Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 03:52 am BST

PDB ID	:	6F2A
Title	:	Crystal structure of the complex Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO1 with Fe(II)/Lysine
Authors	:	Isabet, T.; Stura, E.A.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on	:	2017-11-24
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

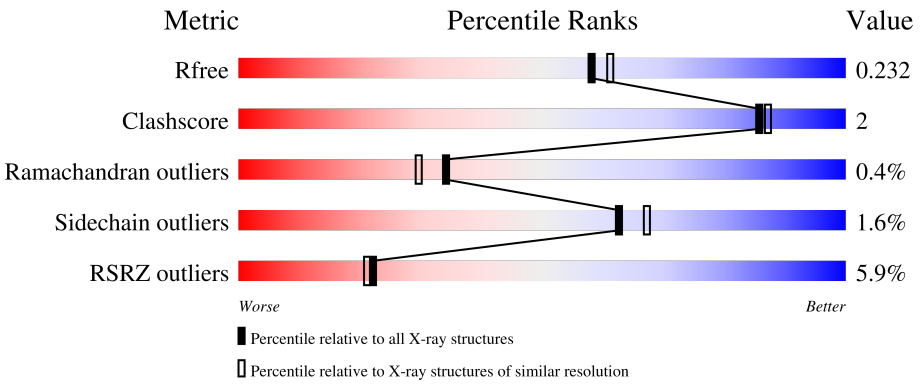
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	3% 84% 7% 9%
1	B	358	8% 84% 6% • 9%
1	C	358	4% 86% 5% 9%
1	D	358	6% 86% • 9%

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
4	ACY	C	403	-	X	-	-
4	ACY	C	404	-	X	-	-
4	ACY	D	403	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10848 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.

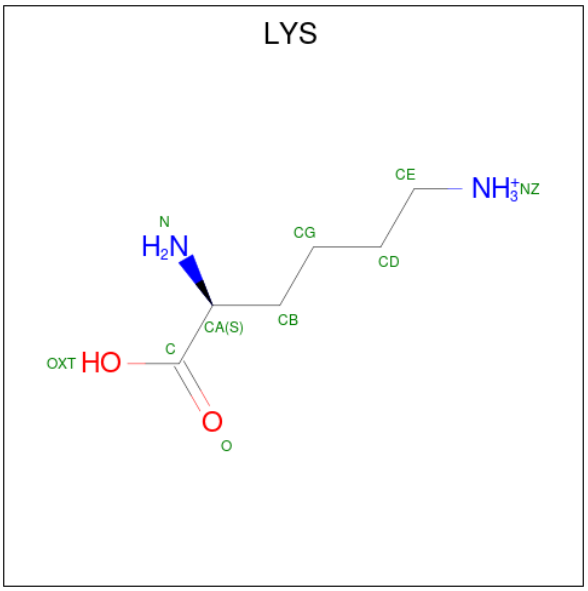
- Molecule 1 is a protein called L-lysine 3-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	325	2525	1585	454	471	15	0	4	0
1	B	324	2529	1587	453	473	16	0	5	0
1	C	326	2513	1579	446	473	15	0	2	0
1	D	324	2500	1570	448	468	14	0	1	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

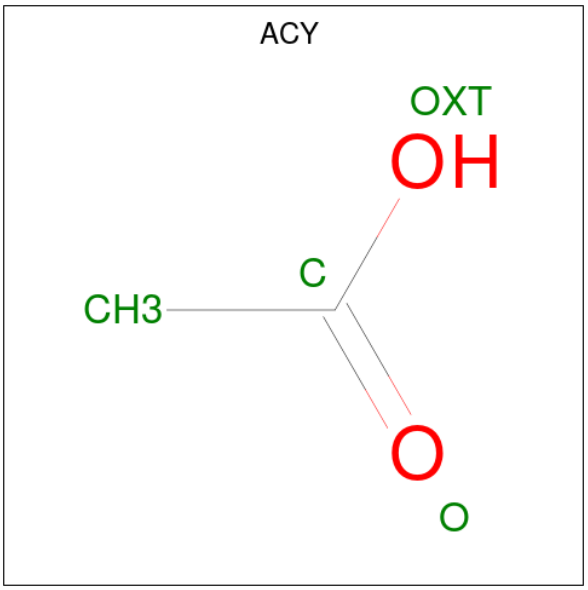
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	6	2	2	0	0
			Total	C	N	O		
3	A	1	10	6	2	2	0	0
			Total	C	N	O		
3	B	1	10	6	2	2	0	0
			Total	C	N	O		
3	C	1	10	6	2	2	0	0
			Total	C	N	O		
3	D	1	10	6	2	2	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 is water.

