



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 PM GMT

PDB ID : 4M27
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

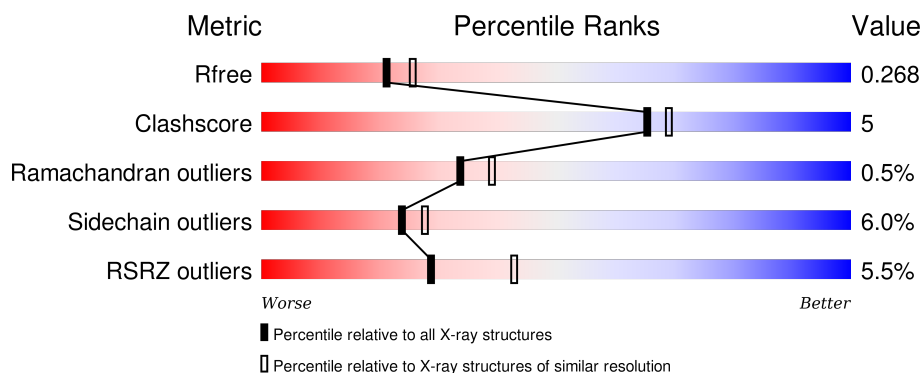
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	B	364	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>14%</div> </div> </div>
1	C	364	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	364	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ARG	C	401	-	-	-	X
3	ARG	D	401	-	-	-	X

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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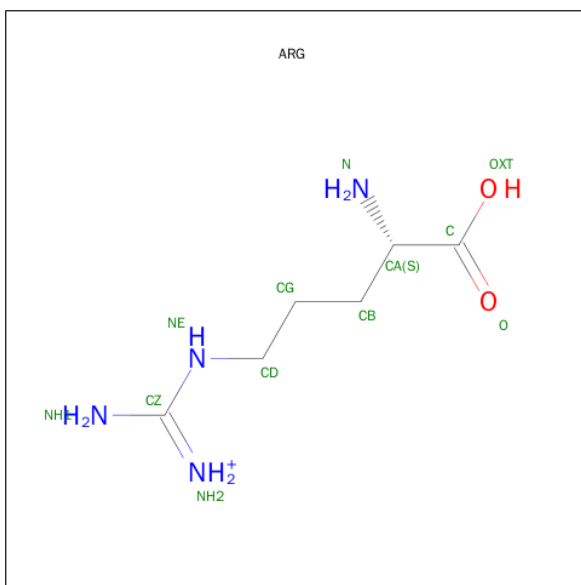
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS	-	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 (three-letter code: FE) (formula: Fe).

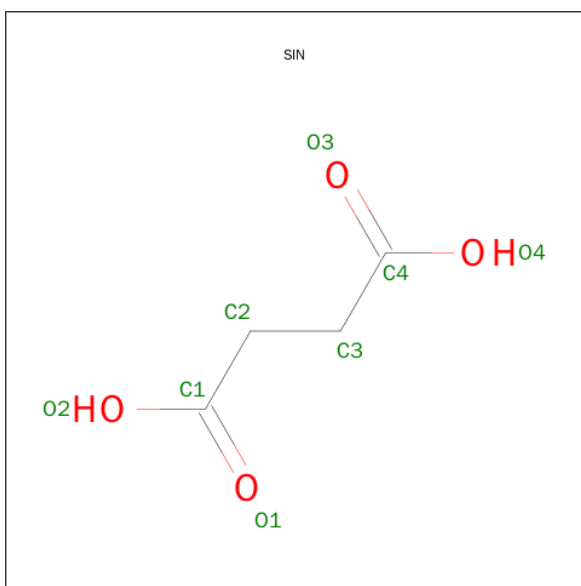
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is ARGinine (three-letter code: 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 (three-letter code: SIN) (formula: C₄H₆O₄).

