B:231:GLN:O	1:B:235:ASP:HB2	1.95	0.66
1:D:54:GLU:OE1	2:D:512:HOH:O	2.13	0.65
1:A:205:ILE:HD12	1:A:253[B]:ARG:HH11	1.61	0.65
1:D:209:GLU:HA	1:D:212:LEU:HD13	1.78	0.65
1:B:234:ILE:HD12	1:B:235:ASP:H	1.61	0.65
1:A:305:ARG:HD3	2:A:610:HOH:O	1.97	0.65
1:D:81:GLN:NE2	1:D:173:ARG:HE	1.95	0.64
1:D:38:ASP:OD1	1:D:40:VAL:HG12	1.98	0.63
1:D:156:GLU:OE2	1:D:321:ARG:NH2	2.31	0.63
1:A:96:ARG:HH11	1:A:127:HIS:CE1	2.17	0.63
1:D:69:HIS:HD2	2:D:546:HOH:O	1.81	0.63
1:D:330:ARG:NH2	2:D:599:HOH:O	2.34	0.61
1:B:162:TYR:CE2	1:B:334:MET:HE3	2.36	0.60
1:A:90:HIS:CD2	1:A:92[A]:ARG:H	2.19	0.60
1:A:90:HIS:CD2	1:A:92[B]:ARG:H	2.19	0.60
1:B:277:LYS:CE	2:B:601:HOH:O	2.45	0.60
1:C:90:HIS:HD2	1:C:92[A]:ARG:H	1.51	0.59
1:A:90:HIS:HD2	1:A:92[B]:ARG:H	1.49	0.59
1:A:247[B]:ARG:HG3	1:A:247[B]:ARG:NH1	2.18	0.58
1:D:230:ILE:H	1:D:230:ILE:HD13	1.69	0.58
1:D:81:GLN:HE22	1:D:173:ARG:HE	1.51	0.58
1:A:90:HIS:HD2	1:A:92[A]:ARG:H	1.49	0.57
1:D:69:HIS:CD2	2:D:546:HOH:O	2.57	0.57
1:A:130:HIS:HE1	2:A:500:HOH:O	1.87	0.57
1:B:284:ARG:HD3	2:B:628:HOH:O	2.05	0.57
1:D:321:ARG:HD3	2:D:558:HOH:O	2.04	0.56
1:C:90:HIS:HD2	1:C:92[B]:ARG:H	1.53	0.56
1:B:234:ILE:HD12	1:B:235:ASP:N	2.21	0.56
1:A:169:LEU:HD21	1:A:321:ARG:HD2	1.87	0.55
1:A:139:GLU:HG2	1:A:148:LYS:HG3	1.88	0.54
1:D:232:ARG:O	1:D:236:GLU:HG2	2.07	0.54
1:B:81:GLN:HE22	1:B:173:ARG:HE	1.56	0.54
1:D:303:HIS:NE2	2:D:565:HOH:O	2.29	0.54
1:D:92:ARG:HB3	2:D:553:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:NE2	1:B:173:ARG:HE	2.05	0.53
1:B:321[A]:ARG:NH1	2:B:648:HOH:O	2.41	0.53
1:A:222:GLU:OE1	1:A:226:ARG:NH1	2.43	0.52
1:B:229:THR:O	1:B:233:MET:HB3	2.09	0.52
1:D:10:PRO:N	2:D:618:HOH:O	2.43	0.52
1:A:177:HIS:HD2	1:A:289:ASP:OD1	1.92	0.52
1:D:305:ARG:NH1	1:D:306:LEU:O	2.44	0.51
1:D:277:LYS:HD2	2:D:577:HOH:O	2.11	0.50
1:D:269:ARG:HD3	2:D:590:HOH:O	2.11	0.49
1:C:81:GLN:NE2	1:C:173:ARG:HE	2.11	0.49
1:A:220:THR:HG23	1:A:223:GLU:H	1.76	0.49
1:C:130:HIS:HE1	2:C:472:HOH:O	1.95	0.49
1:A:139:GLU:CG	1:A:148:LYS:HG3	2.42	0.49
1:C:68:ARG:NH1	2:C:672:HOH:O	2.46	0.48
1:B:230:ILE:HG13	1:B:334:MET:HG2	1.95	0.48
1:C:156:GLU:OE1	2:C:616:HOH:O	2.20	0.48
