



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:52 PM UTC

PDB ID : 4M2C / pdb_00004m2c
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and D-Arg
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on : 2013-08-05
Resolution : 2.35 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
Mogul : 2022.3.0, CSD as543be (2022)
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

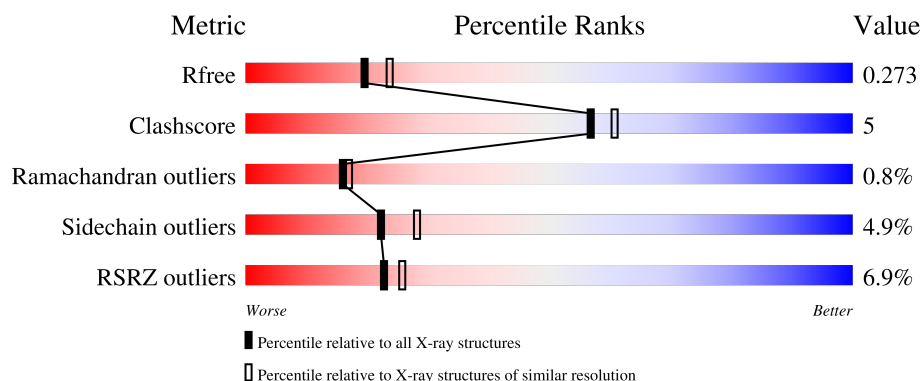
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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	4% 82% 10% 8%
1	B	364	13% 75% 10% 12%
1	C	364	4% 81% 9% 8%
1	D	364	4% 80% 10% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11289 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	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			
1	B	319	Total	C	N	O	S	0	0	0
			2565	1621	465	473	6			
1	C	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			
1	D	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			

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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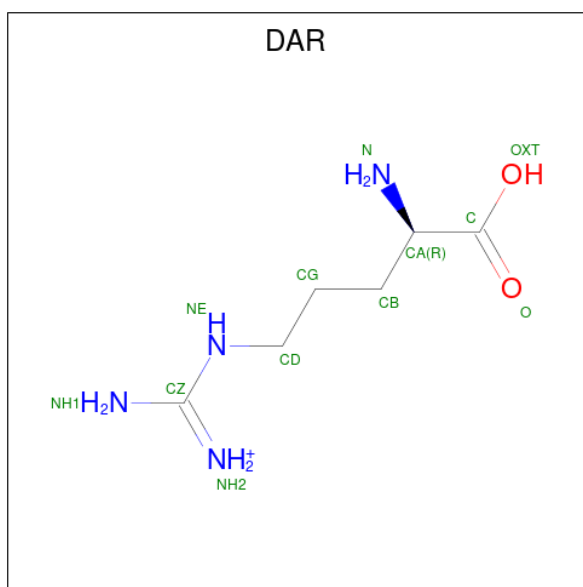
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	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 FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is D-ARGININE (CCD ID: DAR) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			12	6	4	2		
3	D	1	Total	C	N	O	0	0
			12	6	4	2		

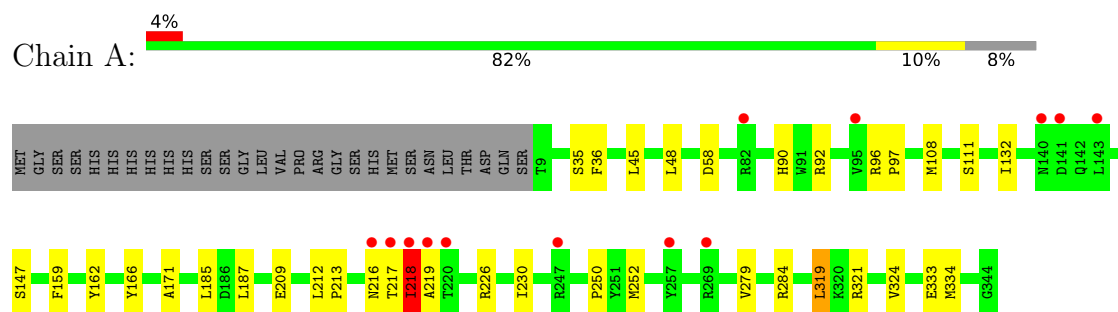
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	131	Total	O	0	0
			131	131		
4	C	163	Total	O	0	0
			163	163		
4	D	149	Total	O	0	0
			149	149		