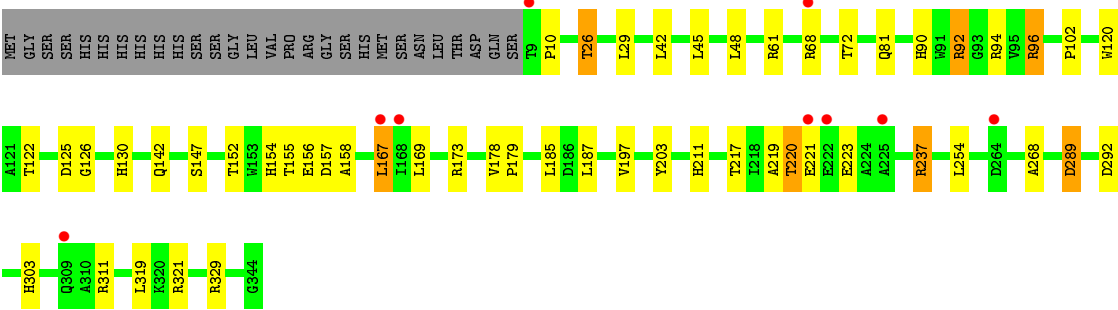
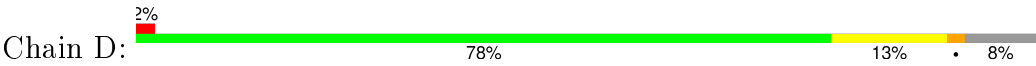


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- 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

● 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 29.49 – 2.35	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-2.35) 84.2 (29.49-2.35)	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 0.201 , 0.268	Depositor DCC
R_{free} test set	2704 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.0	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53469 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.46	1/2779 (0.0%)	0.58	0/3778
1	B	0.47	2/2592 (0.1%)	0.57	0/3523
1	C	0.46	0/2760	0.57	1/3754 (0.0%)
1	D	0.45	0/2760	0.56	1/3754 (0.0%)
All	All	0.46	3/10891 (0.0%)	0.57	2/14809 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	TRP	CD2-CE2	5.11	1.47	1.41
1	B	318	TRP	CD2-CE2	5.04	1.47	1.41
1	A	120	TRP	CD2-CE2	5.02	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	319	LEU	CA-CB-CG	5.11	127.05	115.30

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	2709	0	2626	25	0
1	B	2526	0	2452	26	0
1	C	2690	0	2606	24	0
1	D	2690	0	2606	31	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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	104	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 (104) 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:C:82:ARG:HD2	1:C:82:ARG:O	1.39	1.20
1:B:237:ARG:HB3	1:B:238:PRO:HD3	1.28	1.09
1:C:82:ARG:HD2	1:C:82:ARG:C	1.73	1.05
1:B:82:ARG:HH11	1:B:82:ARG:CG	1.70	1.05
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:B:82:ARG:HH11	1:B:82:ARG:HG3	1.42	0.84
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:B:82:ARG:HH11	1:B:82:ARG:HG2	1.44	0.79
1:C:75:ARG:HD2	5:C:546:HOH:O	1.84	0.78
1:C:82:ARG:C	1:C:82:ARG:CD	2.46	0.76
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:D:92:ARG:NH1	1:D:92:ARG:HG3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.72	0.71
1:C:142:GLN:HE22	1:C:152:THR:H	1.40	0.69
1:B:82:ARG:NH1	1:B:82:ARG:HG2	2.05	0.68
1:C:82:ARG:O	1:C:82:ARG:CD	2.32	0.67
1:B:253:ARG:HG2	1:B:253:ARG:O	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
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:B:82:ARG:NH1	1:B:82:ARG:CG	2.42	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: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:B:139:GLU:HB3	5:B:670:HOH:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HE1	1:A:279:VAL:HG21	1.94	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: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:B:232:ARG:HG3	1:B:235:ASP:OD1	2.15	0.45
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: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: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:D:26:THR:CG2	1:D:102:PRO:HB3	2.40	0.42
1:A:205:ILE:HD12	1:A:253:ARG:NH2	2.35	0.42
1:D:221:GLU:C	1:D:223:GLU:H	2.23	0.42
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.02	0.42
1:B:252:MET:HE2	1:B:254:LEU:HD22	2.01	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:D:154:HIS:NE2	3:D:401:ARG:HG3	2.36	0.41
1:C:178:VAL:HA	1:C:179:PRO:HD3	1.90	0.41
1:A:26:THR:HG21	5:A:522:HOH:O	2.21	0.40
1:D:10:PRO:O	1:D:72:THR:HG22	2.22	0.40
1:C:253:ARG:O	1:C:253:ARG:HG3	2.20	0.40
1:D:130:HIS:CD2	1:D:321:ARG:NH1	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:NH1	5:C:675:HOH:O	2.53	0.40
1:A:311:ARG:NH1	1:A:315:THR:OG1	2.54	0.40
1:A:244:TYR:HE1	1:A:253:ARG:HG2	1.86	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 [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	336/364 (92%)	327 (97%)	7 (2%)	2 (1%)	30	34
1	B	308/364 (85%)	290 (94%)	16 (5%)	2 (1%)	30	34
1	C	334/364 (92%)	323 (97%)	10 (3%)	1 (0%)	46	55
1	D	334/364 (92%)	321 (96%)	11 (3%)	2 (1%)	30	34
All	All	1312/1456 (90%)	1261 (96%)	44 (3%)	7 (0%)	34	39