1:D:156:GLU:OE1	2:D:565:HOH:O	2.20	0.48
1:D:232:ARG:HG2	1:D:236:GLU:OE1	2.13	0.48
1:C:24:GLU:HG3	2:C:659:HOH:O	2.14	0.48
1:C:90:HIS:CD2	1:C:92[B]:ARG:HG2	2.49	0.48
1:D:237:ARG:O	1:D:237:ARG:HG2	2.14	0.48
1:D:231:GLN:HE22	1:D:235:ASP:CG	2.17	0.47
1:C:69:HIS:HD2	2:C:677:HOH:O	1.97	0.47
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.50	0.47
1:A:334:MET:HE1	2:A:618:HOH:O	2.15	0.46
1:C:321:ARG:HD3	2:C:611:HOH:O	2.15	0.46
1:D:230:ILE:HA	1:D:233:MET:HB2	1.95	0.46
1:A:96:ARG:NH1	1:A:127:HIS:CE1	2.84	0.46
1:A:81:GLN:NE2	1:A:173:ARG:HE	2.14	0.45
1:D:327:ASP:OD1	2:D:597:HOH:O	2.21	0.45
1:C:90:HIS:CD2	1:C:92[B]:ARG:CG	3.00	0.45
1:B:96:ARG:NH1	2:B:578:HOH:O	2.49	0.45
1:B:169:LEU:HD21	1:B:321[A]:ARG:HD2	1.99	0.45
1:D:231:GLN:NE2	1:D:235:ASP:OD2	2.49	0.45
1:B:228:ALA:HB1	1:B:232:ARG:HH21	1.81	0.45
1:A:81:GLN:HE22	1:A:173:ARG:HE	1.64	0.44
1:A:177:HIS:HE1	2:A:666:HOH:O	2.01	0.44
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.53	0.44
1:A:187:LEU:HD22	1:A:250:PRO:HD3	2.00	0.43
1:B:308:PHE:HB3	2:B:532:HOH:O	2.17	0.43
1:B:284:ARG:NE	2:B:629:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CD2	1:B:41:LEU:HB2	2.53	0.43
1:A:171:ALA:HA	1:A:319:LEU:HD22	2.00	0.43
1:D:83:ARG:O	1:D:99:PRO:HB2	2.19	0.42
1:B:187:LEU:HD22	1:B:195:ILE:HD11	2.01	0.42
1:B:234:ILE:CG1	1:B:334:MET:HE1	2.48	0.42
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.00	0.42
1:B:234:ILE:CG1	1:B:334:MET:HE2	2.32	0.41
1:B:132:ILE:HD11	1:B:321[A]:ARG:HD3	2.03	0.41
1:B:36:PHE:CE1	1:B:108:MET:HG3	2.56	0.41
1:C:82:ARG:CB	1:C:82:ARG:CZ	2.98	0.41
1:D:77:HIS:CD2	1:D:106:LEU:HD21	2.55	0.41
1:A:220:THR:HG23	1:A:223:GLU:HB2	2.02	0.41
1:A:163:ARG:NH1	1:A:253[B]:ARG:HH21	2.18	0.41
1:D:227:PHE:CD1	1:D:230:ILE:HD11	2.55	0.41
1:A:253[A]:ARG:HG3	1:A:253[A]:ARG:O	2.20	0.41
1:A:213:PRO:HG3	1:A:227:PHE:HB3	2.03	0.41
1:B:148:LYS:C	1:B:148:LYS:HE2	2.41	0.41
1:D:81:GLN:HE22	1:D:173:ARG:HB3	1.85	0.40
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.83	0.40
1:A:253[A]:ARG:NH2	2:A:616:HOH:O	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92[A]:ARG:NH1	2:B:532:HOH:O[2_646]	1.15	1.05

