



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 PM GMT

PDB ID : 4M2F  
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and L-canavanine  
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.  
Deposited on : 2013-08-05  
Resolution : 1.92 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](mailto: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.

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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

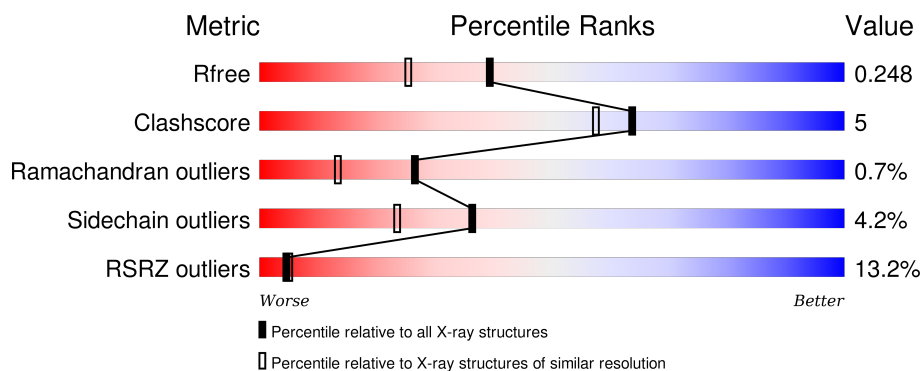
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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  $\geq 3$ , 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>10%</div> <div>80%</div> <div>11%</div> <div>•</div> <div>8%</div> </div>
1	B	364	<div> <div>7%</div> <div>76%</div> <div>9%</div> <div>•</div> <div>14%</div> </div>
1	C	364	<div> <div>14%</div> <div>81%</div> <div>11%</div> <div>•</div> <div>8%</div> </div>
1	D	364	<div> <div>16%</div> <div>80%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11548 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	313	Total	C	N	O	S	0	0	0
			2517	1591	457	463	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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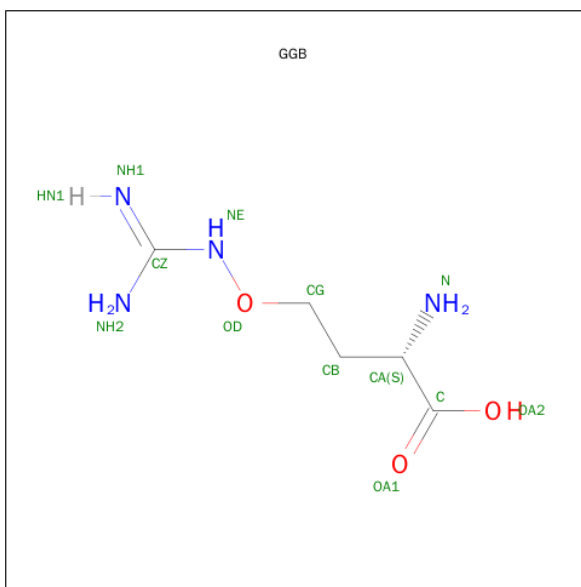
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS	-	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 L-CANAVANINE (three-letter code: GGB) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>4</sub>O<sub>3</sub>).

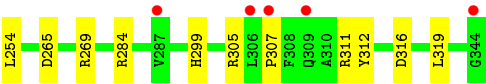


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			12	5	4	3		
3	D	1	Total	C	N	O	0	0
			12	5	4	3		

