



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:55 PM EDT

PDB ID : 6F2E  
Title : Crystal structure of the APO Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO1  
Authors : Isabet, T.; Stura, E.A.; Legrand, P.; Zaparucha, A.; Bastard, K.  
Deposited on : 2017-11-24  
Resolution : 1.90 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

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

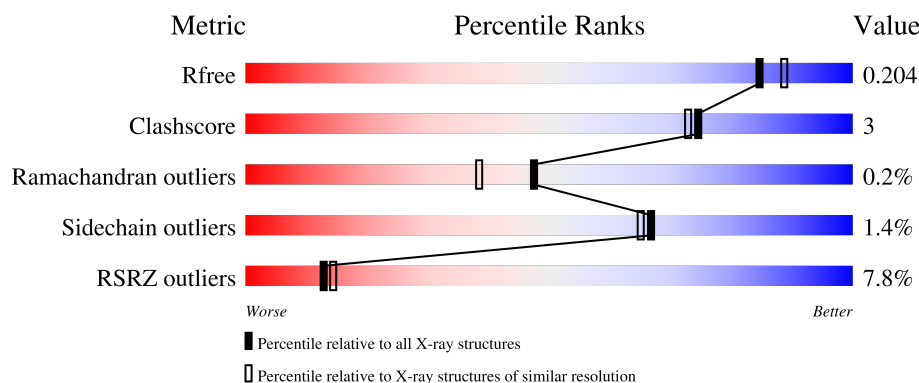
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	358	<div> <div>3%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	B	358	<div> <div>12%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	358	<div> <div>5%</div> <div>86%</div> <div>5%</div> <div>8%</div> </div>
1	D	358	<div> <div>8%</div> <div>83%</div> <div>7%</div> <div>10%</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
2	ACY	D	401	-	X	-	-

## 2 Entry composition [i](#)

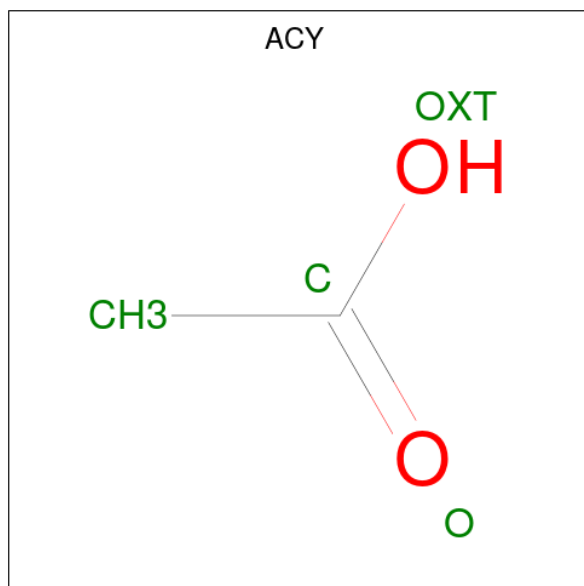
There are 3 unique types of molecules in this entry. The entry contains 11702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-lysine 3-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	5	0
			2579	1614	465	485	15			
1	B	329	Total	C	N	O	S	0	10	0
			2629	1644	480	489	16			
1	C	328	Total	C	N	O	S	0	6	0
			2577	1613	464	485	15			
1	D	322	Total	C	N	O	S	0	8	0
			2557	1602	462	478	15			

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

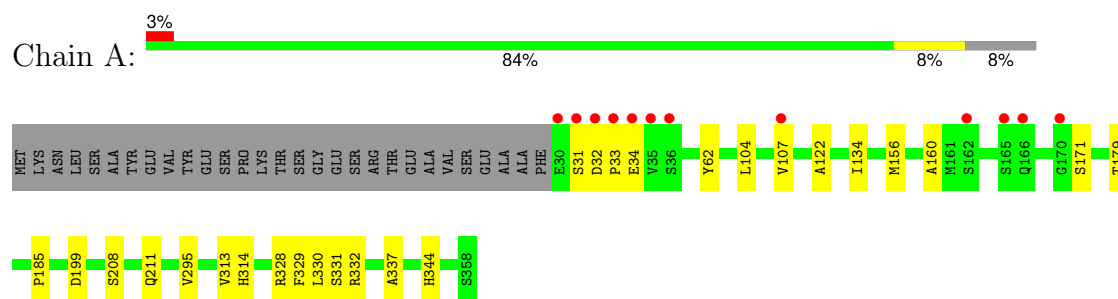
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	383	Total	O	0	2
			384	384		
3	B	292	Total	O	0	2
			292	292		
3	C	379	Total	O	0	2
			379	379		
3	D	289	Total	O	0	0
			289	289		

