



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 PM GMT

PDB ID : 4M2C
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
<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

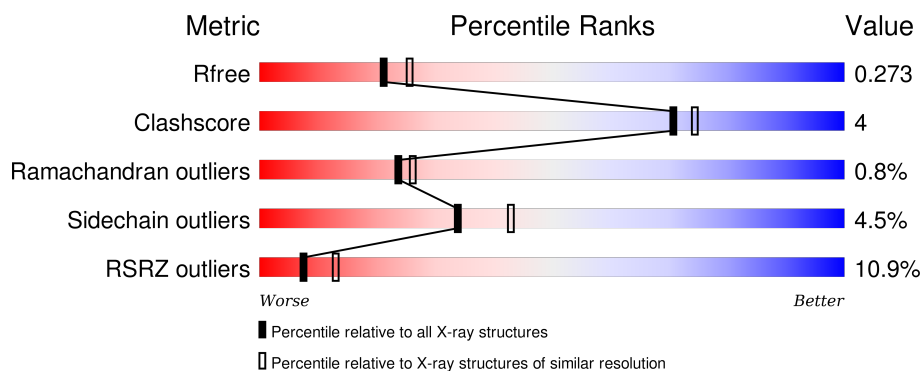
1 Overall quality at a glance

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	
1	B	364	
1	C	364	
1	D	364	

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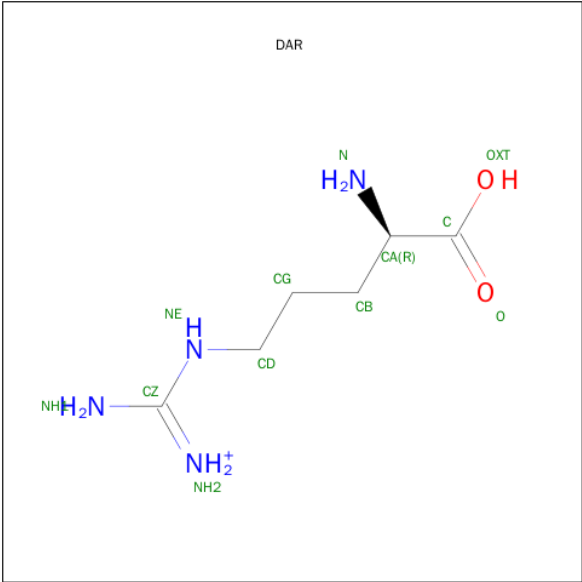
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	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 D-ARGININE (three-letter code: 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		

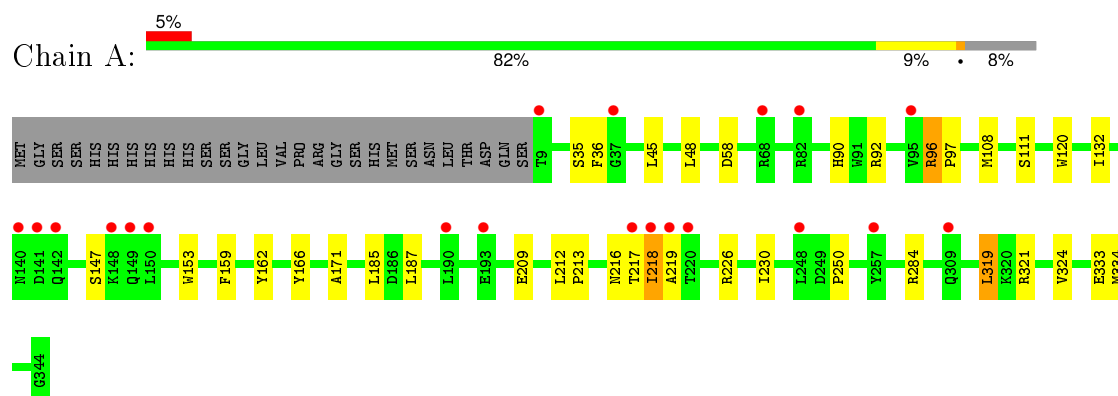
- Molecule 4 is water.

