



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 06:44 PM EDT

PDB ID : 4M25  
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and alpha-ketoglutaric acid  
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.  
Deposited on : 2013-08-05  
Resolution : 1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

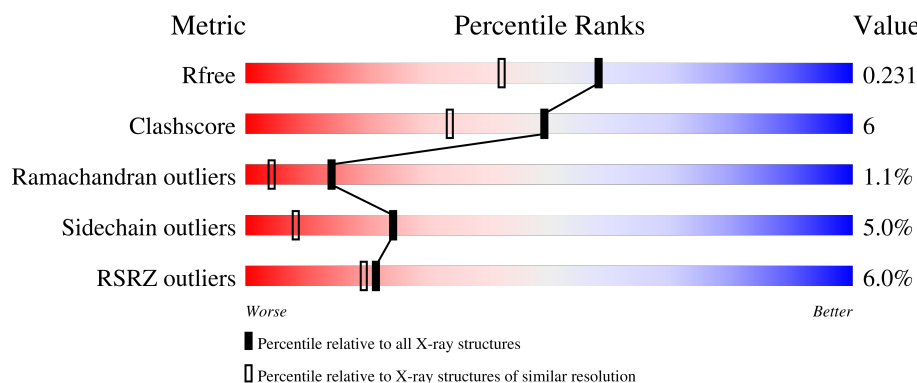
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	364	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	364	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	364	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11546 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	1	0
			2697	1697	488	505	7			
1	B	317	Total	C	N	O	S	0	0	0
			2541	1600	461	473	7			
1	C	317	Total	C	N	O	S	0	0	0
			2541	1600	461	473	7			
1	D	314	Total	C	N	O	S	0	1	0
			2525	1593	456	469	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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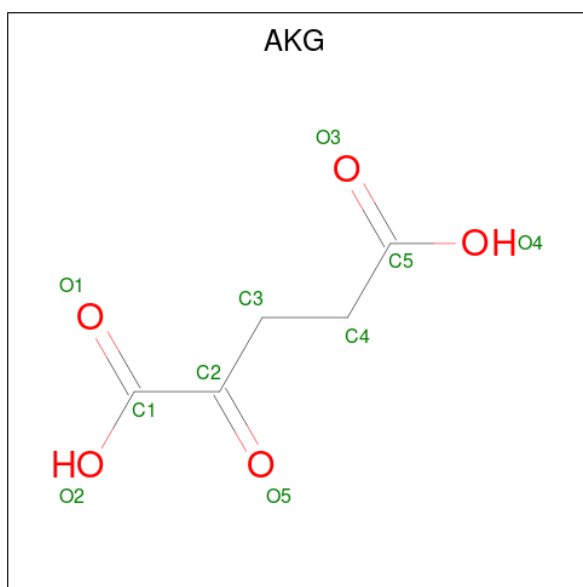
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	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	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

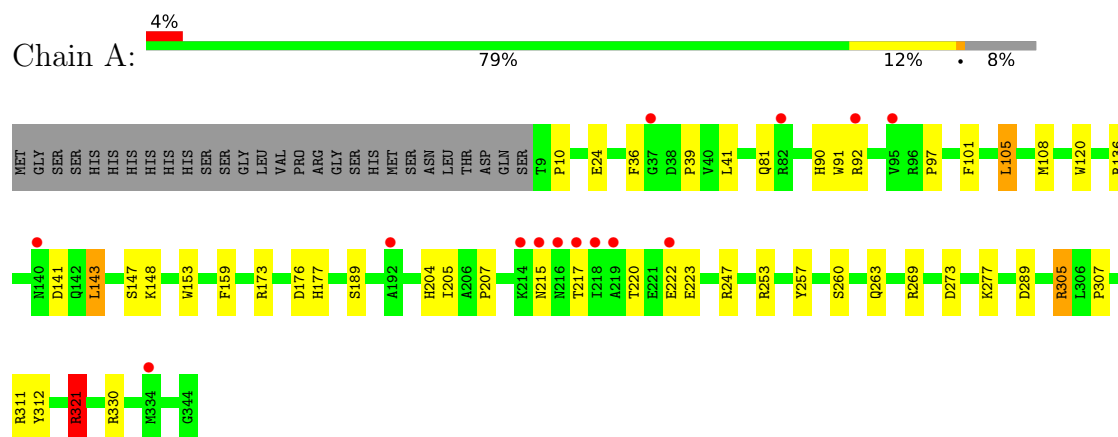
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	404	Total	O	0	0
			404	404		
4	B	263	Total	O	0	0
			263	263		
4	C	291	Total	O	0	0
			291	291		
4	D	236	Total	O	0	0
			236	236		