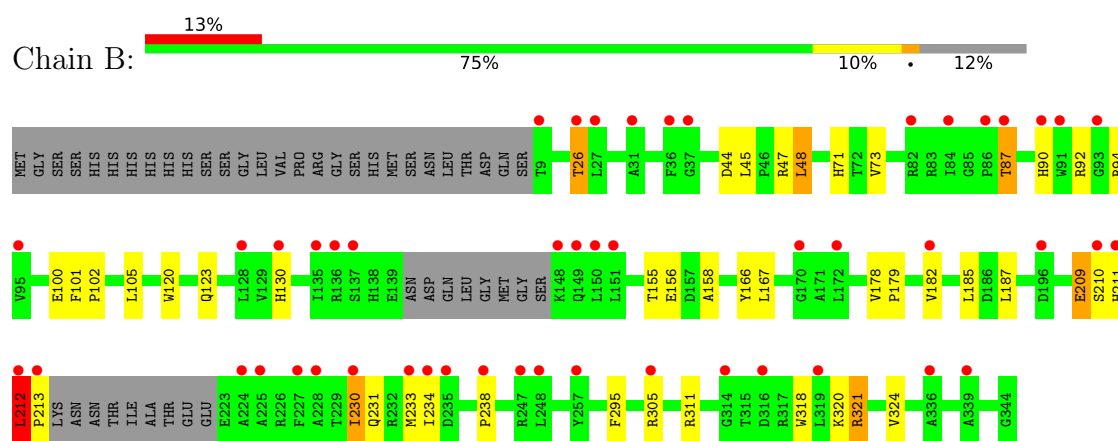
3 Residue-property plots [i](#)

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.

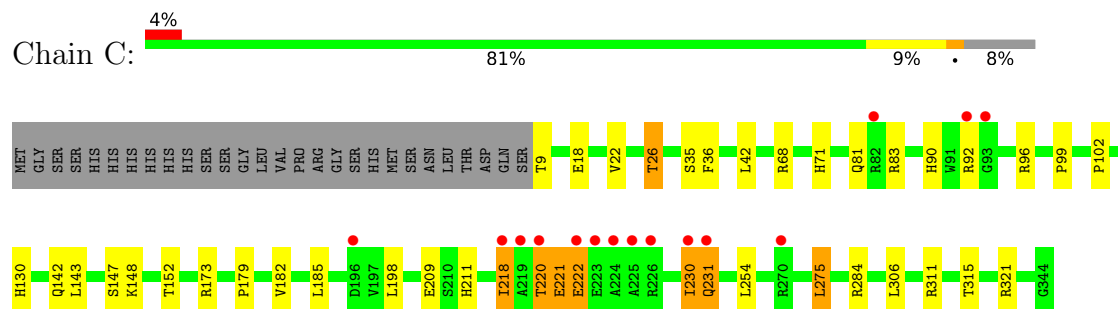
- Molecule 1: L-arginine beta-hydroxylase



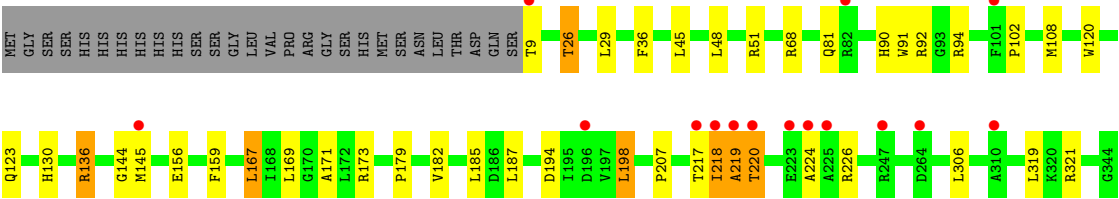
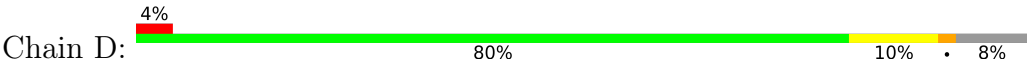
- Molecule 1: L-arginine beta-hydroxylase



