



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:53 AM UTC

PDB ID : 4M2G / pdb_00004m2g
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe, succinate, and (3R,4R)-dihydroxy-L-Arg
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on : 2013-08-05
Resolution : 2.39 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

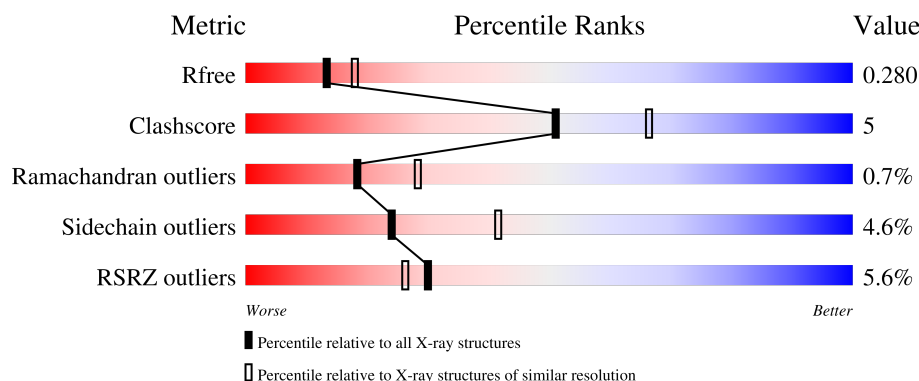
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	3% 83% 9% 8%
1	B	364	4% 74% 9% 15%
1	C	364	7% 79% 11% 9%
1	D	364	7% 80% 12% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11022 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	309	Total	C	N	O	S	0	0	0
			2487	1571	450	460	6			
1	C	331	Total	C	N	O	S	0	0	0
			2651	1671	482	491	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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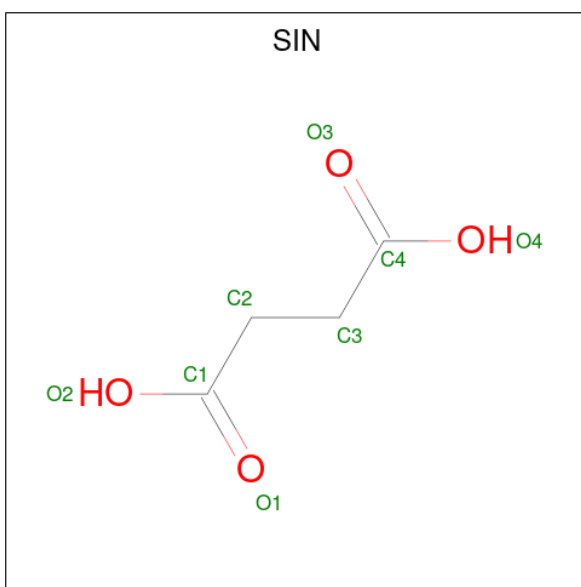
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	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).

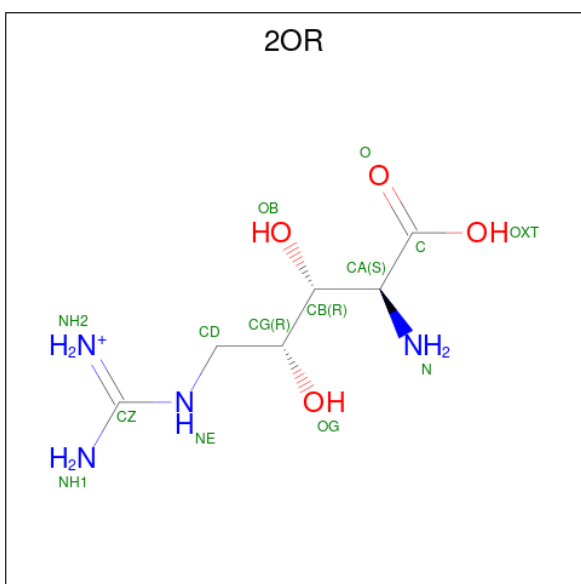
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is amino{[(2R,3R,4S)-4-amino-2,3,5-trihydroxy-5-oxopentyl]amino}methaniminium (CCD ID: 2OR) (formula: C₆H₁₅N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	6	4	4		
4	D	1	Total	C	N	O	0	0
			14	6	4	4		