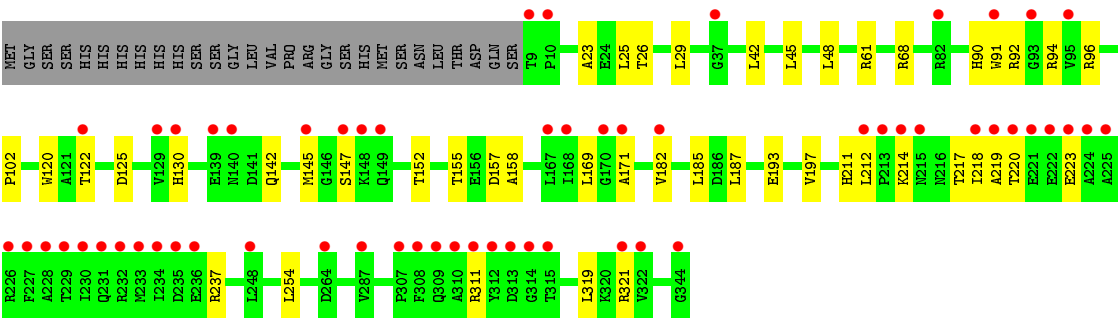
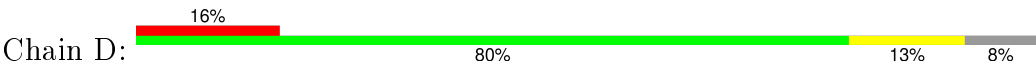
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	249	Total	O	0	0
			249	249		
4	C	222	Total	O	0	0
			222	222		
4	D	187	Total	O	0	0
			187	187		





● 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, $\alpha$ , $\beta$ , $\gamma$	67.99Å 116.61Å 96.18Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	30.00 – 1.92 29.15 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.92) 99.6 (29.15-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.248 0.208 , 0.248	Depositor DCC
$R_{free}$ test set	5687 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.9	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113671 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GGB

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	0.50	1/2760 (0.0%)	0.64	1/3754 (0.0%)
1	B	0.50	1/2583 (0.0%)	0.61	0/3511
1	C	0.50	0/2760	0.61	1/3754 (0.0%)
1	D	0.49	1/2760 (0.0%)	0.61	0/3754
All	All	0.49	3/10863 (0.0%)	0.62	2/14773 (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	5.24	1.47	1.41
1	A	120	TRP	CD2-CE2	5.13	1.47	1.41
1	D	120	TRP	CD2-CE2	5.07	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	319	LEU	CA-CB-CG	5.14	127.12	115.30