- 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	68.03Å 116.37Å 95.80Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.35) 98.3 (30.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.276 0.222 , 0.273	Depositor DCC
R_{free} test set	3086 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11289	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/2760	0.78	0/3754
1	B	0.66	0/2633	0.78	0/3580
1	C	0.65	0/2760	0.78	0/3754
1	D	0.65	0/2760	0.77	1/3754 (0.0%)
All	All	0.65	0/10913	0.78	1/14842 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	ALA	N-CA-C	5.63	116.33	108.00

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	2690	0	2606	24	0
1	B	2565	0	2488	23	0
1	C	2690	0	2606	26	0
1	D	2690	0	2606	25	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	C	12	0	14	0	0
3	D	12	0	14	1	0
4	A	184	0	0	1	0
4	B	131	0	0	0	0
4	C	163	0	0	2	0
4	D	149	0	0	3	0
All	All	11289	0	10334	97	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.

All (97) 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:212:LEU:HB3	1:B:213:PRO:HD3	1.27	1.11
1:A:217:THR:HA	1:A:218:ILE:HG13	1.09	1.08
1:D:219:ALA:O	1:D:220:THR:OG1	1.75	1.04
1:A:217:THR:HA	1:A:218:ILE:CG1	1.99	0.92
1:B:209:GLU:HG2	1:B:210:SER:H	1.34	0.90
1:B:212:LEU:HB3	1:B:213:PRO:CD	2.03	0.88
1:C:90:HIS:HD2	1:C:92:ARG:H	1.21	0.88
1:B:26:THR:HG23	1:B:102:PRO:HB3	1.57	0.85
1:A:217:THR:CA	1:A:218:ILE:HG13	2.03	0.83
1:C:36:PHE:HZ	1:C:96:ARG:HH11	1.28	0.82
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.63	0.81
1:A:132:ILE:HD11	1:A:321:ARG:HD2	1.64	0.80
1:C:36:PHE:HZ	1:C:96:ARG:NH1	1.80	0.78
1:C:142:GLN:NE2	1:C:152:THR:H	1.83	0.76
1:C:221:GLU:HA	1:C:222:GLU:HG3	1.69	0.73
1:A:90:HIS:HD2	1:A:92:ARG:H	1.39	0.71
1:C:142:GLN:HE22	1:C:152:THR:H	1.37	0.70
1:C:36:PHE:CZ	1:C:96:ARG:NH1	2.63	0.67
1:A:96:ARG:NH1	4:A:536:HOH:O	2.28	0.67
1:C:90:HIS:CD2	1:C:92:ARG:H	2.10	0.66
1:A:230:ILE:HD11	1:A:334:MET:HE1	1.78	0.65
1:A:171:ALA:HA	1:A:319:LEU:HD22	1.79	0.64
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.79	0.64
1:D:219:ALA:O	1:D:220:THR:CB	2.47	0.62
1:A:58:ASP:OD1	1:B:47:ARG:NH2	2.32	0.62
1:C:26:THR:HG23	1:C:102:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:THR:HG21	4:C:528:HOH:O	2.02	0.59
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.37	0.59
1:A:90:HIS:CD2	1:A:92:ARG:H	2.20	0.59
1:A:217:THR:HB	1:A:218:ILE:O	2.03	0.58
1:C:26:THR:CG2	1:C:102:PRO:HB3	2.33	0.57
1:A:252:MET:HE1	1:A:279:VAL:HG21	1.86	0.57
1:B:87:THR:CG2	1:B:318:TRP:HB2	2.34	0.57
1:D:130:HIS:CD2	1:D:321:ARG:NH1	2.74	0.56
1:B:26:THR:CG2	1:B:102:PRO:HB3	2.32	0.55
1:B:209:GLU:HG2	1:B:210:SER:N	2.13	0.55