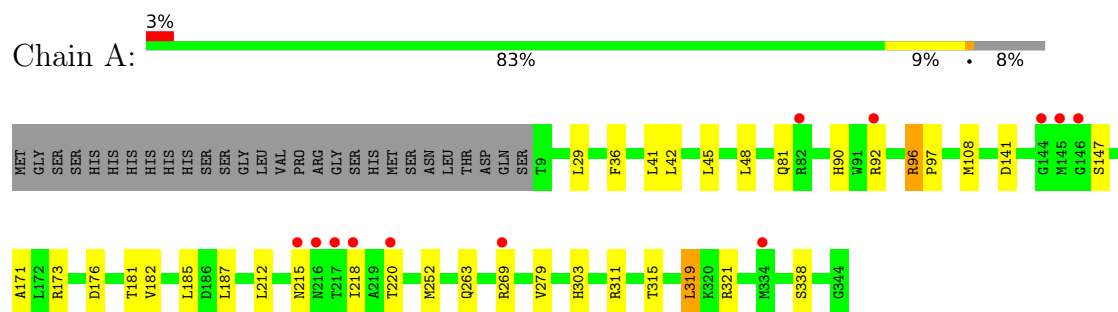
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	106	Total	O	0	0
			106	106		
5	C	113	Total	O	0	0
			113	113		
5	D	79	Total	O	0	0
			79	79		

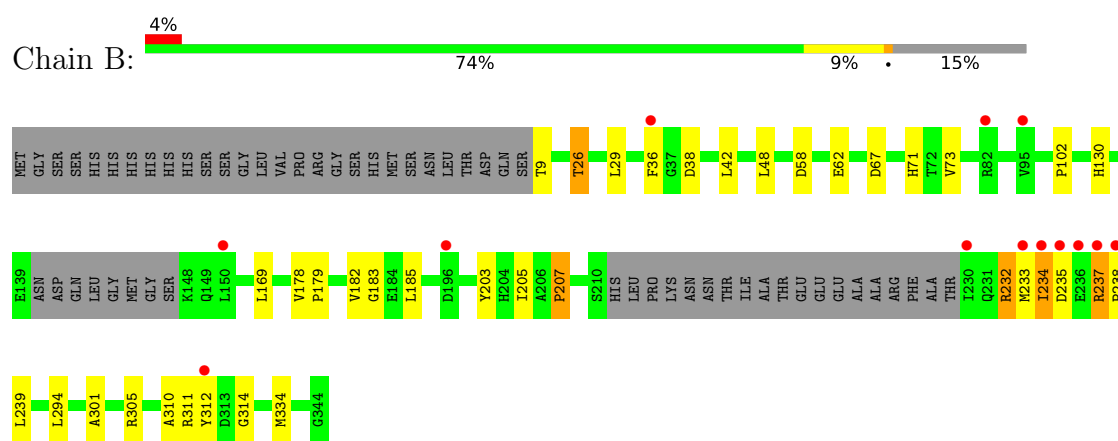
3 Residue-property plots [i](#)

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.

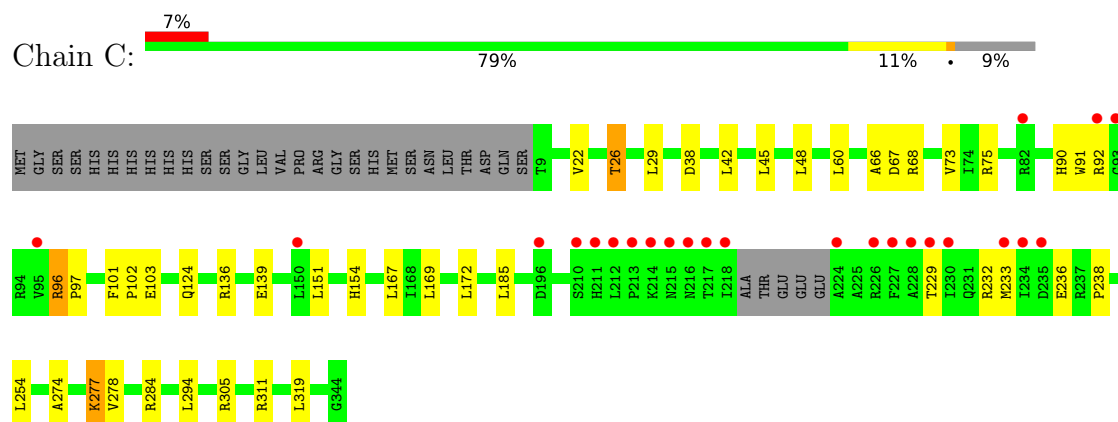
• Molecule 1: L-arginine beta-hydroxylase