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

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Mol	Chain	Res	Type
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%)	272 (94%)	16 (6%)	26	31
1	B	268/311 (86%)	249 (93%)	19 (7%)	18	20
1	C	286/311 (92%)	271 (95%)	15 (5%)	29	35
1	D	286/311 (92%)	269 (94%)	17 (6%)	24	28
All	All	1128/1244 (91%)	1061 (94%)	67 (6%)	24	28

All (67) 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	48	LEU
1	A	60	LEU
1	A	96	ARG
1	A	128	LEU
1	A	141	ASP
1	A	154	HIS
1	A	159	PHE
1	A	182	VAL
1	A	185	LEU
1	A	216	ASN
1	A	253	ARG
1	A	269	ARG
1	B	26	THR
1	B	29	LEU
1	B	42	LEU
1	B	48	LEU

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Mol	Chain	Res	Type
1	B	82	ARG
1	B	105	LEU
1	B	130	HIS
1	B	149	GLN
1	B	154	HIS
1	B	182	VAL
1	B	185	LEU
1	B	208	ASP
1	B	209	GLU
1	B	230	ILE
1	B	232	ARG
1	B	234	ILE
1	B	253	ARG
1	B	305	ARG
1	B	311	ARG
1	C	29	LEU
1	C	42	LEU
1	C	48	LEU
1	C	68	ARG
1	C	82	ARG
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	333	GLU
1	D	26	THR
1	D	29	LEU
1	D	42	LEU
1	D	45	LEU
1	D	48	LEU
1	D	61	ARG
1	D	68	ARG
1	D	92	ARG
1	D	96	ARG
1	D	167	LEU
1	D	185	LEU
1	D	187	LEU

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Mol	Chain	Res	Type
1	D	220	THR
1	D	237	ARG
1	D	254	LEU
1	D	289	ASP
1	D	311	ARG

