



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:29 PM UTC

PDB ID : 4M23 / pdb_00004m23
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

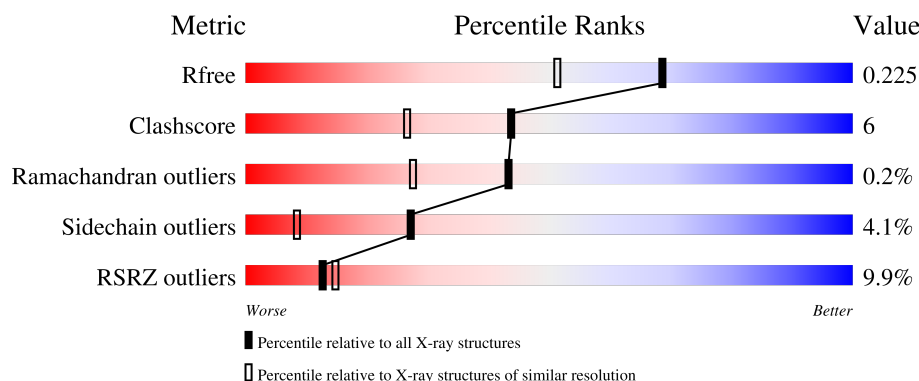
1 Overall quality at a glance

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	364	8% 78% 12% • 9%
1	B	364	6% 76% 8% • 14%
1	C	364	11% 80% 7% 12%
1	D	364	10% 74% 12% • 13%

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

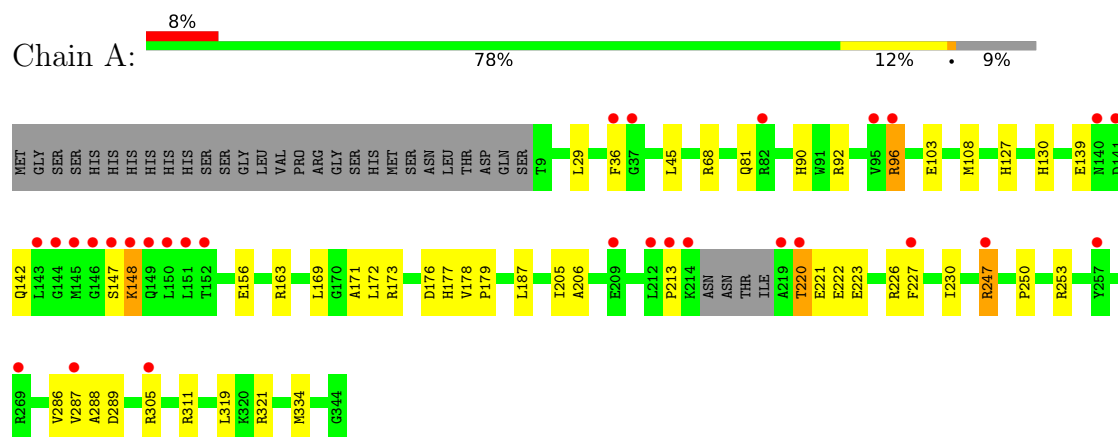
- Molecule 2 is water.

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

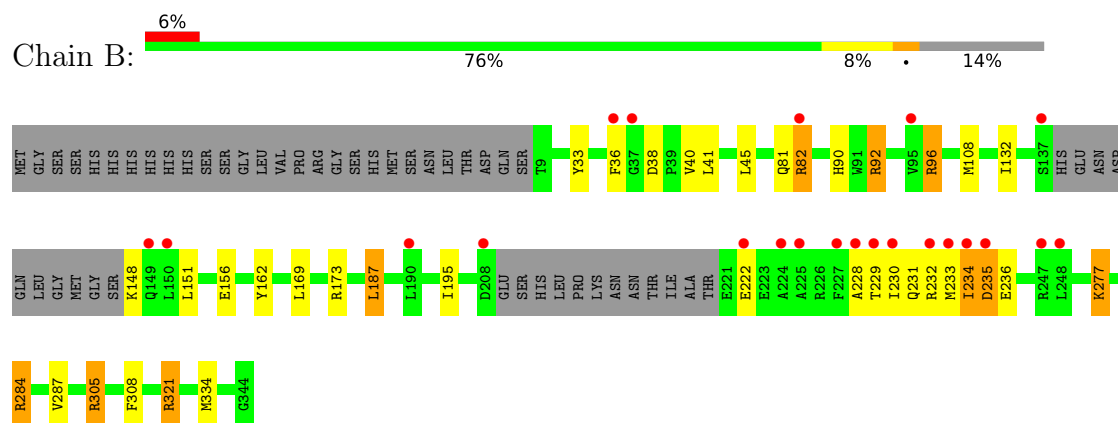
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