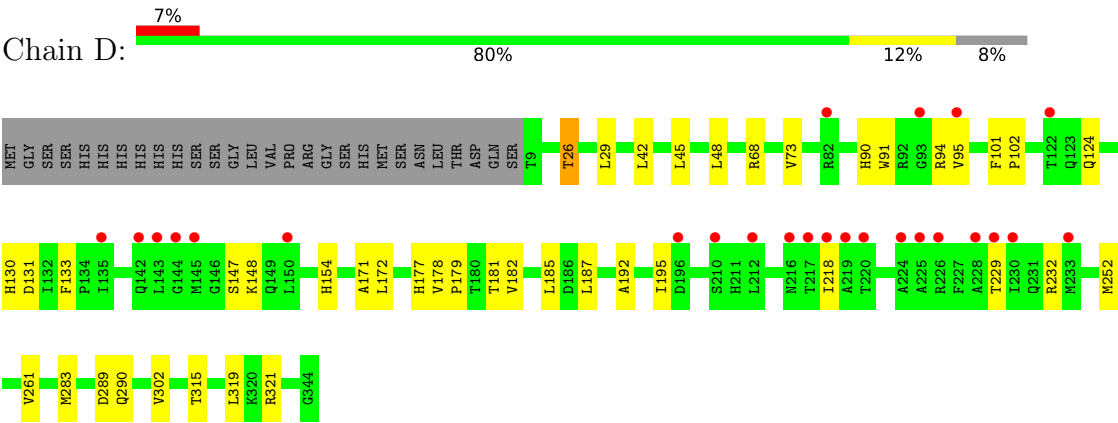
• Molecule 1: L-arginine beta-hydroxylase



• 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	67.29Å 116.21Å 96.16Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	26.15 – 2.39 26.15 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.15-2.39) 99.8 (26.15-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.271 0.218 , 0.280	Depositor DCC
R_{free} test set	2963 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11022	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: SIN, 2OR, FE

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	0.52	0/2760	0.75	0/3754
1	B	0.51	0/2552	0.79	2/3469 (0.1%)
1	C	0.52	0/2720	0.76	0/3698
1	D	0.49	0/2760	0.74	0/3754
All	All	0.51	0/10792	0.76	2/14675 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	CA-C-N	-5.21	113.32	119.84
1	B	237	ARG	C-N-CA	-5.21	113.32	119.84