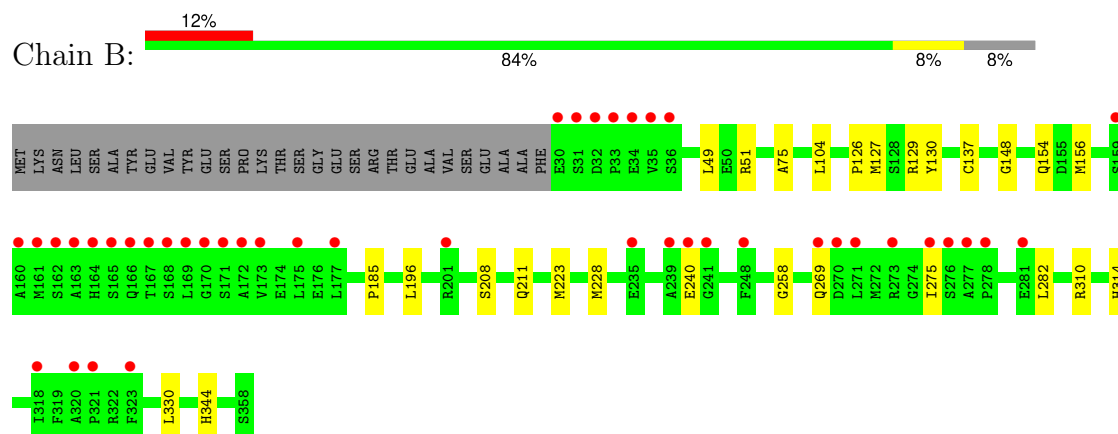
### 3 Residue-property plots

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.

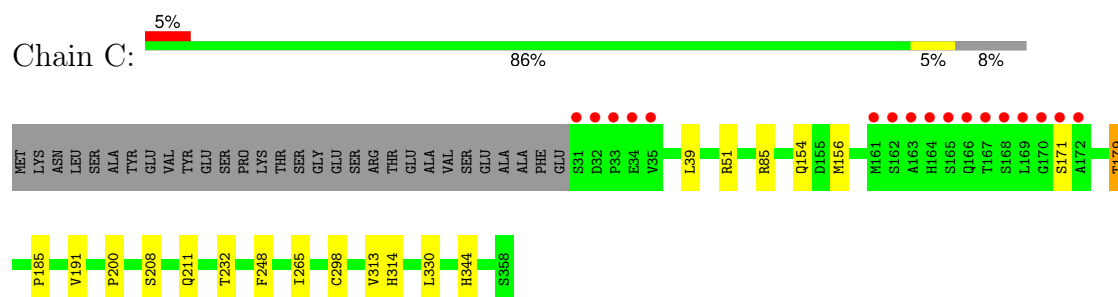
- Molecule 1: L-lysine 3-hydroxylase



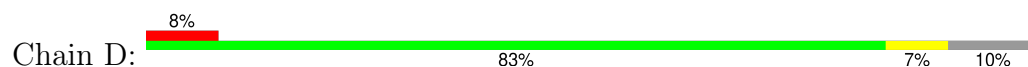
- Molecule 1: L-lysine 3-hydroxylase

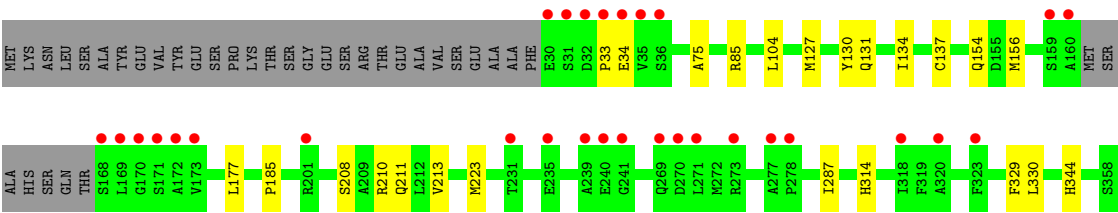


- Molecule 1: L-lysine 3-hydroxylase



- Molecule 1: L-lysine 3-hydroxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.65Å 68.09Å 110.22Å 107.85° 102.84° 93.23°	Depositor
Resolution (Å)	38.00 – 1.90 48.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.00-1.90) 98.6 (48.26-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.177 , 0.203 0.179 , 0.204	Depositor DCC
$R_{free}$ test set	5884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: ACY

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	0.54	0/2634	0.60	0/3575
1	B	0.49	0/2685	0.61	0/3641
1	C	0.52	0/2632	0.61	0/3573
1	D	0.51	0/2611	0.60	0/3541
All	All	0.51	0/10562	0.60	0/14330

There are no bond length outliers.

