



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:29 AM UTC

PDB ID : 4M27 / pdb_00004m27
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and L-Arg
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on : 2013-08-05
Resolution : 2.35 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

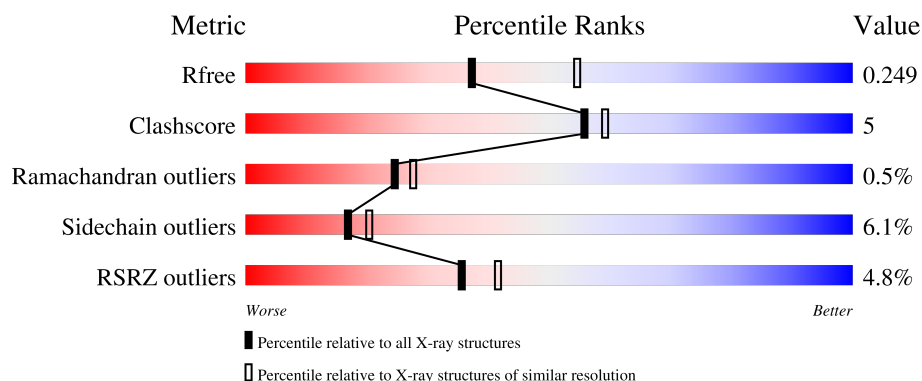
1 Overall quality at a glance

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	
1	B	364	
1	C	364	
1	D	364	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11415 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	2	0
			2709	1704	492	505	8			
1	B	314	Total	C	N	O	S	0	0	0
			2526	1596	458	466	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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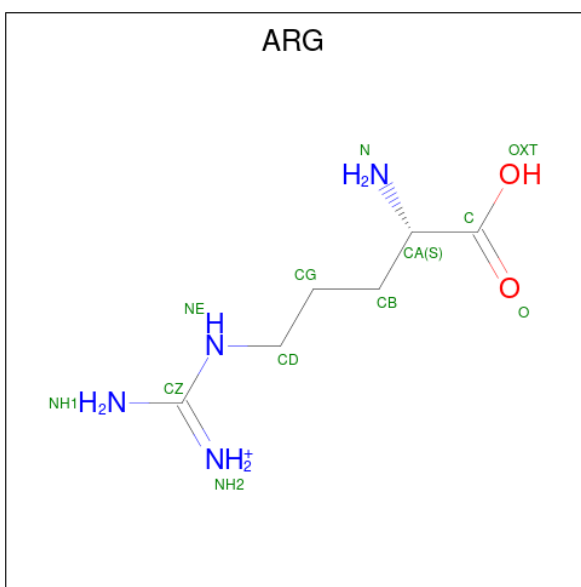
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	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).

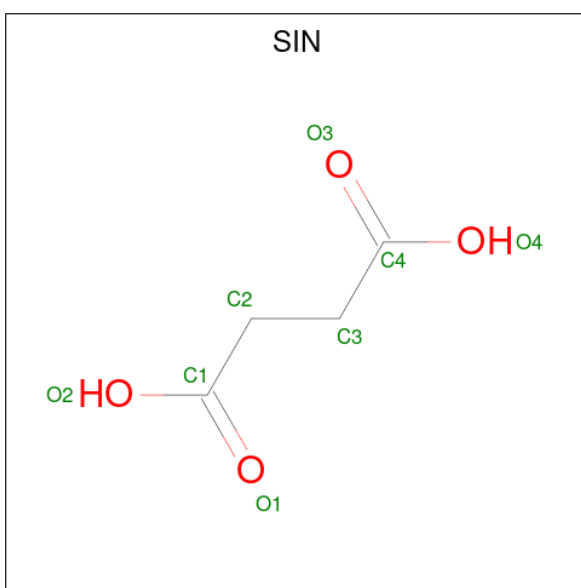
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

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



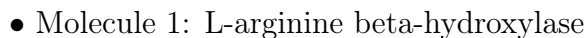
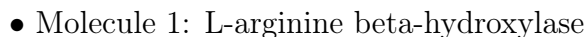
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total 218	O 218	0	0
5	B	174	Total 174	O 174	0	0
5	C	185	Total 185	O 185	0	0
5	D	179	Total 179	O 179	0	0