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	16	0
1	B	2487	0	2413	51	0
1	C	2651	0	2575	23	0
1	D	2690	0	2606	19	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	4	0	0
3	B	8	0	4	0	0
3	C	8	0	4	0	0
3	D	8	0	4	0	0
4	C	14	0	13	1	0
4	D	14	0	13	2	0
5	A	142	0	0	1	0
5	B	106	0	0	1	0
5	C	113	0	0	0	0
5	D	79	0	0	0	0
All	All	11022	0	10242	108	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 (108) 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:207:PRO:HD3	1:B:237:ARG:NH1	1.21	1.48
1:B:207:PRO:CD	1:B:237:ARG:NH1	2.00	1.23
1:B:233:MET:HE2	1:B:334:MET:HE3	1.25	1.13
1:B:233:MET:CG	1:B:334:MET:HG2	1.78	1.12
1:B:233:MET:HE2	1:B:334:MET:CE	1.79	1.11
1:B:207:PRO:CG	1:B:237:ARG:CZ	2.41	0.99
1:B:233:MET:HG3	1:B:334:MET:CG	1.94	0.97
1:B:233:MET:HG3	1:B:334:MET:HG2	1.00	0.96
1:B:233:MET:HE3	1:B:233:MET:HA	1.46	0.96
1:B:233:MET:O	1:B:235:ASP:N	1.99	0.95
1:B:207:PRO:CD	1:B:237:ARG:CZ	2.47	0.92
1:B:207:PRO:HD3	1:B:237:ARG:HH12	1.14	0.90
1:D:154:HIS:CE1	4:D:402:2OR:H9	1.88	0.90
1:B:207:PRO:HG2	1:B:237:ARG:CZ	2.05	0.86
1:B:233:MET:HB3	1:B:334:MET:HE2	1.61	0.82
1:A:92:ARG:NH1	5:A:552:HOH:O	2.14	0.81
1:B:233:MET:HA	1:B:233:MET:CE	2.17	0.74
1:D:154:HIS:CE1	4:D:402:2OR:OG	2.40	0.72
1:C:26:THR:HG23	1:C:102:PRO:HB3	1.71	0.70
1:B:233:MET:HE3	1:B:233:MET:CA	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PRO:HD3	1:B:237:ARG:HH11	1.50	0.66
1:C:26:THR:CG2	1:C:102:PRO:HB3	2.25	0.66
1:B:233:MET:HE2	1:B:334:MET:HE2	1.76	0.65
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.77	0.65
1:B:233:MET:CE	1:B:334:MET:CE	2.68	0.65
1:B:233:MET:CE	1:B:334:MET:HE3	2.17	0.65
1:D:218:ILE:HD12	1:D:218:ILE:H	1.62	0.64
1:B:232:ARG:O	1:B:234:ILE:N	2.28	0.64
1:B:232:ARG:C	1:B:234:ILE:H	2.06	0.64
1:B:233:MET:SD	1:B:334:MET:CG	2.86	0.64
1:B:233:MET:SD	1:B:334:MET:HG2	2.38	0.64
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.29	0.62
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.35	0.61
1:B:203:TYR:C	1:B:239:LEU:HD22	2.24	0.61
1:B:233:MET:CG	1:B:334:MET:CG	2.68	0.60
1:B:26:THR:CG2	1:B:102:PRO:HB3	2.31	0.59
1:B:232:ARG:O	1:B:234:ILE:HD12	2.01	0.59
1:B:207:PRO:CG	1:B:237:ARG:NH1	2.58	0.59
1:B:234:ILE:HG22	1:B:234:ILE:O	2.02	0.59
1:A:90:HIS:CD2	1:A:92:ARG:H	2.20	0.58
1:B:26:THR:HG23	1:B:102:PRO:HB3	1.86	0.58
1:B:233:MET:SD	1:B:334:MET:HG3	2.44	0.57
1:A:81:GLN:HE22	1:A:173:ARG:HE	1.54	0.56
1:B:203:TYR:O	1:B:239:LEU:HA	2.06	0.56
1:B:169:LEU:HD12	1:B:294:LEU:HD23	1.90	0.53
1:A:171:ALA:HA	1:A:319:LEU:HD22	1.89	0.53
1:B:203:TYR:C	1:B:239:LEU:CD2	2.82	0.52
1:B:207:PRO:CD	1:B:237:ARG:HH12	1.92	0.52
1:B:207:PRO:CG	1:B:237:ARG:NE	2.73	0.52
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.93	0.51
1:B:233:MET:CE	1:B:334:MET:HE2	2.39	0.49
1:A:263:GLN:O	1:A:269:ARG:NH2	2.44	0.49
1:B:207:PRO:HG2	1:B:237:ARG:NH2	2.28	0.49
1:A:181:THR:O	1:A:303:HIS:HA	2.13	0.49
1:A:81:GLN:NE2	1:A:173:ARG:HE	2.10	0.49
1:C:154:HIS:NE2	4:C:402:2OR:OG	2.46	0.49
1:C:229:THR:HG22	1:C:232:ARG:HH21	1.78	0.49
1:D:172:LEU:O	1:D:290:GLN:HG3	2.13	0.48
1:A:90:HIS:HD2	1:A:92:ARG:H	1.61	0.48
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.97	0.47
1:C:90:HIS:CD2	1:C:92:ARG:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TRP:CH2	1:C:124:GLN:HA	2.49	0.47
1:C:151:LEU:HB3	1:C:305:ARG:H	1.79	0.47
1:C:274:ALA:O	1:C:278:VAL:HG23	2.15	0.47
1:C:90:HIS:HD2	1:C:92:ARG:H	1.61	0.47
1:C:169:LEU:HD12	1:C:294:LEU:HD23	1.95	0.47
1:B:232:ARG:C	1:B:234:ILE:N	2.70	0.47
1:C:26:THR:HG23	1:C:102:PRO:CB	2.42	0.47
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.97	0.47
1:C:38:ASP:OD1	1:C:38:ASP:C	2.59	0.46
1:D:181:THR:HB	1:D:283:MET:HE3	1.98	0.46
1:B:58:ASP:O	1:B:62:GLU:HG3	2.16	0.45
1:C:232:ARG:HG3	1:C:233:MET:HG3	1.97	0.45
1:D:252:MET:HE3	1:D:302:VAL:HG13	1.98	0.45
1:C:277:LYS:HA	1:C:277:LYS:HD2	1.77	0.45
1:C:66:ALA:O	1:C:67:ASP:C	2.59	0.45
1:C:73:VAL:HG22	1:C:294:LEU:HD12	2.00	0.44
1:A:41:LEU:O	1:A:45:LEU:HG	2.17	0.44
1:C:101:PHE:HB3	1:C:102:PRO:HD3	2.00	0.43
1:B:237:ARG:NE	5:B:584:HOH:O	2.30	0.43
1:D:101:PHE:HB3	1:D:102:PRO:HD3	1.99	0.43
1:A:338:SER:HB3	1:B:67:ASP:HB3	2.00	0.43
1:C:103:GLU:HG2	1:C:172:LEU:HD22	1.99	0.43
1:D:229:THR:HG22	1:D:232:ARG:HH22	1.84	0.43
1:A:212:LEU:O	1:A:215:ASN:HB2	2.19	0.43
1:B:36:PHE:C	1:B:38:ASP:H	2.27	0.43
1:C:136:ARG:O	1:C:139:GLU:HG3	2.18	0.43
1:B:207:PRO:HG3	1:B:237:ARG:HD2	2.01	0.43
1:D:91:TRP:CD2	1:D:124:GLN:HG3	2.54	0.43
1:D:26:THR:HG23	1:D:102:PRO:CB	2.45	0.42
1:D:90:HIS:CD2	1:D:91:TRP:H	2.37	0.42
1:B:183:GLY:O	1:B:301:ALA:HA	2.19	0.42
1:A:252:MET:HE1	1:A:279:VAL:HG21	2.02	0.42
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.53	0.42
1:C:96:ARG:HA	1:C:97:PRO:HA	1.84	0.42
1:B:310:ALA:HB3	1:B:312:TYR:CE1	2.55	0.41
1:A:311:ARG:NH1	1:A:315:THR:OG1	2.53	0.41
1:B:233:MET:CB	1:B:334:MET:HE2	2.43	0.41
1:C:22:VAL:O	1:C:26:THR:HB	2.20	0.41
1:D:130:HIS:HB2	1:D:321:ARG:HB3	2.03	0.41
1:D:178:VAL:HA	1:D:179:PRO:HD3	1.91	0.41
1:D:192:ALA:HA	1:D:195:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HA	1:A:97:PRO:HA	1.89	0.40
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.88	0.40
1:B:207:PRO:HG2	1:B:237:ARG:NE	2.33	0.40
1:D:131:ASP:HB3	1:D:133:PHE:CE2	2.57	0.40
1:B:9:THR:HG21	1:B:71:HIS:CE1	2.56	0.40
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.95	0.40