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	2579	0	2529	22	0
1	B	2629	0	2582	17	0
1	C	2577	0	2527	14	0
1	D	2557	0	2506	15	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
3	A	384	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	292	0	0	3	0
3	C	379	0	0	6	0
3	D	289	0	0	3	0
All	All	11702	0	10156	66	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 3.

All (66) 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:D:127[A]:MET:CE	1:D:131:GLN:HB2	2.25	0.67
1:D:127[A]:MET:HE2	1:D:131:GLN:HB2	1.75	0.66
1:C:208:SER:H	1:C:211:GLN:HE21	1.45	0.63
1:B:208:SER:H	1:B:211:GLN:HE21	1.46	0.62
1:A:208:SER:H	1:A:211:GLN:HE21	1.47	0.61
1:D:208:SER:H	1:D:211:GLN:HE21	1.46	0.61
1:A:160:ALA:HB1	1:D:223[A]:MET:HG2	1.85	0.59
1:A:337:ALA:HB2	3:A:632:HOH:O	2.02	0.59
1:C:191:VAL:HG21	3:C:502:HOH:O	2.05	0.56
1:B:148:GLY:HA2	3:B:540:HOH:O	2.06	0.55
1:B:185:PRO:HD2	3:B:515:HOH:O	2.08	0.54
1:D:104:LEU:HD21	1:D:134:ILE:HD11	1.90	0.53
1:A:185:PRO:HD2	3:A:617:HOH:O	2.06	0.53
1:A:179:THR:HG23	1:A:313:VAL:HG12	1.89	0.53
1:A:314:HIS:HD2	3:A:629:HOH:O	1.92	0.53
1:C:200:PRO:HA	1:C:298:CYS:SG	2.50	0.52
1:A:107:VAL:HG12	3:A:706:HOH:O	2.10	0.51
1:C:185:PRO:HD2	3:C:543:HOH:O	2.10	0.50
1:D:104:LEU:HD21	1:D:134:ILE:CD1	2.41	0.50
1:A:104:LEU:HD21	1:A:134:ILE:HD11	1.94	0.49
1:A:156[B]:MET:HB3	1:A:330:LEU:HB2	1.94	0.49
1:D:185:PRO:HD2	3:D:502:HOH:O	2.13	0.48
1:D:177:LEU:HD21	1:D:287:ILE:HG12	1.94	0.48
1:C:344:HIS:HE1	3:C:677:HOH:O	1.97	0.48
1:C:156[B]:MET:HB3	1:C:330:LEU:HB2	1.96	0.47
1:A:33:PRO:HD2	3:A:670:HOH:O	2.14	0.47
1:B:127[B]:MET:HG2	1:B:196:LEU:CD2	2.44	0.47
1:A:62:TYR:CD1	1:C:248:PHE:HB2	2.51	0.46
1:A:156[A]:MET:HB2	1:A:330:LEU:HB2	1.97	0.46
1:B:127[A]:MET:HG2	1:B:196:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156[A]:MET:HB2	1:C:330:LEU:HB2	1.99	0.45
1:A:31:SER:HB2	1:A:295:VAL:HG12	1.99	0.45
1:B:228[B]:MET:SD	1:B:275:ILE:HD11	2.56	0.45
1:D:33:PRO:HA	3:D:626:HOH:O	2.15	0.45
1:A:156[A]:MET:HG3	1:A:332:ARG:HB2	2.00	0.44
1:B:127[B]:MET:HA	1:B:130:TYR:CD2	2.52	0.44
1:D:344:HIS:HD2	3:D:643:HOH:O	2.00	0.44
1:D:127[B]:MET:HA	1:D:130:TYR:CD2	2.53	0.44
1:A:344:HIS:HB3	1:B:258:GLY:HA2	1.98	0.44
1:A:156[A]:MET:HE1	3:A:645:HOH:O	2.18	0.44
1:C:314:HIS:HB2	3:C:622:HOH:O	2.18	0.43
1:B:344:HIS:HE1	3:B:608:HOH:O	2.01	0.43
1:A:344:HIS:HD2	3:A:703:HOH:O	2.01	0.43
1:C:154:GLN:HB3	1:C:156[A]:MET:CE	2.49	0.43
1:C:39:LEU:HD13	1:C:85[B]:ARG:HG3	1.99	0.43
1:D:154:GLN:HB3	1:D:156:MET:CE	2.48	0.43
1:C:179[A]:THR:HG23	1:C:313:VAL:HG12	2.00	0.43
1:C:208:SER:H	1:C:211:GLN:NE2	2.16	0.43
1:B:148:GLY:HA3	1:B:154:GLN:NE2	2.34	0.42
1:B:154:GLN:HB3	1:B:156:MET:CE	2.49	0.42
1:D:156:MET:HB2	1:D:330:LEU:HB2	2.02	0.42
1:A:208:SER:H	1:A:211:GLN:NE2	2.17	0.42
1:B:75:ALA:HB1	1:B:137[A]:CYS:SG	2.59	0.42
1:B:156:MET:HB2	1:B:330:LEU:HB2	2.02	0.42
1:B:127[B]:MET:HG2	1:B:196:LEU:HD22	2.02	0.41
1:A:104:LEU:HD21	1:A:134:ILE:CD1	2.49	0.41
1:B:126:PRO:HB3	1:B:129:ARG:HH21	1.85	0.41
2:C:401:ACY:H2	3:C:622:HOH:O	2.20	0.41
1:D:75:ALA:HB1	1:D:137[A]:CYS:SG	2.60	0.41
1:D:210:ARG:HA	1:D:213:VAL:HG22	2.02	0.41
1:C:265:ILE:HG23	3:C:514[B]:HOH:O	2.21	0.41
1:A:199:ASP:HB2	1:A:328:ARG:HB2	2.02	0.41
1:A:122:ALA:HB1	1:A:331:SER:HB2	2.03	0.40
1:A:344:HIS:HE1	3:A:642:HOH:O	2.05	0.40
1:B:49[B]:LEU:HD21	1:B:104:LEU:CD2	2.51	0.40
1:B:223:MET:HB3	1:B:282:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 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	332/358 (93%)	324 (98%)	7 (2%)	1 (0%)	41	31
1	B	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
1	C	332/358 (93%)	324 (98%)	7 (2%)	1 (0%)	41	31
1	D	326/358 (91%)	322 (99%)	4 (1%)	0	100	100
All	All	1327/1432 (93%)	1302 (98%)	23 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	171	SER
1	A	171	SER