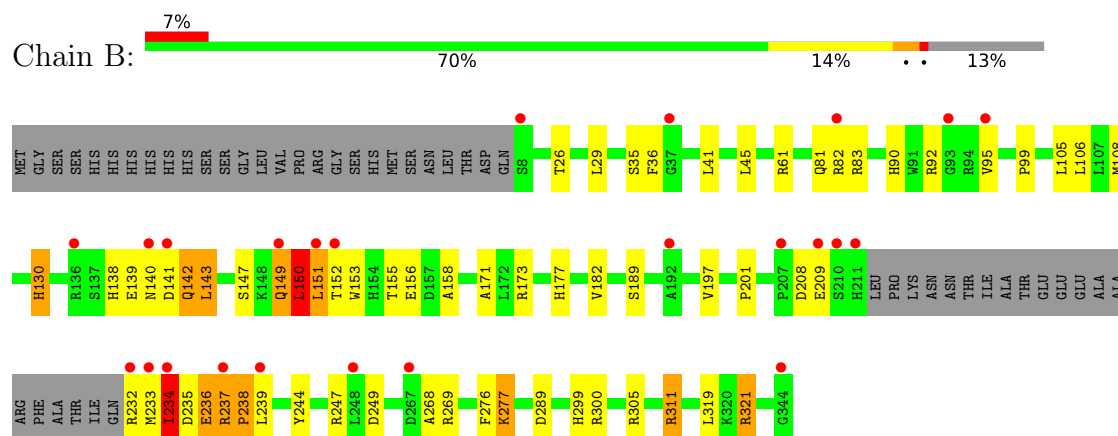
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

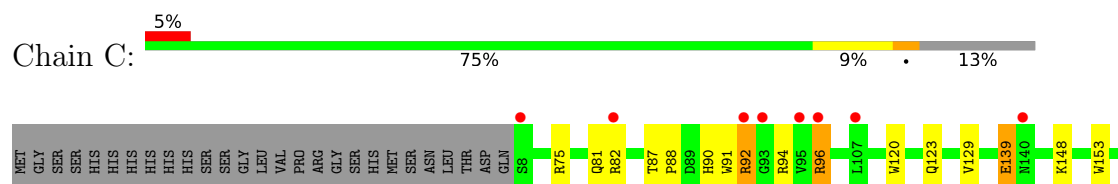
#### • Molecule 1: L-arginine beta-hydroxylase