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		

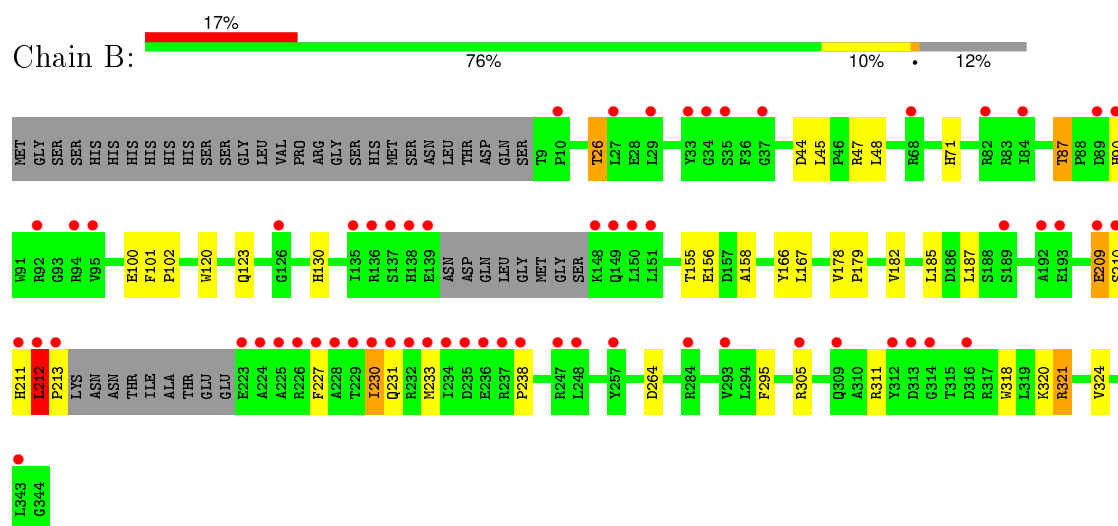
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

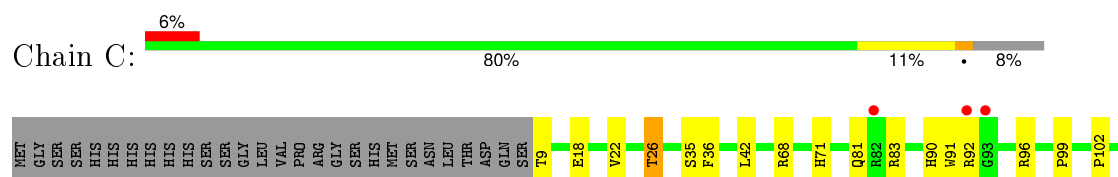
- Molecule 1: L-arginine beta-hydroxylase