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	31	0
1	B	2517	0	2446	26	0
1	C	2690	0	2606	31	0
1	D	2690	0	2606	23	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	10	2	0
3	D	12	0	10	0	0
4	A	275	0	0	5	1
4	B	249	0	0	4	0
4	C	222	0	0	6	0
4	D	187	0	0	1	0
All	All	11548	0	10284	109	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 (109) 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	1.46	1.14
1:B:237:ARG:HB3	1:B:238:PRO:HD3	1.31	1.10
1:B:82:ARG:HH11	1:B:82:ARG:CG	1.71	1.04
1:A:305:ARG:HH21	1:A:317:ARG:HH12	1.08	0.98
1:C:82:ARG:HD2	1:C:82:ARG:C	1.76	0.97
1:B:227:PHE:HB3	1:B:228:ALA:HA	1.48	0.94
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.30	0.92
1:C:236:GLU:CG	4:C:722:HOH:O	2.22	0.88
1:B:331:SER:HB2	1:B:343:LEU:HD11	1.57	0.87
1:D:142:GLN:HE22	1:D:152:THR:H	1.25	0.84
1:B:90:HIS:HD2	1:B:92:ARG:H	1.24	0.84
1:C:82:ARG:C	1:C:82:ARG:CD	2.44	0.82
1:C:236:GLU:HG3	4:C:722:HOH:O	1.81	0.81
1:A:24:GLU:OE1	4:A:739:HOH:O	2.01	0.79
1:C:236:GLU:HG2	4:C:722:HOH:O	1.83	0.79
1:C:82:ARG:O	1:C:82:ARG:CD	2.32	0.76
1:B:253:ARG:NH1	4:B:741:HOH:O	2.19	0.75
1:D:90:HIS:HD2	1:D:92:ARG:H	1.35	0.75
1:B:237:ARG:HB3	1:B:238:PRO:CD	2.14	0.74
1:C:90:HIS:HD2	1:C:92:ARG:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:NH1	1:B:82:ARG:HG2	2.01	0.68
1:C:213:PRO:HB3	1:C:219:ALA:HB2	1.74	0.68
1:D:157:ASP:OD1	1:D:211:HIS:HE1	1.76	0.68
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.77	0.67
1:A:179:PRO:HB3	1:A:287:VAL:HG22	1.77	0.67
1:C:142:GLN:HE22	1:C:152:THR:H	1.40	0.67
1:D:26:THR:HG21	4:D:612:HOH:O	1.96	0.65
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.58	0.65
1:A:305:ARG:HH21	1:A:317:ARG:NH1	1.88	0.63
1:A:151:LEU:HB3	1:A:305:ARG:HB2	1.81	0.62
1:D:26:THR:OG1	1:D:102:PRO:O	2.17	0.62
1:B:90:HIS:CD2	1:B:92:ARG:H	2.12	0.61
1:D:23:ALA:O	1:D:26:THR:HG22	2.00	0.60
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.35	0.60
1:A:92:ARG:NH2	4:A:754:HOH:O	2.35	0.60
1:A:140:ASN:O	1:A:141:ASP:HB2	2.01	0.59
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.84	0.58
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.86	0.58
1:B:227:PHE:CB	1:B:228:ALA:HA	2.26	0.57
1:C:69:HIS:HD2	4:C:668:HOH:O	1.87	0.57
1:A:90:HIS:CD2	1:A:92:ARG:HG3	2.40	0.56
1:B:232:ARG:HG3	1:B:235:ASP:OD1	2.05	0.56
1:A:90:HIS:CD2	1:A:92:ARG:H	2.24	0.56
1:A:96:ARG:NH2	4:A:539:HOH:O	2.39	0.55
1:C:127:HIS:CD2	4:C:637:HOH:O	2.60	0.55
1:D:169:LEU:CD2	1:D:321:ARG:HG3	2.36	0.55
1:C:90:HIS:CD2	1:C:92:ARG:HB2	2.40	0.55
1:C:90:HIS:CD2	1:C:92:ARG:H	2.22	0.55
1:A:209:GLU:HA	1:A:212:LEU:HD13	1.88	0.55
1:A:217:THR:HG22	1:A:219:ALA:H	1.73	0.54
1:B:132:ILE:HD13	1:B:305:ARG:HH12	1.73	0.53
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.90	0.53
1:B:36:PHE:CE1	1:B:108:MET:HG3	2.45	0.51
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.46	0.51
1:A:218:ILE:O	1:A:218:ILE:HG22	2.11	0.51
1:D:130:HIS:HD2	1:D:321:ARG:NH1	2.08	0.51
1:A:90:HIS:HD2	1:A:92:ARG:H	1.59	0.51
1:C:151:LEU:HB3	1:C:305:ARG:H	1.75	0.50
1:A:81:GLN:NE2	1:A:173:ARG:HE	2.09	0.50
1:D:193:GLU:O	1:D:197:VAL:HG23	2.12	0.50
1:B:38:ASP:OD1	1:B:40:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:O	1:A:223:GLU:HG2	2.12	0.49
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.44	0.49
1:A:212:LEU:O	1:A:215:ASN:HB2	2.12	0.49
1:B:208:ASP:HB2	4:B:733:HOH:O	2.13	0.49
1:B:331:SER:CB	1:B:343:LEU:HD11	2.38	0.49
1:D:212:LEU:HD13	1:D:214:LYS:HE2	1.94	0.48
1:C:36:PHE:HZ	1:C:96:ARG:NH1	2.11	0.48
1:D:219:ALA:HB1	1:D:223:GLU:HB3	1.95	0.47
1:A:140:ASN:O	1:A:141:ASP:CB	2.63	0.47
1:B:237:ARG:CB	1:B:238:PRO:HD3	2.23	0.47
1:B:130:HIS:HE1	4:B:678:HOH:O	1.97	0.47
1:A:147:SER:HB2	1:A:308:PHE:O	2.14	0.46
1:A:269:ARG:HD3	4:A:771:HOH:O	2.15	0.46
1:C:244:TYR:OH	1:C:299:HIS:ND1	2.45	0.45
1:D:130:HIS:CD2	1:D:321:ARG:NH1	2.84	0.45
1:C:142:GLN:NE2	1:C:152:THR:H	2.11	0.45
1:B:81:GLN:NE2	1:B:173:ARG:HE	2.16	0.44
1:C:229:THR:HA	4:C:710:HOH:O	2.16	0.44
1:A:132:ILE:HG21	1:A:305:ARG:NH2	2.32	0.44
1:C:36:PHE:CZ	1:C:96:ARG:NH1	2.86	0.44
1:A:132:ILE:HG21	1:A:305:ARG:HH22	1.81	0.44
1:C:147:SER:O	1:C:307:PRO:HA	2.17	0.44
1:C:187:LEU:HD22	1:C:195:ILE:HD11	2.00	0.44
1:A:85:GLY:HA2	4:A:635:HOH:O	2.18	0.44
1:A:81:GLN:HE22	1:A:173:ARG:HE	1.65	0.43
1:A:150:LEU:HA	1:A:307:PRO:HD3	2.00	0.43
1:A:179:PRO:HD2	1:A:306:LEU:HD12	2.00	0.43
1:C:43:ARG:O	1:D:61:ARG:HG2	2.19	0.43
1:C:265:ASP:O	1:C:269:ARG:HG3	2.19	0.43
1:C:123:GLN:NE2	3:C:402:GGB:HN2	2.16	0.43
1:D:155:THR:HB	1:D:158:ALA:HB2	2.01	0.42
1:D:122:THR:OG1	1:D:211:HIS:HD2	2.03	0.42
1:D:91:TRP:HD1	1:D:145:MET:HE2	1.84	0.42
1:C:232:ARG:O	1:C:236:GLU:HG2	2.19	0.42
1:D:125:ASP:OD2	1:D:217:THR:HG23	2.20	0.42
1:C:96:ARG:NH1	1:C:104:GLU:OE1	2.50	0.42
1:B:163:ARG:NH1	1:B:253:ARG:HH21	2.18	0.42
1:D:25:LEU:O	1:D:29:LEU:HG	2.20	0.41
1:C:312:TYR:N	1:C:316:ASP:OD2	2.53	0.41
1:D:90:HIS:CD2	1:D:92:ARG:H	2.25	0.41
1:D:218:ILE:HG13	1:D:218:ILE:H	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:OH	1:C:237:ARG:NH1	2.53	0.41
1:A:90:HIS:NE2	1:A:92:ARG:HG3	2.36	0.40
1:C:123:GLN:HE22	3:C:402:GGB:HN2	1.68	0.40
1:B:101:PHE:HB3	1:B:102:PRO:HD3	2.03	0.40
1:B:9:THR:N	4:B:688:HOH:O	2.53	0.40
1:A:159:PHE:CZ	1:A:207:PRO:HB3	2.56	0.40
1:A:171:ALA:HA	1:A:319:LEU:HD22	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	4:A:735:HOH:O[1_655]	2.00	0.20