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

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	215	ASN
1	B	57	GLN
1	B	90	HIS
1	B	123	GLN
1	B	138	HIS
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	142	GLN
1	C	177	HIS
1	C	204	HIS
1	C	263	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	130	HIS
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 carbohydrates 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	C	401	-	5,11,11	0.18	0	3,13,13	0.30	0
4	SIN	C	403	2	1,7,7	0.01	0	2,8,8	0.49	0
3	ARG	D	401	-	5,11,11	0.18	0	3,13,13	0.21	0
4	SIN	D	403	2	1,7,7	0.05	0	2,8,8	1.02	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	C	401	-	-	0/5/11/11	0/0/0/0
4	SIN	C	403	2	-	0/1/5/5	0/0/0/0
3	ARG	D	401	-	-	0/5/11/11	0/0/0/0
4	SIN	D	403	2	-	0/1/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	0.32	30 (8%) 12 19	13, 26, 79, 126	4 (1%)
1	B	314/364 (86%)	0.25	26 (8%) 14 22	17, 31, 79, 128	3 (0%)
1	C	336/364 (92%)	-0.03	8 (2%) 62 74	15, 24, 44, 96	4 (1%)
1	D	336/364 (92%)	0.11	9 (2%) 58 70	19, 29, 49, 75	3 (0%)
All	All	1322/1456 (90%)	0.16	73 (5%) 29 43	13, 28, 56, 128	14 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	17.7
1	A	216	ASN	9.9
1	C	219	ALA	9.0
1	A	150	LEU	8.9
1	C	220	THR	7.5
1	B	227	PHE	6.3
1	A	149	GLN	5.9
1	B	228	ALA	5.9
1	A	151	LEU	5.6
1	B	138	HIS	5.5
1	A	147	SER	5.3
1	A	218	ILE	5.2
1	A	141	ASP	5.1
1	A	215	ASN	5.0
1	B	230	ILE	4.9
1	C	92	ARG	4.8
1	A	145	MET	4.8
1	B	225	ALA	4.8
1	A	140	ASN	4.7
1	B	229	THR	4.5
1	A	212	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	210	SER	4.5
1	A	219	ALA	4.3
1	C	222	GLU	4.2
1	B	237	ARG	4.1
1	A	143	LEU	3.9
1	A	144	GLY	3.9
1	A	142	GLN	3.8
1	A	148	LYS	3.7
1	B	209	GLU	3.6
1	B	232	ARG	3.5
1	A	223	GLU	3.5
1	D	9	THR	3.3
1	B	95	VAL	3.3
1	B	226	ARG	3.2
1	D	225	ALA	3.2
1	B	248	LEU	3.1
1	D	168	ILE	3.1
1	B	137	SER	3.1
1	D	264	ASP	3.0
1	A	222	GLU	3.0
1	B	139	GLU	3.0
1	C	223	GLU	3.0
1	B	231	GLN	2.9
1	B	89	ASP	2.8
1	D	222	GLU	2.7
1	D	221	GLU	2.7
1	A	214	LYS	2.7
1	A	224	ALA	2.7
1	A	213	PRO	2.7
1	B	93	GLY	2.6
1	C	221	GLU	2.6
1	D	167	LEU	2.6
1	B	238	PRO	2.6
1	B	344	GLY	2.6
1	B	208	ASP	2.5
1	A	269	ARG	2.5
1	C	225	ALA	2.4
1	B	192	ALA	2.4
1	A	210	SER	2.3
1	A	146	GLY	2.3
1	A	82	ARG	2.3
1	A	257	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	PRO	2.2
1	D	68	ARG	2.2
1	A	209	GLU	2.2
1	C	224	ALA	2.2
1	B	135	ILE	2.1
1	A	9	THR	2.1
1	A	287	VAL	2.1
1	B	234	ILE	2.1
1	D	309	GLN	2.1
1	B	37	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	ARG	C	401	12/12	0.86	0.20	3.14	31,33,35,36	0
3	ARG	D	401	12/12	0.90	0.24	2.34	32,33,35,35	0
4	SIN	D	403	8/8	0.91	0.19	0.56	32,33,34,37	0
4	SIN	C	403	8/8	0.96	0.10	-0.98	23,24,25,26	0
2	FE	A	401	1/1	0.99	0.04	-	37,37,37,37	0
2	FE	C	402	1/1	1.00	0.12	-	23,23,23,23	0
2	FE	D	402	1/1	0.99	0.15	-	24,24,24,24	0
2	FE	B	401	1/1	0.98	0.10	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.