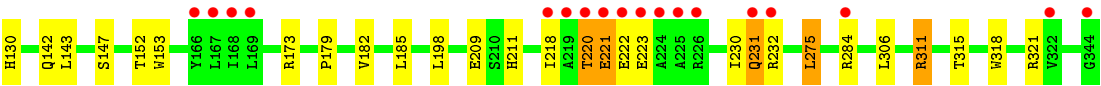


- Molecule 1: L-arginine beta-hydroxylase

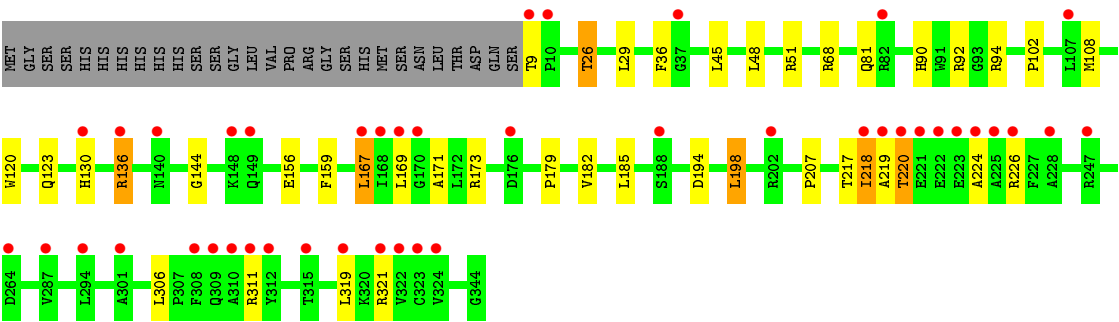
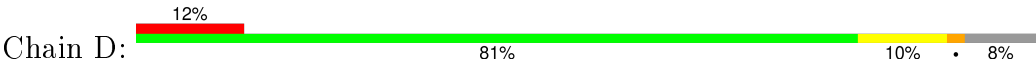


- Molecule 1: L-arginine beta-hydroxylase





● 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 28.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.35) 98.4 (28.31-2.35)	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 (5.34%)	DCC
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 , 36.4	EDS
Estimated twinning fraction	0.027 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 60884 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	2/2760 (0.1%)	0.55	0/3754
1	B	0.47	0/2633	0.54	0/3580
1	C	0.46	3/2760 (0.1%)	0.56	0/3754
1	D	0.45	0/2760	0.55	0/3754
All	All	0.46	5/10913 (0.0%)	0.55	0/14842

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TRP	CD2-CE2	5.33	1.47	1.41
1	C	318	TRP	CD2-CE2	5.20	1.47	1.41
1	C	153	TRP	CD2-CE2	5.02	1.47	1.41
1	A	153	TRP	CD2-CE2	5.01	1.47	1.41
1	C	91	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	22	0
1	B	2565	0	2488	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2690	0	2606	26	0
1	D	2690	0	2606	24	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	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	93	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 4.

All (93) 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:A:230:ILE:HD11	1:A:334:MET:HE1	1.75	0.69
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:171:ALA:HA	1:A:319:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:311:ARG:NH1	1:C:315:THR:OG1	2.45	0.49
1:A:209:GLU:HA	1:A:212:LEU:HD13	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:TRP:HB2	1:D:123:GLN:HB3	1.99	0.45
1:D:179:PRO:HG2	1:D:306:LEU:HD12	2.00	0.44
1:C:35:SER:HB2	4:C:530:HOH:O	2.17	0.44
1:D:159:PHE:CE2	1:D:207:PRO:HB3	2.53	0.44
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.85	0.44
1:D:130:HIS:CE1	4:D:533:HOH:O	2.71	0.44
1:C:211:HIS:HB3	1:C:230:ILE:HD13	2.00	0.44
1:C:143:LEU:HD21	1:C:209:GLU:HG2	1.98	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:162:TYR:CD2	1:A:334:MET:HE3	2.53	0.43
1:A:212:LEU:HA	1:A:213:PRO:HD2	1.92	0.43
1:B:230:ILE:HD13	1:B:230:ILE:H	1.84	0.42
1:B:87:THR:HG23	1:B:318:TRP:HB2	2.01	0.42
1:C:230:ILE:HG13	1:C:231:GLN:N	2.33	0.42
1:A:35:SER:HB3	1:A:97:PRO:HD3	2.00	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:HB3	1:D:136:ARG:HE	1.68	0.41
1:D:224:ALA:C	1:D:226:ARG:H	2.23	0.41
1:D:217:THR:O	1:D:218:ILE:HG12	2.20	0.41
1:B:166:TYR:HB2	1:B:324:VAL:HB	2.02	0.41
1:B:44:ASP:HB3	1:B:48:LEU:HD13	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%)	21	22
1	B	313/364 (86%)	301 (96%)	10 (3%)	2 (1%)	30	34
1	C	334/364 (92%)	315 (94%)	16 (5%)	3 (1%)	21	22
1	D	334/364 (92%)	324 (97%)	7 (2%)	3 (1%)	21	22
All	All	1315/1456 (90%)	1264 (96%)	40 (3%)	11 (1%)	24	26