1:D:169:LEU:CD2	1:D:321:ARG:HG3	2.38	0.53
1:B:209:GLU:CG	1:B:210:SER:H	2.15	0.53
1:B:120:TRP:HB2	1:B:123:GLN:HB2	1.91	0.53
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.44	0.53
1:B:26:THR:HG23	1:B:102:PRO:CB	2.32	0.52
1:C:130:HIS:HB2	1:C:321:ARG:HB3	1.93	0.51
1:D:123:GLN:NE2	1:D:321:ARG:HH12	2.08	0.51
1:C:130:HIS:CD2	1:C:321:ARG:HH11	2.28	0.51
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.92	0.50
1:D:51:ARG:HD2	4:D:526:HOH:O	2.12	0.50
1:A:209:GLU:HA	1:A:212:LEU:HD13	1.92	0.49
1:C:311:ARG:NH1	1:C:315:THR:OG1	2.45	0.49
1:C:198:LEU:HD22	1:C:275:LEU:HD12	1.94	0.49
1:B:101:PHE:HB3	1:B:102:PRO:HD3	1.95	0.49
1:D:81:GLN:NE2	1:D:173:ARG:HE	2.11	0.49
1:B:233:MET:HA	1:B:238:PRO:HD3	1.94	0.48
1:C:81:GLN:NE2	1:C:173:ARG:HE	2.12	0.48
1:D:123:GLN:HE22	1:D:321:ARG:HH12	1.61	0.48
1:A:132:ILE:HB	1:A:319:LEU:HB2	1.95	0.47
1:A:187:LEU:HD22	1:A:250:PRO:HD3	1.95	0.47
1:C:22:VAL:O	1:C:26:THR:HB	2.15	0.47
1:B:156:GLU:OE2	1:B:321:ARG:NH2	2.48	0.47
1:C:83:ARG:O	1:C:99:PRO:HB2	2.14	0.46
1:D:156:GLU:HB3	1:D:167:LEU:HD21	1.97	0.46
1:C:221:GLU:HA	1:C:222:GLU:CG	2.41	0.46
1:D:224:ALA:C	1:D:226:ARG:H	2.23	0.46
1:D:90:HIS:HD2	1:D:92:ARG:H	1.63	0.45
1:D:194:ASP:O	1:D:198:LEU:HD22	2.17	0.45
1:C:18:GLU:O	1:C:22:VAL:HG23	2.17	0.45
1:D:120:TRP:HB2	1:D:123:GLN:HB3	1.99	0.45
1:C:35:SER:HB2	4:C:530:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:PRO:HG2	1:D:306:LEU:HD12	2.00	0.44
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.85	0.44
1:D:159:PHE:CE2	1:D:207:PRO:HB3	2.53	0.44
1:C:211:HIS:HB3	1:C:230:ILE:HD13	2.00	0.44
1:D:130:HIS:CE1	4:D:533:HOH:O	2.71	0.44
1:C:143:LEU:HD21	1:C:209:GLU:HG2	1.98	0.44
1:D:91:TRP:HD1	1:D:145:MET:HE2	1.82	0.44
1:D:144:GLY:N	3:D:402:DAR:OXT	2.35	0.44
1:A:111:SER:HB2	1:A:324:VAL:HG22	2.00	0.43
1:B:100:GLU:HG3	1:B:320:LYS:HE3	2.00	0.43
1:C:179:PRO:HG2	1:C:306:LEU:HD12	1.99	0.43
1:A:212:LEU:HA	1:A:213:PRO:HD2	1.92	0.43
1:A:162:TYR:CE2	1:A:334:MET:HE3	2.54	0.43
1:B:230:ILE:H	1:B:230:ILE:HD13	1.84	0.42
1:A:162:TYR:CD2	1:A:334:MET:HE3	2.54	0.42
1:B:87:THR:HG23	1:B:318:TRP:HB2	2.01	0.42
1:A:35:SER:HB3	1:A:97:PRO:HD3	2.00	0.42
1:C:230:ILE:HG13	1:C:231:GLN:N	2.33	0.42
1:A:166:TYR:HB2	1:A:324:VAL:HB	2.01	0.42
1:B:155:THR:HB	1:B:158:ALA:HB2	2.01	0.42
1:A:226:ARG:HG3	1:A:333:GLU:O	2.19	0.42
1:B:71:HIS:HA	1:B:295:PHE:O	2.20	0.42
1:D:130:HIS:HE1	4:D:533:HOH:O	2.03	0.41
1:D:136:ARG:HE	1:D:136:ARG:HB3	1.68	0.41
1:D:217:THR:O	1:D:218:ILE:HG12	2.20	0.41
1:B:92:ARG:C	1:B:94:ARG:H	2.29	0.41
1:B:44:ASP:HB3	1:B:48:LEU:HD13	2.02	0.41
1:B:166:TYR:HB2	1:B:324:VAL:HB	2.02	0.41
1:A:90:HIS:CD2	1:A:92:ARG:HG3	2.56	0.41
1:C:9:THR:HG21	1:C:71:HIS:CE1	2.56	0.40