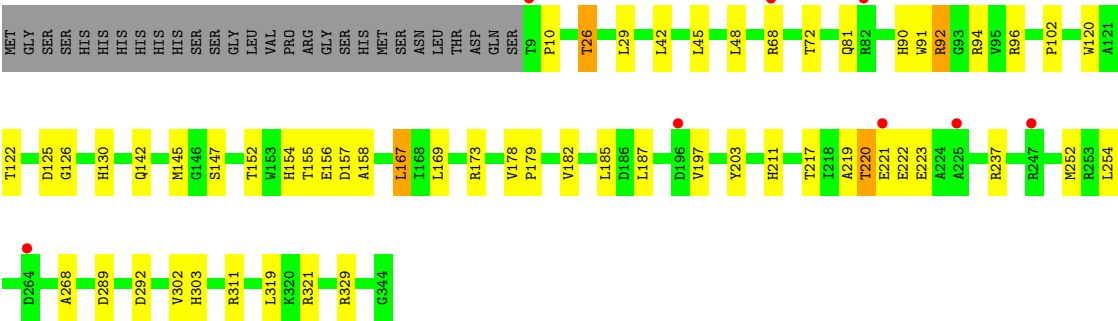
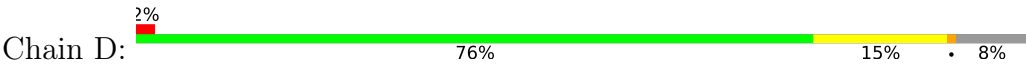
i

- 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	68.58Å 117.00Å 96.31Å 90.00° 92.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-2.35) 84.5 (30.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.270 (Not available) , 0.249	Depositor DCC
R_{free} test set	2708 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11415	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 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	0.65	0/2779	0.81	0/3778
1	B	0.65	0/2592	0.78	0/3523
1	C	0.65	0/2760	0.80	0/3754
1	D	0.64	0/2760	0.77	1/3754 (0.0%)
All	All	0.65	0/10891	0.79	1/14809 (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	222	GLU	N-CA-C	-5.15	107.02	113.15

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	2709	0	2626	25	0
1	B	2526	0	2452	21	0
1	C	2690	0	2606	22	0
1	D	2690	0	2606	33	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0
4	C	8	0	4	0	0
4	D	8	0	4	1	0
5	A	218	0	0	1	1
5	B	174	0	0	3	0
5	C	185	0	0	3	0
5	D	179	0	0	1	0
All	All	11415	0	10322	99	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 5.