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	334/364 (92%)	325 (97%)	6 (2%)	3 (1%)	14	22
1	B	303/364 (83%)	284 (94%)	15 (5%)	4 (1%)	9	14
1	C	327/364 (90%)	311 (95%)	16 (5%)	0	100	100
1	D	334/364 (92%)	317 (95%)	15 (4%)	2 (1%)	21	32
All	All	1298/1456 (89%)	1237 (95%)	52 (4%)	9 (1%)	18	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	ILE
1	B	238	PRO
1	B	314	GLY
1	D	94	ARG
1	A	147	SER
1	B	207	PRO
1	D	95	VAL
1	A	220	THR
1	A	218	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	286/311 (92%)	276 (96%)	10 (4%)	32	53
1	B	265/311 (85%)	253 (96%)	12 (4%)	24	42
1	C	282/311 (91%)	267 (95%)	15 (5%)	20	36
1	D	286/311 (92%)	272 (95%)	14 (5%)	22	39
All	All	1119/1244 (90%)	1068 (95%)	51 (5%)	24	41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	42	LEU
1	A	48	LEU
1	A	96	ARG
1	A	141	ASP
1	A	182	VAL
1	A	185	LEU
1	A	187	LEU
1	A	319	LEU
1	A	321	ARG
1	B	26	THR
1	B	29	LEU
1	B	42	LEU
1	B	48	LEU
1	B	73	VAL
1	B	130	HIS
1	B	182	VAL
1	B	185	LEU
1	B	205	ILE
1	B	232	ARG
1	B	305	ARG
1	B	311	ARG
1	C	26	THR
1	C	29	LEU