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	334/364 (92%)	324 (97%)	7 (2%)	3 (1%)	14	14
1	B	313/364 (86%)	301 (96%)	10 (3%)	2 (1%)	21	24
1	C	334/364 (92%)	315 (94%)	16 (5%)	3 (1%)	14	14
1	D	334/364 (92%)	324 (97%)	7 (2%)	3 (1%)	14	14
All	All	1315/1456 (90%)	1264 (96%)	40 (3%)	11 (1%)	16	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ILE
1	B	212	LEU
1	C	220	THR
1	D	218	ILE
1	B	209	GLU
1	C	218	ILE
1	D	94	ARG
1	D	220	THR
1	A	147	SER
1	A	219	ALA
1	C	147	SER

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	286/311 (92%)	278 (97%)	8 (3%)	38	51
1	B	272/311 (88%)	252 (93%)	20 (7%)	13	14
1	C	286/311 (92%)	271 (95%)	15 (5%)	21	25
1	D	286/311 (92%)	274 (96%)	12 (4%)	26	35
All	All	1130/1244 (91%)	1075 (95%)	55 (5%)	22	28

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	48	LEU
1	A	159	PHE
1	A	185	LEU
1	A	216	ASN
1	A	218	ILE
1	A	284	ARG
1	A	319	LEU
1	B	26	THR
1	B	45	LEU
1	B	48	LEU
1	B	73	VAL
1	B	87	THR
1	B	90	HIS
1	B	105	LEU
1	B	130	HIS
1	B	167	LEU
1	B	182	VAL
1	B	185	LEU
1	B	187	LEU
1	B	211	HIS
1	B	212	LEU
1	B	230	ILE
1	B	231	GLN
1	B	234	ILE
1	B	305	ARG
1	B	311	ARG
1	B	321	ARG
1	C	26	THR
1	C	42	LEU
1	C	68	ARG
1	C	148	LYS
1	C	182	VAL
1	C	185	LEU
1	C	218	ILE
1	C	220	THR
1	C	221	GLU
1	C	222	GLU
1	C	230	ILE
1	C	231	GLN
1	C	254	LEU
1	C	275	LEU

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Mol	Chain	Res	Type
1	C	284	ARG
1	D	9	THR
1	D	26	THR
1	D	29	LEU
1	D	45	LEU
1	D	48	LEU
1	D	68	ARG
1	D	136	ARG
1	D	167	LEU
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	71	HIS
1	A	81	GLN
1	A	90	HIS
1	A	142	GLN
1	A	177	HIS
1	A	216	ASN
1	B	57	GLN
1	B	69	HIS
1	B	177	HIS
1	C	57	GLN
1	C	69	HIS
1	C	81	GLN
1	C	90	HIS
1	C	130	HIS
1	C	142	GLN
1	C	215	ASN
1	D	57	GLN
1	D	71	HIS
1	D	81	GLN
1	D	90	HIS
1	D	123	GLN
1	D	130	HIS
1	D	216	ASN
1	D	263	GLN

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Mol	Chain	Res	Type
1	D	290	GLN
1	D	303	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DAR	D	402	-	10,11,11	0.80	1 (10%)	9,13,13	1.12	1 (11%)
3	DAR	C	402	-	10,11,11	0.71	1 (10%)	9,13,13	1.10	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAR	D	402	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAR	C	402	-	-	3/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	DAR	OXT-C	-2.38	1.23	1.30
3	C	402	DAR	OXT-C	-2.01	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	DAR	OXT-C-O	-3.03	117.21	124.08
3	C	402	DAR	OXT-C-O	-2.45	118.53	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	DAR	N-CA-CB-CG
3	D	402	DAR	C-CA-CB-CG
3	C	402	DAR	OXT-C-CA-N
3	C	402	DAR	C-CA-CB-CG
3	D	402	DAR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	DAR	1	0