All (99) 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:237:ARG:HB3	1:B:238:PRO:HD3	1.28	1.09
1:B:227:PHE:HB3	1:B:228:ALA:HA	1.47	0.95
1:D:92:ARG:HH11	1:D:92:ARG:HG3	1.36	0.88
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.60	0.84
1:B:237:ARG:HB3	1:B:238:PRO:CD	2.09	0.82
1:A:140:ASN:O	1:A:141:ASP:HB2	1.81	0.81
1:C:75:ARG:HD2	5:C:546:HOH:O	1.84	0.78
1:A:26:THR:HG23	1:A:102:PRO:HB3	1.66	0.76
1:C:213:PRO:HB3	1:C:219:ALA:HB2	1.67	0.76
1:B:26:THR:HG23	1:B:102:PRO:HB3	1.70	0.72
1:C:90:HIS:HD2	1:C:92:ARG:H	1.38	0.72
1:C:91:TRP:CD1	1:C:145:MET:HE3	2.25	0.71
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.72	0.71
1:D:92:ARG:HG3	1:D:92:ARG:NH1	2.05	0.71
1:C:142:GLN:HE22	1:C:152:THR:H	1.40	0.69
1:B:253:ARG:O	1:B:253:ARG:HG2	1.94	0.66
1:D:125:ASP:OD2	1:D:217:THR:HG23	1.95	0.66
1:C:90:HIS:CD2	1:C:92:ARG:H	2.17	0.62
1:D:90:HIS:HD2	1:D:92:ARG:H	1.48	0.61
1:A:26:THR:CG2	1:A:102:PRO:HB3	2.31	0.61
1:D:157:ASP:OD1	1:D:211:HIS:HE1	1.84	0.61
1:B:90:HIS:HD2	1:B:92:ARG:H	1.48	0.60
1:B:331:SER:HB2	1:B:343:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:HIS:CD2	4:D:403:SIN:O4	2.54	0.59
1:B:227:PHE:CB	1:B:228:ALA:HA	2.23	0.58
1:D:156:GLU:HB2	1:D:167:LEU:HD21	1.84	0.58
1:D:122:THR:OG1	1:D:211:HIS:HD2	1.88	0.56
1:D:142:GLN:HE22	1:D:152:THR:H	1.53	0.55
1:D:156:GLU:HG2	1:D:167:LEU:HD11	1.89	0.54
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.90	0.53
1:D:91:TRP:HD1	1:D:145:MET:HE2	1.73	0.53
1:D:120:TRP:O	1:D:126:GLY:HA2	2.10	0.52
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.45	0.52
1:C:200:GLU:OE2	1:C:202:ARG:NH1	2.40	0.52
1:A:90:HIS:CD2	1:A:92[A]:ARG:HG3	2.45	0.52
1:B:26:THR:CG2	1:B:102:PRO:HB3	2.38	0.51
1:B:38:ASP:OD1	1:B:40:VAL:HG12	2.10	0.51
1:A:90:HIS:HD2	1:A:92[B]:ARG:H	1.56	0.51
1:A:90:HIS:CD2	1:A:92[B]:ARG:H	2.29	0.51
1:B:139:GLU:HB3	5:B:670:HOH:O	2.11	0.50
1:B:253:ARG:NH1	5:B:612:HOH:O	2.44	0.50
1:D:197:VAL:HG12	1:D:203:TYR:OH	2.11	0.50
1:A:90:HIS:HD2	1:A:92[A]:ARG:H	1.57	0.50
1:A:90:HIS:CD2	1:A:92[A]:ARG:H	2.29	0.50
1:C:169:LEU:HD12	1:C:294:LEU:HD23	1.94	0.50
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.45	0.49
1:A:26:THR:HG23	1:A:102:PRO:CB	2.38	0.49
1:D:130:HIS:HD2	1:D:321:ARG:NH1	2.11	0.49
1:D:219:ALA:HB1	1:D:223:GLU:HB3	1.95	0.49
1:A:159:PHE:CE1	1:A:207:PRO:HB3	2.47	0.49
1:A:333:GLU:HG3	1:A:334[A]:MET:HG3	1.96	0.48
1:A:151:LEU:HB3	1:A:305:ARG:H	1.77	0.48
1:D:81:GLN:HE22	1:D:173:ARG:HE	1.62	0.48
1:C:297:ASP:OD2	1:D:329:ARG:NH1	2.46	0.47
1:A:132:ILE:HB	1:A:319:LEU:HB2	1.96	0.47
1:A:252:MET:HE1	1:A:279:VAL:HG21	1.96	0.47
1:D:96:ARG:NH1	5:D:601:HOH:O	2.47	0.47
1:C:265:ASP:O	1:C:269:ARG:HG3	2.15	0.46
1:D:220:THR:HG22	1:D:221:GLU:H	1.81	0.46
1:C:177:HIS:HD2	1:C:289:ASP:OD1	1.98	0.46
1:A:150:LEU:HA	1:A:307:PRO:HD3	1.98	0.45
1:D:221:GLU:C	1:D:223:GLU:H	2.23	0.45
1:D:252:MET:HE3	1:D:302:VAL:HG13	1.98	0.45
1:B:232:ARG:HG3	1:B:235:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:THR:HG21	1:C:230:ILE:HD12	1.97	0.45
1:A:43:ARG:HD2	1:B:62:GLU:HG3	1.99	0.45
1:C:91:TRP:HD1	1:C:145:MET:HE3	1.79	0.45
1:C:274:ALA:O	1:C:278:VAL:HG23	2.16	0.45
1:C:264:ASP:HB2	5:C:642:HOH:O	2.16	0.44
1:C:91:TRP:CH2	1:C:124:GLN:HA	2.53	0.44
1:C:18:GLU:O	1:C:22:VAL:HG23	2.17	0.44
1:B:252:MET:HE2	1:B:254:LEU:HD22	1.99	0.44
1:D:130:HIS:HD2	1:D:321:ARG:HH11	1.65	0.43
1:D:289:ASP:O	1:D:292:ASP:HB2	2.19	0.43
1:B:107:LEU:HD11	1:B:320:LYS:HB2	2.00	0.43
1:A:171:ALA:HA	1:A:319:LEU:HD22	2.01	0.43
1:B:156:GLU:OE1	1:B:303:HIS:CE1	2.72	0.43
1:D:178:VAL:HA	1:D:179:PRO:HD3	1.90	0.42
1:A:205:ILE:HD12	1:A:253:ARG:NH2	2.35	0.42
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.40	0.42
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.02	0.42
1:B:111:SER:HB2	1:B:324:VAL:HG22	2.01	0.42
1:B:101:PHE:HB3	1:B:102:PRO:HD3	2.02	0.41
1:C:213:PRO:HB3	1:C:219:ALA:CB	2.45	0.41
1:B:229:THR:HB	1:B:233:MET:SD	2.60	0.41
1:D:81:GLN:NE2	1:D:173:ARG:HE	2.18	0.41
1:B:82:ARG:HD3	5:B:557:HOH:O	2.21	0.41
1:D:203:TYR:CE2	1:D:268:ALA:HB1	2.56	0.41
1:A:132:ILE:HD11	1:A:321:ARG:HD2	2.03	0.41
1:C:178:VAL:HA	1:C:179:PRO:HD3	1.90	0.41
1:D:154:HIS:NE2	3:D:401:ARG:HG3	2.36	0.41
1:A:26:THR:HG21	5:A:522:HOH:O	2.21	0.40
1:C:253:ARG:O	1:C:253:ARG:HG3	2.20	0.40
1:D:10:PRO:O	1:D:72:THR:HG22	2.22	0.40
1:D:130:HIS:CD2	1:D:321:ARG:NH1	2.88	0.40
1:C:96:ARG:NH1	5:C:675:HOH:O	2.53	0.40
1:A:244:TYR:HE1	1:A:253:ARG:HG2	1.86	0.40
1:A:311:ARG:NH1	1:A:315:THR:OG1	2.54	0.40
1:D:155:THR:HB	1:D:158:ALA:HB2	2.02	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:D:237:ARG:NH2	5:A:519:HOH:O[1_655]	2.16	0.04