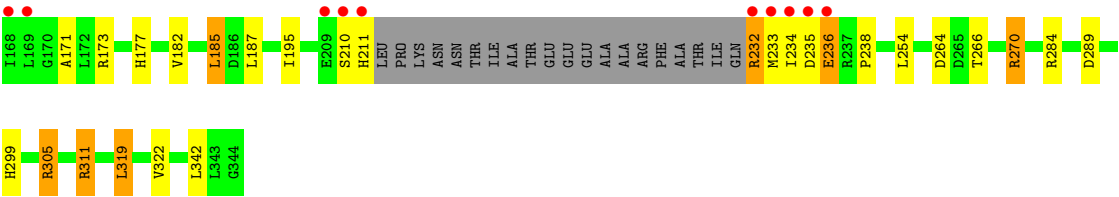


#### • Molecule 1: L-arginine beta-hydroxylase

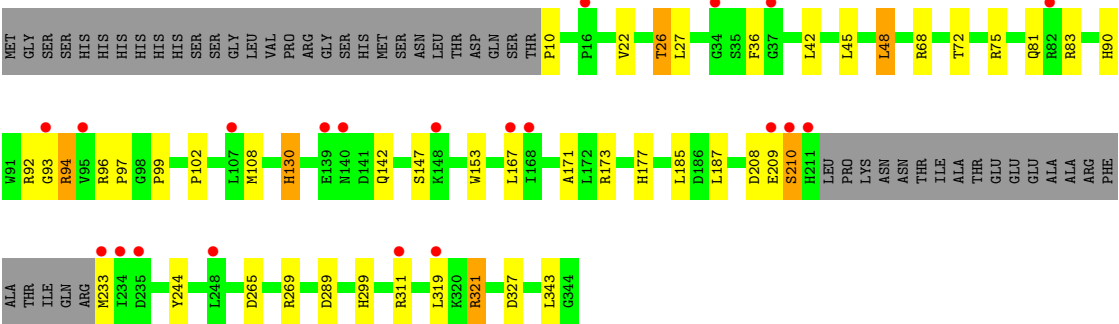


#### • Molecule 1: L-arginine beta-hydroxylase





● Molecule 1: L-arginine beta-hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.20Å 117.26Å 96.56Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	30.00 – 1.84 26.70 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.84) 99.4 (26.70-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.194 , 0.232 0.195 , 0.231	Depositor DCC
$R_{free}$ test set	6600 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.333 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: AKG, 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	0.69	3/2767 (0.1%)	0.80	2/3764 (0.1%)
1	B	0.68	1/2608 (0.0%)	0.79	3/3545 (0.1%)
1	C	0.70	1/2608 (0.0%)	0.84	3/3545 (0.1%)
1	D	0.65	1/2592 (0.0%)	0.77	1/3523 (0.0%)
All	All	0.68	6/10575 (0.1%)	0.80	9/14377 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TRP	CD2-CE2	5.86	1.48	1.41
1	A	91	TRP	CD2-CE2	5.56	1.48	1.41
1	D	153	TRP	CD2-CE2	5.46	1.47	1.41
1	C	153	TRP	CD2-CE2	5.26	1.47	1.41
1	B	153	TRP	CD2-CE2	5.15	1.47	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	305	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	321	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	319	LEU	CA-CB-CG	5.80	128.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	GLN	Peptide

## 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	2697	0	2612	29	1
1	B	2541	0	2456	40	0
1	C	2541	0	2456	24	1
1	D	2525	0	2442	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	404	0	0	10	0
4	B	263	0	0	9	0
4	C	291	0	0	4	0
4	D	236	0	0	7	0
All	All	11546	0	9982	120	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 6.

The worst 5 of 120 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:75:ARG:HD2	4:C:754:HOH:O	1.53	1.06
1:B:239:LEU:HB2	4:B:665:HOH:O	1.60	1.00
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.51	0.93
1:D:244:TYR:OH	1:D:299:HIS:ND1	2.02	0.92
1:B:90:HIS:HD2	1:B:92:ARG:H	1.20	0.88

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:A:257:TYR:OH	1:C:270:ARG:NH2[2_546]	2.03	0.17

## 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	335/364 (92%)	326 (97%)	7 (2%)	2 (1%)	25	12
1	B	313/364 (86%)	293 (94%)	14 (4%)	6 (2%)	8	1
1	C	313/364 (86%)	300 (96%)	10 (3%)	3 (1%)	15	5
1	D	311/364 (85%)	303 (97%)	5 (2%)	3 (1%)	15	5
All	All	1272/1456 (87%)	1222 (96%)	36 (3%)	14 (1%)	14	4

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LEU
1	B	237	ARG
1	C	235	ASP
1	D	94	ARG
1	B	150	LEU