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	336/364 (92%)	0.28	13 (3%) 43 49	13, 37, 63, 98	4 (1%)
1	B	319/364 (87%)	1.07	49 (15%) 5 6	26, 46, 110, 129	3 (0%)
1	C	336/364 (92%)	0.32	15 (4%) 38 44	18, 35, 63, 96	4 (1%)
1	D	336/364 (92%)	0.56	15 (4%) 38 44	26, 44, 65, 123	3 (0%)
All	All	1327/1456 (91%)	0.55	92 (6%) 23 26	13, 40, 73, 129	14 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	ARG	6.8
1	D	82	ARG	6.2
1	D	220	THR	5.9
1	A	82	ARG	5.3
1	C	82	ARG	5.3
1	A	269	ARG	5.1
1	B	82	ARG	5.0
1	C	224	ALA	4.9
1	B	227	PHE	4.7
1	D	218	ILE	4.6
1	B	212	LEU	4.5
1	D	224	ALA	4.3
1	C	220	THR	3.9
1	B	213	PRO	3.8
1	B	37	GLY	3.8
1	C	93	GLY	3.7
1	A	217	THR	3.6
1	C	218	ILE	3.6
1	A	220	THR	3.5
1	D	219	ALA	3.5
1	C	219	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	314	GLY	3.4
1	B	148	LYS	3.3
1	A	216	ASN	3.3
1	B	151	LEU	3.3
1	B	233	MET	3.2
1	B	95	VAL	3.2
1	B	137	SER	3.2
1	B	316	ASP	3.2
1	B	234	ILE	3.2
1	B	170	GLY	3.1
1	D	196	ASP	3.1
1	B	150	LEU	3.1
1	B	238	PRO	3.1
1	B	90	HIS	3.0
1	A	247	ARG	2.9
1	A	218	ILE	2.9
1	C	225	ALA	2.8
1	B	36	PHE	2.8
1	A	219	ALA	2.7
1	D	9	THR	2.7
1	B	247	ARG	2.7
1	C	226	ARG	2.6
1	B	248	LEU	2.6
1	B	135	ILE	2.6
1	C	230	ILE	2.6
1	B	228	ALA	2.6
1	B	84	ILE	2.6
1	D	225	ALA	2.5
1	B	235	ASP	2.5
1	B	93	GLY	2.5
1	D	247	ARG	2.5
1	B	172	LEU	2.5
1	D	217	THR	2.5
1	B	224	ALA	2.5
1	B	225	ALA	2.5
1	C	196	ASP	2.5
1	B	196	ASP	2.5
1	D	310	ALA	2.5
1	B	27	LEU	2.4
1	B	128	LEU	2.4
1	A	140	ASN	2.4
1	B	339	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	136	ARG	2.4
1	B	87	THR	2.4
1	A	143	LEU	2.4
1	B	91	TRP	2.4
1	C	222	GLU	2.4
1	D	223	GLU	2.4
1	B	9	THR	2.3
1	B	182	VAL	2.3
1	B	230	ILE	2.3
1	B	305	ARG	2.3
1	C	270	ARG	2.3
1	B	26	THR	2.3
1	D	145	MET	2.3
1	B	86	PRO	2.3
1	C	231	GLN	2.3
1	D	264	ASP	2.2
1	C	223	GLU	2.2
1	B	210	SER	2.2
1	B	149	GLN	2.2
1	B	257	TYR	2.2
1	B	31	ALA	2.2
1	A	95	VAL	2.1
1	A	141	ASP	2.1
1	D	101	PHE	2.1
1	B	130	HIS	2.1
1	B	319	LEU	2.0
1	A	257	TYR	2.0
1	B	336	ALA	2.0
1	B	211	HIS	2.0

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	FE	B	401	1/1	0.84	0.09	94,94,94,94	0
3	DAR	D	402	12/12	0.89	0.11	42,45,50,53	0
3	DAR	C	402	12/12	0.90	0.11	38,45,53,54	0
2	FE	C	401	1/1	0.95	0.07	70,70,70,70	0
2	FE	D	401	1/1	0.99	0.05	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.