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	336/364 (92%)	327 (97%)	7 (2%)	2 (1%)	21	24
1	B	308/364 (85%)	290 (94%)	16 (5%)	2 (1%)	21	24
1	C	334/364 (92%)	323 (97%)	10 (3%)	1 (0%)	36	43
1	D	334/364 (92%)	321 (96%)	11 (3%)	2 (1%)	21	24
All	All	1312/1456 (90%)	1261 (96%)	44 (3%)	7 (0%)	24	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	B	237	ARG
1	C	218	ILE
1	D	94	ARG
1	A	147	SER
1	B	207	PRO
1	D	147	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%)	271 (94%)	17 (6%)	18	22
1	B	268/311 (86%)	250 (93%)	18 (7%)	15	17
1	C	286/311 (92%)	267 (93%)	19 (7%)	15	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	286/311 (92%)	271 (95%)	15 (5%)	21	25
All	All	1128/1244 (91%)	1059 (94%)	69 (6%)	17	20

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	26	THR
1	A	29	LEU
1	A	42	LEU
1	A	45	LEU
1	A	48	LEU
1	A	60	LEU
1	A	128	LEU
1	A	154	HIS
1	A	159	PHE
1	A	182	VAL
1	A	185	LEU
1	A	209	GLU
1	A	216	ASN
1	A	223	GLU
1	A	253	ARG
1	A	287	VAL
1	B	26	THR
1	B	29	LEU
1	B	42	LEU
1	B	48	LEU
1	B	82	ARG
1	B	105	LEU
1	B	130	HIS
1	B	149	GLN
1	B	182	VAL
1	B	185	LEU
1	B	208	ASP
1	B	230	ILE
1	B	234	ILE
1	B	236	GLU
1	B	253	ARG
1	B	305	ARG
1	B	311	ARG
1	B	321	ARG
1	C	29	LEU

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	48	LEU
1	C	54	GLU
1	C	68	ARG
1	C	75	ARG
1	C	82	ARG
1	C	95	VAL
1	C	96	ARG
1	C	182	VAL
1	C	185	LEU
1	C	218	ILE
1	C	223	GLU
1	C	254	LEU
1	C	277	LYS
1	C	284	ARG
1	C	311	ARG
1	C	319	LEU
1	C	333	GLU
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	92	ARG
1	D	167	LEU
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	220	THR
1	D	254	LEU
1	D	311	ARG
1	D	319	LEU

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	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	215	ASN
1	B	57	GLN