## 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%)	326 (98%)	6 (2%)	2 (1%)	30	16
1	B	307/364 (84%)	293 (95%)	11 (4%)	3 (1%)	19	7
1	C	334/364 (92%)	320 (96%)	12 (4%)	2 (1%)	30	16
1	D	334/364 (92%)	327 (98%)	5 (2%)	2 (1%)	30	16
All	All	1309/1456 (90%)	1266 (97%)	34 (3%)	9 (1%)	26	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	B	237	ARG
1	A	147	SER

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Mol	Chain	Res	Type
1	C	218	ILE
1	D	94	ARG
1	B	231	GLN
1	C	80	ASP
1	B	137	SER
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	286/311 (92%)	273 (96%)	13 (4%)	34	21
1	B	267/311 (86%)	255 (96%)	12 (4%)	34	21
1	C	286/311 (92%)	275 (96%)	11 (4%)	40	27
1	D	286/311 (92%)	275 (96%)	11 (4%)	40	27
All	All	1125/1244 (90%)	1078 (96%)	47 (4%)	36	23

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	45	LEU
1	A	96	ARG
1	A	97	PRO
1	A	128	LEU
1	A	154	HIS
1	A	159	PHE
1	A	185	LEU
1	A	215	ASN
1	A	216	ASN
1	A	221	GLU
1	A	253	ARG
1	A	311	ARG
1	B	45	LEU
1	B	82	ARG