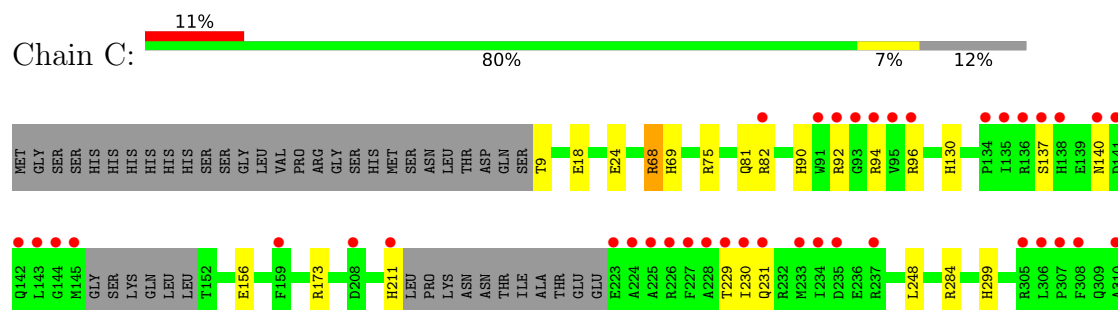
• Molecule 1: L-arginine beta-hydroxylase



• Molecule 1: L-arginine beta-hydroxylase

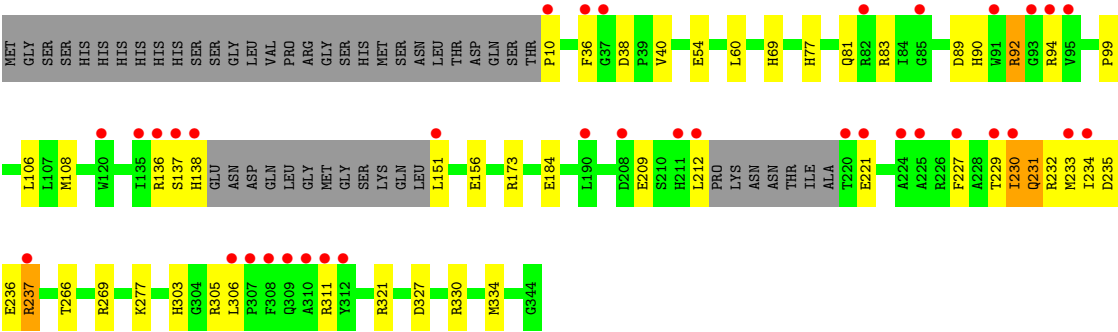


• Molecule 1: L-arginine beta-hydroxylase





● 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, α , β , γ	68.31Å 117.17Å 96.60Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	30.00 – 1.76 30.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.76) 99.9 (30.00-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	7533 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11527	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.89	0/2789	0.93	8/3786 (0.2%)
1	B	0.86	0/2624	0.89	1/3565 (0.0%)
1	C	0.89	0/2659	0.89	0/3612
1	D	0.86	0/2636	0.89	2/3582 (0.1%)
All	All	0.87	0/10708	0.90	11/14545 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-CB	6.84	118.18	110.72
1	B	287	VAL	N-CA-CB	6.16	117.43	110.72
1	A	288	ALA	N-CA-C	-6.00	95.81	107.62
1	A	206	ALA	CA-C-N	5.55	125.48	119.76
1	A	206	ALA	C-N-CA	5.55	125.48	119.76
1	A	45	LEU	CA-C-N	-5.28	113.60	119.19
1	A	45	LEU	C-N-CA	-5.28	113.60	119.19
1	D	237	ARG	CA-C-N	-5.14	114.66	119.85
1	D	237	ARG	C-N-CA	-5.14	114.66	119.85
1	A	286	VAL	CA-C-N	-5.11	115.77	122.37
1	A	286	VAL	C-N-CA	-5.11	115.77	122.37

There are no chirality outliers.

There are no planarity outliers.