### 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	274/293 (94%)	271 (99%)	3 (1%)	73	73
1	B	279/293 (95%)	271 (97%)	8 (3%)	42	35
1	C	274/293 (94%)	269 (98%)	5 (2%)	59	55
1	D	271/293 (92%)	266 (98%)	5 (2%)	59	55
All	All	1098/1172 (94%)	1077 (98%)	21 (2%)	67	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	34	GLU
1	A	329	PHE
1	B	51[A]	ARG
1	B	51[B]	ARG
1	B	240	GLU
1	B	269	GLN
1	B	310[A]	ARG
1	B	310[B]	ARG
1	B	314[A]	HIS
1	B	314[B]	HIS
1	C	51[A]	ARG
1	C	51[B]	ARG
1	C	179[A]	THR
1	C	179[B]	THR
1	C	232	THR
1	D	34	GLU
1	D	85	ARG
1	D	314[A]	HIS
1	D	314[B]	HIS
1	D	329	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	314	HIS
1	A	344	HIS
1	B	106	GLN
1	B	211	GLN
1	B	344	HIS
1	C	211	GLN
1	C	314	HIS
1	C	344	HIS
1	D	211	GLN
1	D	344	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	ACY	D	401	-	3,3,3	1.76	1 (33%)	3,3,3	2.65	2 (66%)
2	ACY	A	401	-	3,3,3	0.09	0	3,3,3	1.27	0
2	ACY	C	401	-	3,3,3	0.58	0	3,3,3	0.94	0
2	ACY	B	401	-	3,3,3	0.65	0	3,3,3	0.82	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ACY	O-C	2.47	1.33	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ACY	OXT-C-CH3	3.51	129.75	115.05
2	D	401	ACY	O-C-CH3	-2.87	110.74	122.53