### 5.3.2 Protein sidechains [i](#)

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	287/311 (92%)	282 (98%)	5 (2%)	60	47
1	B	271/311 (87%)	253 (93%)	18 (7%)	16	4
1	C	271/311 (87%)	255 (94%)	16 (6%)	19	5
1	D	269/311 (86%)	253 (94%)	16 (6%)	19	5
All	All	1098/1244 (88%)	1043 (95%)	55 (5%)	24	8

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	LEU
1	C	284	ARG
1	D	321	ARG
1	D	185	LEU
1	C	211	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	HIS
1	C	177	HIS
1	C	142	GLN
1	D	57	GLN
1	B	57	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	AKG	A	403	2	9,9,9	1.69	1 (11%)	11,11,11	1.41	2 (18%)
3	AKG	B	403	2	9,9,9	2.32	2 (22%)	11,11,11	1.29	2 (18%)
3	AKG	C	403	2	9,9,9	1.98	1 (11%)	11,11,11	1.62	2 (18%)
3	AKG	D	403	2	9,9,9	1.84	1 (11%)	11,11,11	2.23	4 (36%)

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	AKG	A	403	2	-	1/9/9/9	-
3	AKG	B	403	2	-	1/9/9/9	-
3	AKG	C	403	2	-	1/9/9/9	-
3	AKG	D	403	2	-	3/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	AKG	C2-C1	-5.58	1.46	1.53
3	C	403	AKG	C2-C1	-5.01	1.46	1.53
3	D	403	AKG	C2-C1	-4.87	1.47	1.53
3	A	403	AKG	C2-C1	-4.04	1.48	1.53
3	B	403	AKG	O1-C1	2.52	1.29	1.22

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	AKG	O1-C1-C2	-5.22	114.75	121.72
3	D	403	AKG	O2-C1-C2	2.90	121.91	113.97
3	B	403	AKG	C3-C2-C1	2.84	121.25	115.97
3	C	403	AKG	C3-C2-C1	2.82	121.21	115.97
3	C	403	AKG	O2-C1-C2	2.73	121.43	113.97

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	AKG	C1-C2-C3-C4
3	D	403	AKG	C1-C2-C3-C4
3	A	403	AKG	C1-C2-C3-C4
3	C	403	AKG	C1-C2-C3-C4
3	D	403	AKG	C3-C4-C5-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.02	14 (4%) 36 33	16, 27, 53, 116	6 (1%)
1	B	317/364 (87%)	0.21	24 (7%) 13 12	19, 32, 72, 97	3 (0%)
1	C	317/364 (87%)	0.04	18 (5%) 23 21	16, 27, 57, 92	4 (1%)
1	D	314/364 (86%)	0.15	21 (6%) 17 15	17, 32, 61, 80	3 (0%)
All	All	1284/1456 (88%)	0.10	77 (5%) 21 19	16, 30, 61, 116	16 (1%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	15.9
1	A	216	ASN	10.0
1	C	234	ILE	6.6
1	C	236	GLU	5.7
1	A	214	LYS	5.6

### 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AKG	D	403	10/10	0.95	0.10	27,29,32,32	0
3	AKG	B	403	10/10	0.96	0.08	29,30,34,36	0
3	AKG	A	403	10/10	0.96	0.09	24,25,26,27	0
3	AKG	C	403	10/10	0.97	0.16	26,26,27,28	0
2	FE	B	402	1/1	0.98	0.07	48,48,48,48	0
2	FE	D	402	1/1	0.98	0.12	47,47,47,47	0
2	FE	B	401	1/1	0.98	0.06	30,30,30,30	0
2	FE	C	402	1/1	0.99	0.08	48,48,48,48	0
2	FE	A	402	1/1	0.99	0.02	26,26,26,26	0
2	FE	D	401	1/1	1.00	0.08	23,23,23,23	0
2	FE	C	401	1/1	1.00	0.09	22,22,22,22	0
2	FE	A	401	1/1	1.00	0.07	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.