## 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	334/364 (92%)	327 (98%)	6 (2%)	1 (0%)	46 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/364 (86%)	303 (97%)	9 (3%)	0	100	100
1	C	316/364 (87%)	307 (97%)	9 (3%)	0	100	100
1	D	313/364 (86%)	302 (96%)	10 (3%)	1 (0%)	46	25
All	All	1275/1456 (88%)	1239 (97%)	34 (3%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	D	137	SER

### 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	288/311 (93%)	279 (97%)	9 (3%)	47	21
1	B	271/311 (87%)	257 (95%)	14 (5%)	29	7
1	C	274/311 (88%)	259 (94%)	15 (6%)	27	7
1	D	272/311 (88%)	256 (94%)	16 (6%)	24	6
All	All	1105/1244 (89%)	1051 (95%)	54 (5%)	34	9

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	68	ARG
1	A	96	ARG
1	A	130	HIS
1	A	142	GLN
1	A	148	LYS
1	A	220	THR
1	A	247[A]	ARG
1	A	247[B]	ARG

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	82	ARG
1	B	92	ARG
1	B	96	ARG
1	B	151	LEU
1	B	187	LEU
1	B	222	GLU
1	B	234	ILE
1	B	235	ASP
1	B	236	GLU
1	B	284	ARG
1	B	305	ARG
1	B	321[A]	ARG
1	B	321[B]	ARG
1	C	68	ARG
1	C	82	ARG
1	C	92[A]	ARG
1	C	92[B]	ARG
1	C	94	ARG
1	C	130	HIS
1	C	133	PHE
1	C	137	SER
1	C	140	ASN
1	C	211	HIS
1	C	229	THR
1	C	230	ILE
1	C	248	LEU
1	C	270	ARG
1	C	311	ARG
1	D	60	LEU
1	D	61	ARG
1	D	89[A]	ASP
1	D	89[B]	ASP
1	D	92	ARG
1	D	94[A]	ARG
1	D	94[B]	ARG
1	D	133	PHE
1	D	151	LEU
1	D	221	GLU
1	D	230	ILE
1	D	231	GLN
1	D	234	ILE

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Mol	Chain	Res	Type
1	D	266	THR
1	D	311	ARG
1	D	321	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	69	HIS
1	A	81	GLN
1	A	90	HIS
1	A	130	HIS
1	A	177	HIS
1	A	263	GLN
1	B	57	GLN
1	B	81	GLN
1	B	90	HIS
1	B	154	HIS
1	B	177	HIS
1	B	290	GLN
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	130	HIS
1	C	177	HIS
1	C	299	HIS
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	231	GLN