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	45	LEU
1	C	48	LEU
1	C	68	ARG
1	C	75	ARG
1	C	96	ARG
1	C	167	LEU
1	C	185	LEU
1	C	254	LEU
1	C	277	LYS
1	C	284	ARG
1	C	311	ARG
1	C	319	LEU
1	D	26	THR
1	D	29	LEU
1	D	42	LEU
1	D	45	LEU
1	D	48	LEU
1	D	68	ARG
1	D	73	VAL
1	D	147	SER
1	D	148	LYS
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	261	VAL
1	D	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	90	HIS
1	A	138	HIS
1	A	140	ASN
1	A	142	GLN
1	A	177	HIS
1	A	231	GLN
1	B	57	GLN
1	B	90	HIS
1	B	231	GLN
1	C	57	GLN

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Mol	Chain	Res	Type
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	130	HIS
1	C	142	GLN
1	C	177	HIS
1	C	216	ASN
1	D	142	GLN
1	D	177	HIS
1	D	216	ASN

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SIN	A	402	-	7,7,7	1.12	0	8,8,8	1.15	0
3	SIN	D	403	2	7,7,7	1.06	0	8,8,8	1.14	0
3	SIN	C	403	2	7,7,7	1.10	0	8,8,8	1.03	0
3	SIN	B	402	-	7,7,7	1.02	0	8,8,8	1.56	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2OR	C	402	2	13,13,13	0.85	0	14,17,17	0.87	1 (7%)
4	2OR	D	402	2	13,13,13	0.89	0	14,17,17	0.80	0

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	SIN	A	402	-	-	5/5/5/5	-
3	SIN	D	403	2	-	5/5/5/5	-
3	SIN	C	403	2	-	2/5/5/5	-
3	SIN	B	402	-	-	5/5/5/5	-
4	2OR	C	402	2	-	8/17/17/17	-
4	2OR	D	402	2	-	0/17/17/17	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	SIN	C3-C2-C1	-2.58	106.82	113.67
4	C	402	2OR	OG-CG-CD	2.06	113.71	109.67