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Mol	Chain	Res	Type
1	B	130	HIS
1	B	136	ARG
1	B	154	HIS
1	B	189	SER
1	B	208	ASP
1	B	230	ILE
1	B	232	ARG
1	B	234	ILE
1	B	284	ARG
1	B	311	ARG
1	C	48	LEU
1	C	68	ARG
1	C	82	ARG
1	C	96	ARG
1	C	133	PHE
1	C	185	LEU
1	C	218	ILE
1	C	223	GLU
1	C	254	LEU
1	C	284	ARG
1	C	311	ARG
1	D	42	LEU
1	D	45	LEU
1	D	48	LEU
1	D	68	ARG
1	D	96	ARG
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	220	THR
1	D	254	LEU
1	D	311	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	69	HIS
1	A	81	GLN
1	A	90	HIS
1	A	177	HIS
1	A	216	ASN

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	81	GLN
1	B	90	HIS
1	B	130	HIS
1	B	177	HIS
1	C	57	GLN
1	C	69	HIS
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	142	GLN
1	C	177	HIS
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	263	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 6 ligands modelled in this entry, 4 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	GGB	C	402	-	4,11,11	4.56	1 (25%)	1,13,13	0.36	0
3	GGB	D	402	-	4,11,11	4.74	1 (25%)	1,13,13	0.29	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	GGB	C	402	-	-	0/5/11/11	0/0/0/0
3	GGB	D	402	-	-	0/5/11/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	GGB	OD-NE	-9.42	1.34	1.45
3	C	402	GGB	OD-NE	-9.06	1.34	1.45