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 ⓘ

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%)	51	65
1	B	272/311 (88%)	254 (93%)	18 (7%)	21	23
1	C	286/311 (92%)	273 (96%)	13 (4%)	34	43
1	D	286/311 (92%)	274 (96%)	12 (4%)	36	46
All	All	1130/1244 (91%)	1079 (96%)	51 (4%)	34	43

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

Mol	Chain	Res	Type
1	A	45	LEU
1	A	48	LEU
1	A	96	ARG
1	A	159	PHE
1	A	185	LEU
1	A	216	ASN
1	A	284	ARG
1	A	319	LEU
1	B	26	THR
1	B	45	LEU
1	B	87	THR
1	B	90	HIS
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	227	PHE
1	B	230	ILE
1	B	231	GLN
1	B	264	ASP
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	182	VAL
1	C	185	LEU
1	C	220	THR
1	C	221	GLU
1	C	223	GLU
1	C	231	GLN
1	C	232	ARG
1	C	275	LEU
1	C	284	ARG
1	C	311	ARG
1	D	9	THR
1	D	26	THR
1	D	29	LEU

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Mol	Chain	Res	Type
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	198	LEU
1	D	311	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	142	GLN
1	A	149	GLN
1	A	177	HIS
1	A	216	ASN
1	B	57	GLN
1	B	149	GLN
1	B	177	HIS
1	B	231	GLN
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	130	HIS
1	C	142	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	123	GLN
1	D	130	HIS
1	D	177	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	C	402	-	5,11,11	0.35	0	3,13,13	0.75	0
3	DAR	D	402	-	5,11,11	0.36	0	3,13,13	0.70	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	DAR	C	402	-	-	0/5/11/11	0/0/0/0
3	DAR	D	402	-	-	0/5/11/11	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.