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	2720	0	2639	38	1
1	B	2559	0	2487	36	0
1	C	2592	0	2497	18	0
1	D	2569	0	2478	34	0
2	A	292	0	0	9	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	126	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 (126) 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:HG2	1:B:321[A]:ARG:HH11	1.04	1.14
1:A:334:MET:CE	2:A:619:HOH:O	1.99	1.09
1:B:234:ILE:HG12	1:B:334:MET:HE2	1.30	1.07
1:A:92[B]:ARG:NH1	2:A:591:HOH:O	1.85	1.01
1:A:156:GLU:OE2	1:A:321:ARG:NH2	1.96	0.98
1:A:334:MET:HE3	2:A:619:HOH:O	1.60	0.97
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:HG2	1:B:321[A]:ARG:NH1	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:B:234:ILE:CG1	1:B:334:MET:HE2	2.13	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:HH11	1:A:247[B]:ARG:HG3	1.51	0.74
1:A:334:MET:HE2	2:A:619:HOH:O	1.74	0.74
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.21	0.73
1:C:9:THR:N	2:C:675:HOH:O	2.23	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:229:THR:HG22	1:B:233:MET:HE3	1.85	0.58
1:D:230:ILE:HD13	1:D:230:ILE:H	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: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:69:HIS:CD2	2:D:546:HOH:O	2.57	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:B:162:TYR:CE2	1:B:334:MET:HE3	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:GLN:HE22	1:D:235:ASP:CG	2.17	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:A:220:THR:HG23	1:A:223:GLU:H	1.76	0.49
1:C:81:GLN:NE2	1:C:173:ARG:HE	2.11	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: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: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:B:148:LYS:HE2	1:B:148:LYS:C	2.41	0.45
1:D:327:ASP:OD1	2:D:597:HOH:O	2.21	0.45
1:B:96:ARG:NH1	2:B:578:HOH:O	2.49	0.45
1:C:90:HIS:CD2	1:C:92[B]:ARG:CG	3.00	0.45
1:B:169:LEU:HD21	1:B:321[A]:ARG:HD2	1.99	0.45
1:D:229:THR:HB	1:D:334:MET:HE2	1.98	0.45
1:B:228:ALA:HB1	1:B:232:ARG:HH21	1.81	0.45
1:D:231:GLN:NE2	1:D:235:ASP:OD2	2.49	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:162:TYR:HE2	1:B:334:MET:HE3	1.83	0.43
1:B:308:PHE:HB3	2:B:532:HOH:O	2.17	0.43
1:B:33:TYR:CD2	1:B:41:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:NE	2:B:629:HOH:O	2.50	0.43
1:A:230:ILE:HD11	1:A:334:MET:HE1	2.01	0.43
1:A:171:ALA:HA	1:A:319:LEU:HD22	2.00	0.43
1:B:187:LEU:HD22	1:B:195:ILE:HD11	2.01	0.42
1:D:83:ARG:O	1:D:99:PRO:HB2	2.19	0.42
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.00	0.42
1:B:36:PHE:CE1	1:B:108:MET:HG3	2.56	0.41
1:B:132:ILE:HD11	1:B:321[A]:ARG:HD3	2.03	0.41
1:D:136:ARG:C	1:D:138:HIS:H	2.29	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:213:PRO:HG3	1:A:227:PHE:HB3	2.03	0.41
1:A:253[A]:ARG:O	1:A:253[A]:ARG:HG3	2.20	0.41
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.83	0.40
1:D:81:GLN:HE22	1:D:173:ARG:HB3	1.85	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 [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	334/364 (92%)	327 (98%)	6 (2%)	1 (0%)	36 21
1	B	312/364 (86%)	303 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	316/364 (87%)	307 (97%)	9 (3%)	0	100	100
1	D	313/364 (86%)	302 (96%)	10 (3%)	1 (0%)	36	21
All	All	1275/1456 (88%)	1239 (97%)	34 (3%)	2 (0%)	43	27

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%)	35	15
1	B	271/311 (87%)	256 (94%)	15 (6%)	19	4
1	C	274/311 (88%)	262 (96%)	12 (4%)	25	7
1	D	272/311 (88%)	259 (95%)	13 (5%)	23	6
All	All	1105/1244 (89%)	1056 (96%)	49 (4%)	27	7

All (49) 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	142	GLN
1	A	148	LYS
1	A	220	THR
1	A	221	GLU
1	A	247[A]	ARG
1	A	247[B]	ARG
1	B	45	LEU

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Mol	Chain	Res	Type
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	277	LYS
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	94	ARG
1	C	137	SER
1	C	140	ASN
1	C	211	HIS
1	C	229	THR
1	C	230	ILE
1	C	231	GLN
1	C	248	LEU
1	C	284	ARG
1	C	311	ARG
1	D	60	LEU
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	151	LEU
1	D	221	GLU
1	D	230	ILE
1	D	231	GLN
1	D	234	ILE
1	D	266	THR
1	D	311	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	81	GLN
1	A	90	HIS
1	A	130	HIS
1	A	177	HIS
1	B	57	GLN
1	B	69	HIS
1	B	81	GLN
1	B	90	HIS
1	B	154	HIS
1	B	177	HIS
1	B	290	GLN
1	B	309	GLN
1	C	81	GLN
1	C	90	HIS
1	C	130	HIS
1	C	177	HIS
1	C	211	HIS
1	C	299	HIS
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	177	HIS
1	D	231	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 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