### 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 [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	332/364 (91%)	0.37	25 (7%)	17 22	13, 23, 52, 83	2 (0%)
1	B	314/364 (86%)	0.56	32 (10%)	9 11	15, 24, 62, 98	3 (0%)
1	C	319/364 (87%)	0.70	41 (12%)	5 6	14, 23, 71, 115	2 (0%)
1	D	316/364 (86%)	0.92	47 (14%)	3 5	15, 28, 64, 101	3 (0%)
All	All	1281/1456 (87%)	0.63	145 (11%)	7 9	13, 25, 64, 115	10 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	ILE	18.1
1	D	212	LEU	13.2
1	C	140	ASN	10.8
1	B	227	PHE	10.4
1	D	308	PHE	9.7
1	A	150	LEU	9.6
1	C	138	HIS	9.0
1	C	145	MET	8.6
1	D	306	LEU	8.0
1	D	221	GLU	7.9
1	C	224	ALA	7.9
1	D	138	HIS	7.8
1	C	143	LEU	7.6
1	C	141	ASP	7.4
1	C	234	ILE	7.4
1	D	137	SER	7.3
1	B	233	MET	7.1
1	C	227	PHE	7.0
1	A	149	GLN	6.8
1	C	308	PHE	6.7
1	D	151	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	37	GLY	6.6
1	D	136	ARG	6.1
1	C	306	LEU	6.0
1	A	219	ALA	5.9
1	D	230	ILE	5.7
1	D	37	GLY	5.7
1	C	228	ALA	5.7
1	D	307	PRO	5.7
1	A	143	LEU	5.5
1	A	148	LYS	5.4
1	C	144	GLY	5.4
1	A	212	LEU	5.3
1	D	227	PHE	5.3
1	C	211	HIS	5.3
1	B	137	SER	5.2
1	D	309	GLN	5.2
1	D	311	ARG	5.2
1	D	220	THR	5.2
1	C	95	VAL	5.1
1	C	225	ALA	5.0
1	D	224	ALA	5.0
1	D	310	ALA	5.0
1	B	235	ASP	4.9
1	A	151	LEU	4.8
1	A	147	SER	4.8
1	D	312	TYR	4.7
1	A	140	ASN	4.7
1	B	224	ALA	4.6
1	A	213	PRO	4.6
1	C	309	GLN	4.5
1	C	230	ILE	4.4
1	B	228	ALA	4.4
1	B	222	GLU	4.3
1	C	307	PRO	4.1
1	D	234	ILE	4.1
1	C	226	ARG	4.1
1	C	137	SER	4.1
1	D	209	GLU	4.0
1	C	142	GLN	4.0
1	A	37	GLY	3.9
1	B	231	GLN	3.9
1	C	139	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	209	GLU	3.9
1	A	141	ASP	3.8
1	B	225	ALA	3.8
1	A	146	GLY	3.8
1	D	10	PRO	3.7
1	D	167	LEU	3.4
1	B	237	ARG	3.4
1	B	223	GLU	3.3
1	C	136	ARG	3.3
1	B	230	ILE	3.3
1	B	149	GLN	3.3
1	B	208	ASP	3.2
1	D	228	ALA	3.2
1	A	145	MET	3.2
1	D	93	GLY	3.1
1	C	305	ARG	3.1
1	D	233	MET	3.1
1	D	229	THR	3.1
1	C	223	GLU	3.1
1	B	95	VAL	3.1
1	B	150	LEU	3.1
1	A	82	ARG	3.0
1	B	122	THR	3.0
1	B	221	GLU	3.0
1	C	232	ARG	3.0
1	C	229	THR	2.9
1	B	232	ARG	2.9
1	C	311	ARG	2.9
1	D	305	ARG	2.9
1	A	222	GLU	2.9
1	C	235	ASP	2.9
1	B	248	LEU	2.9
1	C	82	ARG	2.9
1	D	107	LEU	2.8
1	D	193	GLU	2.8
1	B	82	ARG	2.8
1	C	231	GLN	2.8
1	D	232	ARG	2.7
1	A	95	VAL	2.7
1	D	82	ARG	2.7
1	C	236	GLU	2.7
1	D	172	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	121	ALA	2.6
1	D	135	ILE	2.6
1	D	222	GLU	2.6
1	C	312	TYR	2.6
1	C	233	MET	2.6
1	A	227	PHE	2.6
1	C	310	ALA	2.6
1	D	296	ILE	2.6
1	D	236	GLU	2.6
1	D	211	HIS	2.6
1	A	214	LYS	2.6
1	D	168	ILE	2.6
1	A	142	GLN	2.6
1	B	229	THR	2.5
1	D	225	ALA	2.5
1	A	221	GLU	2.5
1	D	322	VAL	2.5
1	A	209	GLU	2.4
1	B	257	TYR	2.4
1	D	210	SER	2.4
1	C	135	ILE	2.4
1	D	294	LEU	2.3
1	D	315	THR	2.3
1	D	237	ARG	2.3
1	D	169	LEU	2.3
1	D	223	GLU	2.3
1	C	169	LEU	2.3
1	D	319	LEU	2.3
1	B	92	ARG	2.2
1	B	148	LYS	2.2
1	B	226	ARG	2.2
1	B	236	GLU	2.2
1	B	34	GLY	2.1
1	B	136	ARG	2.1
1	B	36	PHE	2.1
1	A	257	TYR	2.1
1	A	192	ALA	2.1
1	A	307	PRO	2.0
1	C	134	PRO	2.0
1	C	237	ARG	2.0

## 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 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.