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Mol	Chain	Res	Type
1	B	90	HIS
1	B	138	HIS
1	B	177	HIS
1	C	81	GLN
1	C	90	HIS
1	C	142	GLN
1	C	177	HIS
1	C	204	HIS
1	C	231	GLN
1	C	263	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	130	HIS
1	D	140	ASN
1	D	142	GLN
1	D	177	HIS
1	D	211	HIS
1	D	290	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ARG	D	401	-	10,11,11	0.75	1 (10%)	9,13,13	0.98	1 (11%)
4	SIN	D	403	2	7,7,7	1.14	0	8,8,8	1.13	0
3	ARG	C	401	-	10,11,11	0.74	1 (10%)	9,13,13	0.95	1 (11%)
4	SIN	C	403	2	7,7,7	1.10	0	8,8,8	1.10	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	ARG	D	401	-	-	3/11/11/11	-
4	SIN	D	403	2	-	2/5/5/5	-
3	ARG	C	401	-	-	2/11/11/11	-
4	SIN	C	403	2	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ARG	OXT-C	-2.26	1.23	1.30
3	C	401	ARG	OXT-C	-2.22	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ARG	OXT-C-O	-2.75	117.83	124.08
3	D	401	ARG	OXT-C-O	-2.69	117.98	124.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	ARG	C-CA-CB-CG
3	D	401	ARG	NE-CD-CG-CB
3	C	401	ARG	NE-CD-CG-CB
4	C	403	SIN	O1-C1-C2-C3
4	D	403	SIN	C2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	C	403	SIN	O2-C1-C2-C3
4	D	403	SIN	C2-C3-C4-O4
3	C	401	ARG	OXT-C-CA-N
3	D	401	ARG	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ARG	1	0
4	D	403	SIN	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%)	0.37	28 (8%)	17 19	8, 26, 79, 126	6 (1%)
1	B	314/364 (86%)	0.39	18 (5%)	29 34	16, 31, 79, 128	3 (0%)
1	C	336/364 (92%)	0.06	10 (2%)	52 59	13, 24, 44, 96	4 (1%)
1	D	336/364 (92%)	0.17	8 (2%)	59 66	17, 29, 49, 75	3 (0%)
All	All	1322/1456 (90%)	0.25	64 (4%)	35 41	8, 27, 56, 128	16 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	7.8
1	A	218	ILE	6.3
1	A	143	LEU	5.9
1	C	92	ARG	5.8
1	B	230	ILE	5.8
1	A	269	ARG	5.6
1	C	220	THR	5.5
1	A	150	LEU	5.5
1	A	144	GLY	5.5
1	C	219	ALA	5.4
1	B	225	ALA	5.0
1	A	216	ASN	4.8
1	B	227	PHE	4.8
1	B	234	ILE	4.7
1	A	82	ARG	4.5
1	A	145	MET	4.5
1	B	210	SER	3.8
1	A	219	ALA	3.8
1	B	82	ARG	3.7
1	C	82	ARG	3.6
1	A	223	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	147	SER	3.5
1	B	229	THR	3.5
1	A	151	LEU	3.5
1	D	82	ARG	3.4
1	A	215	ASN	3.4
1	A	213	PRO	3.3
1	A	146	GLY	3.2
1	A	141	ASP	3.0
1	D	196	ASP	2.9
1	D	225	ALA	2.9
1	A	224	ALA	2.9
1	B	226	ARG	2.9
1	A	212	LEU	2.8
1	C	221	GLU	2.8
1	B	232	ARG	2.8
1	B	138	HIS	2.7
1	B	238	PRO	2.7
1	A	214	LYS	2.7
1	A	210	SER	2.7
1	B	228	ALA	2.6
1	C	196	ASP	2.6
1	C	93	GLY	2.5
1	B	247	ARG	2.5
1	A	148	LYS	2.5
1	A	142	GLN	2.5
1	C	222	GLU	2.4
1	A	149	GLN	2.4
1	D	264	ASP	2.3
1	C	247	ARG	2.3
1	B	36	PHE	2.3
1	A	209	GLU	2.3
1	B	196	ASP	2.2
1	D	68	ARG	2.2
1	D	247	ARG	2.2
1	A	247	ARG	2.2
1	A	287	VAL	2.2
1	D	221	GLU	2.2
1	A	140	ASN	2.2
1	D	9	THR	2.2
1	B	233	MET	2.1
1	B	235	ASP	2.1
1	C	223	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	209	GLU	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($\text{\AA}^2$)	Q<0.9
3	ARG	D	401	12/12	0.81	0.12	32,33,35,35	0
3	ARG	C	401	12/12	0.86	0.12	31,33,35,36	0
4	SIN	D	403	8/8	0.89	0.13	32,33,34,37	0
4	SIN	C	403	8/8	0.94	0.09	23,24,25,26	0
2	FE	A	401	1/1	0.99	0.04	37,37,37,37	0
2	FE	B	401	1/1	0.99	0.04	38,38,38,38	0
2	FE	C	402	1/1	0.99	0.04	23,23,23,23	0
2	FE	D	402	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.