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, 95th 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 ²)	Q<0.9
1	A	332/364 (91%)	0.18	29 (8%)	16	19	7, 23, 52, 83	8 (2%)
1	B	314/364 (86%)	0.28	22 (7%)	22	26	11, 24, 62, 98	7 (2%)
1	C	319/364 (87%)	0.36	40 (12%)	8	9	10, 23, 71, 115	5 (1%)
1	D	316/364 (86%)	0.57	36 (11%)	10	11	15, 28, 64, 101	6 (1%)
All	All	1281/1456 (87%)	0.34	127 (9%)	13	15	7, 24, 64, 115	26 (2%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	ILE	9.2
1	D	212	LEU	6.4
1	C	95	VAL	6.1
1	A	219	ALA	5.9
1	D	82	ARG	5.5
1	C	234	ILE	5.5
1	A	143	LEU	5.3
1	C	138	HIS	5.2
1	C	143	LEU	5.1
1	C	144	GLY	5.1
1	B	224	ALA	5.0
1	C	227	PHE	5.0
1	C	82	ARG	4.9
1	B	82	ARG	4.8
1	B	225	ALA	4.7
1	A	150	LEU	4.7
1	C	224	ALA	4.5
1	A	151	LEU	4.5
1	A	144	GLY	4.5
1	B	227	PHE	4.5
1	D	230	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLY	4.3
1	C	145	MET	4.3
1	C	225	ALA	4.3
1	C	230	ILE	4.2
1	A	82	ARG	4.2
1	C	308	PHE	4.2
1	D	308	PHE	4.2
1	A	212	LEU	4.1
1	D	306	LEU	4.1
1	D	234	ILE	4.1
1	A	37	GLY	4.0
1	A	147	SER	4.0
1	A	213	PRO	4.0
1	B	228	ALA	4.0
1	C	306	LEU	3.9
1	B	37	GLY	3.9
1	D	93	GLY	3.9
1	B	235	ASP	3.7
1	B	233	MET	3.7
1	D	220	THR	3.7
1	B	36	PHE	3.6
1	C	142	GLN	3.6
1	C	92[A]	ARG	3.6
1	D	151	LEU	3.6
1	C	211	HIS	3.5
1	A	145	MET	3.5
1	D	190	LEU	3.4
1	B	95	VAL	3.3
1	C	233	MET	3.3
1	A	220	THR	3.2
1	B	230	ILE	3.2
1	C	140	ASN	3.2
1	D	227	PHE	3.1
1	A	269[A]	ARG	3.0
1	D	221	GLU	3.0
1	D	224	ALA	3.0
1	C	307	PRO	3.0
1	A	95	VAL	2.9
1	C	229	THR	2.9
1	C	208	ASP	2.9
1	B	190	LEU	2.9
1	D	307	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	91	TRP	2.8
1	D	138	HIS	2.8
1	A	149	GLN	2.8
1	A	152	THR	2.8
1	D	37	GLY	2.8
1	D	310	ALA	2.7
1	D	95	VAL	2.7
1	B	137	SER	2.7
1	D	233	MET	2.7
1	D	120	TRP	2.7
1	B	150	LEU	2.7
1	D	225	ALA	2.6
1	A	96	ARG	2.6
1	C	137	SER	2.5
1	C	94	ARG	2.5
1	C	228	ALA	2.5
1	C	311	ARG	2.5
1	C	159	PHE	2.5
1	A	141	ASP	2.5
1	D	208	ASP	2.5
1	D	312	TYR	2.5
1	D	136	ARG	2.5
1	A	148	LYS	2.4
1	B	222	GLU	2.4
1	D	229	THR	2.4
1	C	235	ASP	2.4
1	D	85	GLY	2.4
1	C	134	PRO	2.4
1	D	137	SER	2.4
1	C	141	ASP	2.4
1	A	214	LYS	2.4
1	C	93	GLY	2.4
1	A	36	PHE	2.4
1	C	237	ARG	2.4
1	D	237	ARG	2.4
1	A	287	VAL	2.4
1	D	10	PRO	2.3
1	D	94[A]	ARG	2.3
1	A	257	TYR	2.3
1	B	149	GLN	2.3
1	C	226	ARG	2.3
1	B	208	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	96	ARG	2.2
1	C	305	ARG	2.2
1	D	36	PHE	2.2
1	D	311	ARG	2.2
1	C	91	TRP	2.2
1	B	232	ARG	2.2
1	B	229	THR	2.2
1	A	305	ARG	2.2
1	A	140	ASN	2.2
1	C	135	ILE	2.2
1	C	223	GLU	2.1
1	D	309	GLN	2.1
1	B	248	LEU	2.1
1	A	209	GLU	2.1
1	B	247	ARG	2.1
1	D	135	ILE	2.1
1	C	310	ALA	2.1
1	C	231	GLN	2.1
1	C	136	ARG	2.1
1	A	227	PHE	2.1
1	A	247[A]	ARG	2.0
1	D	211	HIS	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 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.