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
2	C	401	ACY	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, 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	329/358 (91%)	-0.07	12 (3%) 42 45	18, 28, 53, 103	0
1	B	329/358 (91%)	0.63	43 (13%) 3 3	21, 36, 85, 119	6 (1%)
1	C	328/358 (91%)	0.04	17 (5%) 27 30	19, 28, 61, 95	0
1	D	322/358 (89%)	0.46	30 (9%) 8 10	22, 35, 72, 99	0
All	All	1308/1432 (91%)	0.27	102 (7%) 13 14	18, 32, 69, 119	6 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	VAL	14.4
1	B	173	VAL	12.3
1	B	172	ALA	10.5
1	B	35	VAL	10.0
1	B	161	MET	9.7
1	D	173	VAL	9.5
1	B	165	SER	9.0
1	D	172	ALA	8.9
1	B	166	GLN	8.6
1	A	35	VAL	8.6
1	D	36	SER	8.3
1	B	162	SER	8.2
1	B	36	SER	7.8
1	C	35	VAL	7.5
1	B	32	ASP	7.5
1	C	165	SER	7.3
1	B	163	ALA	7.2
1	B	168	SER	7.2
1	D	30	GLU	7.1
1	C	170	GLY	6.6
1	D	168	SER	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	318	ILE	6.5
1	D	241	GLY	6.3
1	B	34	GLU	6.0
1	C	34	GLU	5.9
1	A	30	GLU	5.8
1	B	160	ALA	5.8
1	B	169	LEU	5.7
1	D	318	ILE	5.6
1	D	160	ALA	5.5
1	D	34	GLU	5.4
1	B	277	ALA	5.4
1	A	34	GLU	5.4
1	D	170	GLY	5.3
1	B	30	GLU	5.2
1	C	172	ALA	5.2
1	B	323	PHE	5.0
1	B	31	SER	5.0
1	D	323	PHE	4.9
1	D	320	ALA	4.7
1	B	164	HIS	4.7
1	D	32	ASP	4.5
1	B	271	LEU	4.5
1	C	166	GLN	4.5
1	C	162	SER	4.5
1	B	170	GLY	4.4
1	D	169	LEU	4.4
1	A	32	ASP	4.3
1	C	32	ASP	4.2
1	B	171	SER	4.1
1	B	273	ARG	4.1
1	C	164	HIS	4.1
1	D	235	GLU	4.0
1	A	107	VAL	4.0
1	D	240	GLU	3.9
1	B	320	ALA	3.7
1	D	239	ALA	3.7
1	C	31	SER	3.7
1	B	175	LEU	3.6
1	A	31	SER	3.6
1	B	240	GLU	3.6
1	A	162	SER	3.5
1	D	269	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	271	LEU	3.5
1	D	171	SER	3.5
1	B	167	THR	3.4
1	A	165	SER	3.3
1	B	235	GLU	3.3
1	D	231	THR	3.2
1	B	278	PRO	3.1
1	B	241	GLY	3.1
1	A	166	GLN	3.1
1	C	33	PRO	3.1
1	C	169	LEU	3.1
1	A	36	SER	3.0
1	B	269	GLN	3.0
1	A	170	GLY	3.0
1	D	33	PRO	3.0
1	C	171	SER	2.7
1	D	270	ASP	2.7
1	D	277	ALA	2.6
1	B	33	PRO	2.6
1	D	31	SER	2.6
1	C	163	ALA	2.6
1	B	201	ARG	2.6
1	A	33	PRO	2.5
1	B	159	SER	2.5
1	B	239	ALA	2.4
1	C	167	THR	2.4
1	B	281	GLU	2.4
1	B	270	ASP	2.4
1	D	273	ARG	2.3
1	D	278	PRO	2.3
1	C	168	SER	2.3
1	B	321	PRO	2.2
1	B	275	ILE	2.2
1	D	201	ARG	2.2
1	B	177	LEU	2.2
1	B	276	SER	2.2
1	C	161	MET	2.1
1	B	248	PHE	2.1
1	D	159	SER	2.1

## 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
2	ACY	B	401	4/4	0.90	0.15	37,40,40,43	0
2	ACY	D	401	4/4	0.94	0.14	44,47,49,49	0
2	ACY	A	401	4/4	0.96	0.10	30,31,32,36	0
2	ACY	C	401	4/4	0.97	0.10	30,34,36,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.