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%)	0.36	20 (5%) 25 38	23, 37, 63, 98	4 (1%)
1	B	319/364 (87%)	1.12	61 (19%) 2 3	31, 46, 110, 129	3 (0%)
1	C	336/364 (92%)	0.41	21 (6%) 23 35	23, 35, 63, 96	4 (1%)
1	D	336/364 (92%)	0.77	43 (12%) 5 9	26, 45, 65, 123	3 (0%)
All	All	1327/1456 (91%)	0.66	145 (10%) 7 13	23, 41, 73, 129	14 (1%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	LEU	11.2
1	B	213	PRO	9.5
1	D	221	GLU	9.2
1	D	220	THR	9.0
1	C	224	ALA	8.4
1	B	234	ILE	8.3
1	B	210	SER	6.5
1	B	233	MET	6.0
1	B	82	ARG	5.9
1	B	211	HIS	5.9
1	D	219	ALA	5.8
1	D	224	ALA	5.8
1	B	37	GLY	5.7
1	A	217	THR	5.6
1	C	219	ALA	5.6
1	A	140	ASN	5.5
1	B	149	GLN	5.5
1	B	224	ALA	5.2
1	B	150	LEU	5.1
1	D	82	ARG	5.0
1	B	90	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	151	LEU	4.9
1	C	92	ARG	4.9
1	C	221	GLU	4.8
1	B	192	ALA	4.7
1	B	230	ILE	4.7
1	C	223	GLU	4.5
1	D	9	THR	4.5
1	D	218	ILE	4.4
1	A	218	ILE	4.4
1	D	168	ILE	4.3
1	B	235	ASP	4.3
1	B	209	GLU	4.3
1	B	312	TYR	4.3
1	D	222	GLU	4.2
1	B	237	ARG	4.1
1	B	314	GLY	4.1
1	A	220	THR	4.1
1	D	223	GLU	4.0
1	B	138	HIS	4.0
1	B	137	SER	3.9
1	B	257	TYR	3.9
1	B	89	ASP	3.8
1	D	225	ALA	3.8
1	B	227	PHE	3.7
1	B	316	ASP	3.7
1	B	27	LEU	3.6
1	C	82	ARG	3.5
1	B	238	PRO	3.5
1	A	248	LEU	3.5
1	B	225	ALA	3.5
1	A	219	ALA	3.5
1	D	37	GLY	3.4
1	C	225	ALA	3.4
1	B	232	ARG	3.4
1	D	226	ARG	3.4
1	B	193	GLU	3.3
1	D	309	GLN	3.3
1	A	141	ASP	3.2
1	B	92	ARG	3.2
1	B	34	GLY	3.2
1	D	324	VAL	3.2
1	D	319	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	ILE	3.1
1	D	167	LEU	3.1
1	C	226	ARG	3.1
1	D	10	PRO	3.1
1	B	226	ARG	3.1
1	D	169	LEU	3.0
1	A	9	THR	3.0
1	B	33	TYR	3.0
1	B	148	LYS	3.0
1	D	310	ALA	3.0
1	B	343	LEU	3.0
1	A	148	LYS	3.0
1	C	222	GLU	2.9
1	B	248	LEU	2.9
1	B	136	ARG	2.9
1	C	284	ARG	2.8
1	C	218	ILE	2.8
1	D	228	ALA	2.8
1	C	220	THR	2.8
1	A	150	LEU	2.8
1	C	344	GLY	2.8
1	D	188	SER	2.8
1	C	169	LEU	2.8
1	A	257	TYR	2.8
1	D	176	ASP	2.7
1	B	84	ILE	2.7
1	B	247	ARG	2.7
1	D	148	LYS	2.7
1	B	309	GLN	2.6
1	C	93	GLY	2.6
1	B	228	ALA	2.6
1	A	309	GLN	2.6
1	D	308	PHE	2.6
1	C	232	ARG	2.5
1	B	95	VAL	2.5
1	C	322	VAL	2.5
1	B	236	GLU	2.5
1	B	94	ARG	2.4
1	A	142	GLN	2.4
1	A	149	GLN	2.4
1	D	312	TYR	2.4
1	D	323	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	35	SER	2.4
1	D	311	ARG	2.4
1	B	229	THR	2.4
1	A	193	GLU	2.4
1	B	293	VAL	2.4
1	D	322	VAL	2.4
1	B	10	PRO	2.4
1	A	82	ARG	2.4
1	D	140	ASN	2.4
1	B	139	GLU	2.4
1	D	130	HIS	2.3
1	B	223	GLU	2.3
1	C	168	ILE	2.3
1	A	68	ARG	2.3
1	A	95	VAL	2.3
1	D	136	ARG	2.2
1	C	167	LEU	2.2
1	D	264	ASP	2.2
1	C	231	GLN	2.2
1	D	170	GLY	2.2
1	B	305	ARG	2.2
1	B	284	ARG	2.2
1	B	313	ASP	2.1
1	D	247	ARG	2.1
1	D	321	ARG	2.1
1	B	231	GLN	2.1
1	D	294	LEU	2.1
1	D	202	ARG	2.1
1	B	29	LEU	2.1
1	A	190	LEU	2.1
1	D	315	THR	2.1
1	D	107	LEU	2.1
1	D	149	GLN	2.1
1	B	189	SER	2.1
1	D	287	VAL	2.1
1	A	37	GLY	2.0
1	B	126	GLY	2.0
1	B	68	ARG	2.0
1	D	301	ALA	2.0
1	C	166	TYR	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(\AA^2)	Q<0.9
3	DAR	D	402	12/12	0.93	0.22	1.07	42,45,50,53	0
3	DAR	C	402	12/12	0.94	0.20	1.05	38,45,53,54	0
2	FE	D	401	1/1	0.95	0.12	-	67,67,67,67	0
2	FE	C	401	1/1	0.93	0.09	-	70,70,70,70	0
2	FE	B	401	1/1	0.83	0.10	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.