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402	2OR	O-C-CA-CB
4	C	402	2OR	OXT-C-CA-CB
4	C	402	2OR	CA-CB-CG-OG
4	C	402	2OR	CA-CB-CG-CD
4	C	402	2OR	OB-CB-CG-OG
4	C	402	2OR	OB-CB-CG-CD
3	A	402	SIN	C1-C2-C3-C4
3	D	403	SIN	C1-C2-C3-C4
4	C	402	2OR	OXT-C-CA-N
3	B	402	SIN	C1-C2-C3-C4
4	C	402	2OR	O-C-CA-N
3	A	402	SIN	O1-C1-C2-C3
3	D	403	SIN	C2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	402	SIN	C2-C3-C4-O3
3	A	402	SIN	C2-C3-C4-O4
3	D	403	SIN	C2-C3-C4-O4
3	B	402	SIN	C2-C3-C4-O3
3	B	402	SIN	C2-C3-C4-O4
3	A	402	SIN	O2-C1-C2-C3
3	D	403	SIN	O2-C1-C2-C3
3	B	402	SIN	O2-C1-C2-C3
3	C	403	SIN	O2-C1-C2-C3
3	D	403	SIN	O1-C1-C2-C3
3	C	403	SIN	O1-C1-C2-C3
3	B	402	SIN	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	2OR	1	0
4	D	402	2OR	2	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%)	0.06	12 (3%)	46 42	13, 42, 83, 158	6 (1%)
1	B	309/364 (84%)	0.42	13 (4%)	40 36	24, 52, 90, 131	3 (0%)
1	C	331/364 (90%)	0.28	24 (7%)	21 17	27, 45, 127, 178	4 (1%)
1	D	336/364 (92%)	0.59	25 (7%)	20 17	35, 60, 127, 155	3 (0%)
All	All	1312/1456 (90%)	0.34	74 (5%)	30 26	13, 49, 112, 178	16 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	6.7
1	D	224	ALA	5.6
1	C	218	ILE	5.4
1	B	233	MET	5.2
1	B	236	GLU	5.1
1	D	225	ALA	5.1
1	A	92	ARG	5.1
1	D	218	ILE	4.9
1	A	334	MET	4.7
1	B	237	ARG	4.6
1	A	218	ILE	4.6
1	B	234	ILE	4.6
1	A	217	THR	4.6
1	B	230	ILE	4.5
1	C	92	ARG	4.3
1	D	230	ILE	4.3
1	C	82	ARG	4.2
1	A	82	ARG	4.1
1	D	217	THR	4.0
1	A	215	ASN	4.0
1	A	269	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	ASN	3.9
1	B	36	PHE	3.8
1	B	82	ARG	3.7
1	C	224	ALA	3.6
1	D	228	ALA	3.6
1	A	144	GLY	3.5
1	D	82	ARG	3.4
1	C	212	LEU	3.3
1	C	229	THR	3.3
1	C	217	THR	3.2
1	C	230	ILE	3.2
1	C	228	ALA	3.2
1	C	235	ASP	3.2
1	D	229	THR	3.2
1	C	95	VAL	3.1
1	D	210	SER	3.0
1	C	210	SER	3.0
1	A	220	THR	3.0
1	D	233	MET	3.0
1	C	213	PRO	2.9
1	C	227	PHE	2.9
1	D	95	VAL	2.8
1	C	93	GLY	2.8
1	C	150	LEU	2.7
1	B	150	LEU	2.7
1	C	211	HIS	2.6
1	D	219	ALA	2.6
1	D	150	LEU	2.6
1	D	144	GLY	2.6
1	C	216	ASN	2.5
1	B	238	PRO	2.5
1	D	142	GLN	2.5
1	D	196	ASP	2.5
1	A	145	MET	2.5
1	B	196	ASP	2.5
1	D	220	THR	2.5
1	D	212	LEU	2.5
1	C	196	ASP	2.4
1	D	93	GLY	2.4
1	B	95	VAL	2.4
1	D	145	MET	2.4
1	D	135	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	226	ARG	2.3
1	D	216	ASN	2.3
1	B	312	TYR	2.3
1	C	233	MET	2.3
1	C	215	ASN	2.2
1	C	214	LYS	2.1
1	A	146	GLY	2.1
1	C	226	ARG	2.1
1	D	143	LEU	2.1
1	C	234	ILE	2.0
1	D	122	THR	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](#)

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
3	SIN	A	402	8/8	0.76	0.14	50,54,61,61	0
4	2OR	C	402	14/14	0.80	0.14	67,79,94,96	0
4	2OR	D	402	14/14	0.82	0.14	74,80,88,89	0
3	SIN	B	402	8/8	0.85	0.13	56,59,62,63	0
3	SIN	D	403	8/8	0.87	0.13	63,74,82,83	0
2	FE	B	401	1/1	0.88	0.10	85,85,85,85	0
3	SIN	C	403	8/8	0.91	0.10	52,58,68,69	0
2	FE	D	401	1/1	0.96	0.05	76,76,76,76	0
2	FE	C	401	1/1	0.97	0.04	73,73,73,73	0
2	FE	A	401	1/1	0.99	0.08	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.