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	GGB	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	336/364 (92%)	0.70	38 (11%) 7 8	15, 26, 78, 113	6 (1%)
1	B	313/364 (85%)	0.58	27 (8%) 13 15	19, 29, 77, 132	3 (0%)
1	C	336/364 (92%)	0.75	51 (15%) 3 3	17, 29, 61, 116	4 (1%)
1	D	336/364 (92%)	0.98	59 (17%) 2 2	19, 37, 62, 100	3 (0%)
All	All	1321/1456 (90%)	0.76	175 (13%) 4 5	15, 30, 65, 132	16 (1%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	12.9
1	B	228	ALA	12.5
1	A	150	LEU	11.9
1	A	216	ASN	11.8
1	A	143	LEU	11.6
1	C	220	THR	11.2
1	C	219	ALA	10.1
1	B	227	PHE	9.9
1	A	215	ASN	9.7
1	A	141	ASP	9.6
1	B	225	ALA	9.5
1	B	138	HIS	8.8
1	D	224	ALA	8.7
1	C	230	ILE	8.3
1	D	230	ILE	7.9
1	A	149	GLN	7.8
1	D	225	ALA	7.6
1	C	222	GLU	7.5
1	A	145	MET	7.5
1	A	151	LEU	7.3
1	A	218	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLU	7.2
1	D	220	THR	6.9
1	A	213	PRO	6.8
1	B	237	ARG	6.6
1	A	214	LYS	6.5
1	A	142	GLN	6.2
1	C	225	ALA	6.1
1	C	218	ILE	6.1
1	A	140	ASN	6.0
1	B	230	ILE	6.0
1	A	219	ALA	6.0
1	B	229	THR	5.9
1	D	219	ALA	5.9
1	B	232	ARG	5.8
1	C	92	ARG	5.7
1	C	221	GLU	5.6
1	A	92	ARG	5.6
1	B	234	ILE	5.5
1	D	227	PHE	5.5
1	B	226	ARG	5.4
1	D	228	ALA	5.4
1	A	144	GLY	5.4
1	D	9	THR	5.3
1	B	231	GLN	5.1
1	A	220	THR	4.9
1	C	233	MET	4.9
1	C	224	ALA	4.9
1	D	226	ARG	4.9
1	C	223	GLU	4.6
1	B	150	LEU	4.6
1	A	146	GLY	4.5
1	A	147	SER	4.5
1	A	334	MET	4.5
1	D	218	ILE	4.3
1	D	148	LYS	4.3
1	C	236	GLU	4.2
1	A	212	LEU	4.2
1	C	210	SER	4.1
1	D	223	GLU	4.1
1	C	228	ALA	4.1
1	D	309	GLN	4.1
1	D	222	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	306	LEU	3.8
1	D	139	GLU	3.8
1	A	148	LYS	3.8
1	C	148	LYS	3.8
1	B	137	SER	3.7
1	D	82	ARG	3.6
1	C	344	GLY	3.6
1	D	344	GLY	3.6
1	C	287	VAL	3.6
1	A	82	ARG	3.5
1	B	136	ARG	3.4
1	D	140	ASN	3.4
1	C	151	LEU	3.4
1	B	37	GLY	3.3
1	D	307	PRO	3.3
1	D	147	SER	3.3
1	A	284	ARG	3.3
1	D	213	PRO	3.3
1	B	82	ARG	3.3
1	A	257	TYR	3.2
1	D	168	ILE	3.2
1	D	214	LYS	3.2
1	C	229	THR	3.2
1	C	307	PRO	3.2
1	B	210	SER	3.1
1	D	231	GLN	3.1
1	D	10	PRO	3.1
1	D	315	THR	3.0
1	A	95	VAL	3.0
1	A	269	ARG	3.0
1	C	95	VAL	3.0
1	D	233	MET	3.0
1	A	305	ARG	2.9
1	D	122	THR	2.9
1	D	234	ILE	2.9
1	C	94	ARG	2.9
1	C	136	ARG	2.9
1	D	215	ASN	2.9
1	D	145	MET	2.9
1	D	129	VAL	2.8
1	C	226	ARG	2.8
1	C	149	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	310	ALA	2.8
1	C	9	THR	2.8
1	B	148	LYS	2.7
1	D	95	VAL	2.7
1	C	217	THR	2.7
1	D	321	ARG	2.7
1	D	314	GLY	2.7
1	C	145	MET	2.6
1	A	287	VAL	2.6
1	B	95	VAL	2.6
1	D	212	LEU	2.6
1	D	167	LEU	2.6
1	D	312	TYR	2.6
1	B	287	VAL	2.5
1	B	247	ARG	2.5
1	C	82	ARG	2.5
1	C	146	GLY	2.5
1	D	322	VAL	2.5
1	D	149	GLN	2.5
1	A	247	ARG	2.5
1	B	319	LEU	2.5
1	D	229	THR	2.5
1	A	277	LYS	2.5
1	C	93	GLY	2.5
1	D	311	ARG	2.4
1	C	135	ILE	2.4
1	C	231	GLN	2.4
1	D	182	VAL	2.4
1	C	122	THR	2.4
1	A	227	PHE	2.4
1	A	222	GLU	2.4
1	C	134	PRO	2.4
1	D	91	TRP	2.4
1	D	130	HIS	2.4
1	C	227	PHE	2.4
1	D	232	ARG	2.3
1	D	236	GLU	2.3
1	D	248	LEU	2.3
1	D	37	GLY	2.3
1	C	214	LYS	2.3
1	B	135	ILE	2.3
1	C	215	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	264	ASP	2.2
1	D	171	ALA	2.2
1	D	235	ASP	2.2
1	C	232	ARG	2.2
1	B	233	MET	2.2
1	C	168	ILE	2.2
1	B	248	LEU	2.2
1	C	140	ASN	2.2
1	A	209	GLU	2.2
1	A	152	THR	2.2
1	D	93	GLY	2.1
1	C	234	ILE	2.1
1	C	150	LEU	2.1
1	C	36	PHE	2.1
1	D	313	ASP	2.1
1	C	309	GLN	2.1
1	D	170	GLY	2.1
1	C	166	TYR	2.1
1	C	143	LEU	2.1
1	D	287	VAL	2.1
1	C	89	ASP	2.1
1	B	122	THR	2.1
1	A	10	PRO	2.1
1	A	37	GLY	2.1
1	C	141	ASP	2.0
1	D	308	PHE	2.0
1	C	212	LEU	2.0
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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GGB	D	402	12/12	0.88	0.15	0.04	31,39,43,44	0
3	GGB	C	402	12/12	0.89	0.14	-0.33	37,41,43,44	0
2	FE	B	401	1/1	0.99	0.03	-	33,33,33,33	0
2	FE	C	401	1/1	0.96	0.04	-	49,49,49,49	0
2	FE	D	401	1/1	0.95	0.06	-	51,51,51,51	0
2	FE	A	401	1/1	0.99	0.03	-	42,42,42,42	0

## 6.5 Other polymers

There are no such residues in this entry.