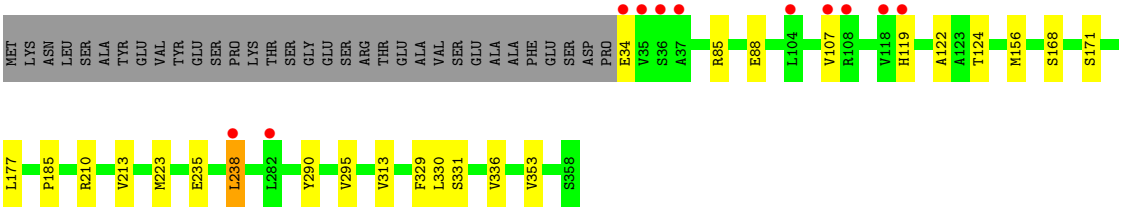
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	197	197	197	0	0
			Total	O		
6	B	150	150	150	0	0
			Total	O		
6	C	202	202	202	0	0
			Total	O		
6	D	157	157	157	0	0

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.

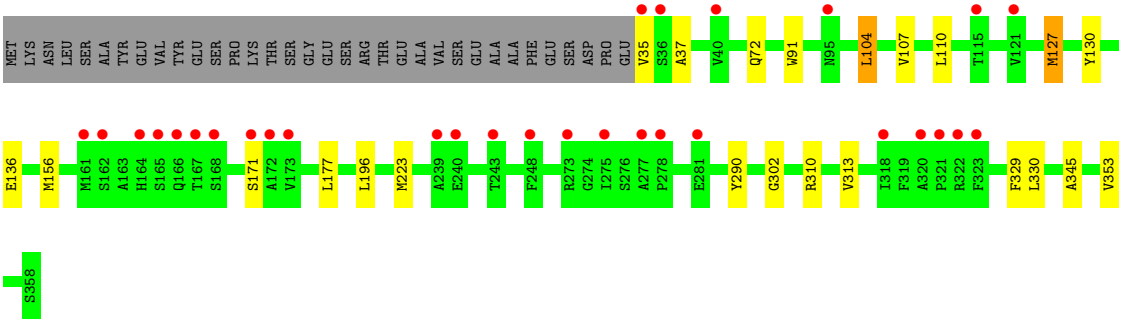
• Molecule 1: L-lysine 3-hydroxylase

Chain A:



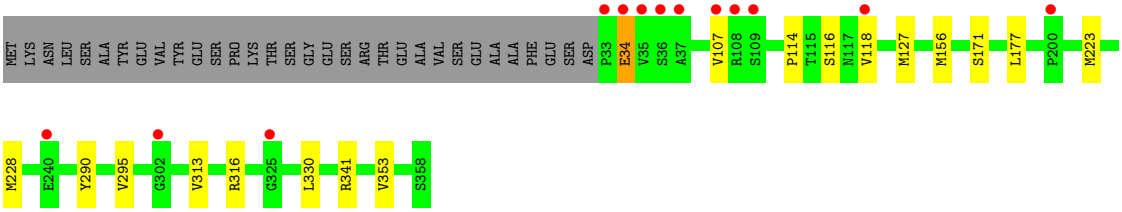
• Molecule 1: L-lysine 3-hydroxylase

Chain B:



• Molecule 1: L-lysine 3-hydroxylase

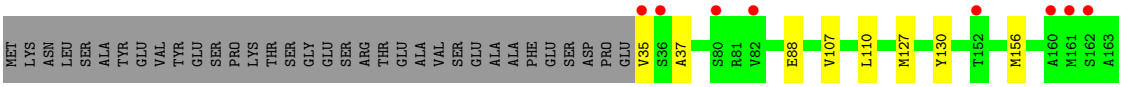
Chain C:

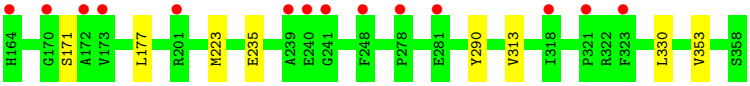


• Molecule 1: L-lysine 3-hydroxylase

Chain D:

6%
86%
9%


MET LYS ASN LEU SER ALA TYR GLU VAL TYR GLU SER PRO LYS THR SER GLY GLU SER ARG THR GLU ALA VAL SER GLU ALA ALA PHE GLU SER ASP PRO GLU
V35 S36 A37 S80 R81 V82 E88 V107 L110 M127 Y130 T152 M156 A160 M161 S162 A163


H164 G170 S171 A172 V173 L177 R201 M223 E235 A239 E240 G241 F248 P278 E281 Y290 V313 I318 P321 R322 F323 L330 V353 S358

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.94Å 67.02Å 110.75Å 107.48° 102.76° 93.74°	Depositor
Resolution (Å)	20.16 – 2.00 47.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.16-2.00) 98.0 (47.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.203 , 0.231 0.204 , 0.232	Depositor DCC
R_{free} test set	4963 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10848	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, ACY, FE2

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	0.53	0/2580	0.66	0/3504
1	B	0.50	0/2583	0.64	0/3506
1	C	0.51	0/2568	0.64	0/3489
1	D	0.50	0/2554	0.64	0/3468
All	All	0.51	0/10285	0.65	0/13967

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	2525	0	2473	14	0
1	B	2529	0	2485	12	0
1	C	2513	0	2462	11	0
1	D	2500	0	2461	8	0
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	A	20	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	0	0
3	C	10	0	12	0	0
3	D	10	0	12	0	0
4	A	8	0	6	1	0
4	C	8	0	6	1	0
4	D	4	0	3	0	0
5	A	1	0	0	1	0
6	A	197	0	0	1	0
6	B	150	0	0	0	0
6	C	202	0	0	2	0
6	D	157	0	0	0	0
All	All	10848	0	9956	45	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 2.

All (45) 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:107:VAL:HG11	1:B:110:LEU:HD13	1.80	0.63
1:D:107:VAL:HG11	1:D:110:LEU:HD13	1.81	0.63
1:C:223[B]:MET:HG3	1:C:228:MET:CE	2.28	0.62
4:A:404:ACY:H2	1:B:91:TRP:HB2	1.84	0.60
1:A:235:GLU:O	1:A:238:LEU:HG	2.02	0.59
1:C:34:GLU:HB3	1:C:295:VAL:HB	1.85	0.59
1:C:223[B]:MET:HG3	1:C:228:MET:HE1	1.84	0.58
1:C:107:VAL:HG21	1:C:127:MET:HB2	1.84	0.58
1:D:177:LEU:HD13	1:D:290:TYR:CE1	2.39	0.58
1:B:177:LEU:HD13	1:B:290:TYR:CE1	2.39	0.57
1:C:177:LEU:HD13	1:C:290:TYR:CE1	2.39	0.56
1:D:35:VAL:HG13	1:D:37:ALA:H	1.70	0.56
1:A:34:GLU:HB3	1:A:295:VAL:HB	1.86	0.56
1:A:177:LEU:HD13	1:A:290:TYR:CE1	2.40	0.55
1:A:156[A]:MET:CE	1:A:168:SER:HB2	2.39	0.53
1:C:177:LEU:HD11	1:C:313:VAL:HG23	1.92	0.52
1:A:177:LEU:HD11	1:A:313:VAL:HG23	1.92	0.52
1:D:177:LEU:HD11	1:D:313:VAL:HG23	1.92	0.51
1:A:85[B]:ARG:NH1	1:A:88:GLU:HG3	2.26	0.51
1:B:177:LEU:HD11	1:B:313:VAL:HG23	1.94	0.50
1:B:35:VAL:HG13	1:B:37:ALA:H	1.76	0.50
1:C:223[B]:MET:CG	1:C:228:MET:HE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HB2	1:B:330:LEU:HB2	1.96	0.47
1:C:156:MET:HB2	1:C:330:LEU:HB2	1.97	0.47
1:D:156:MET:HB2	1:D:330:LEU:HB2	1.96	0.47
1:A:122:ALA:HB1	1:A:331:SER:HB2	1.95	0.46
1:B:104:LEU:HB2	1:B:302:GLY:O	2.16	0.46
1:A:185:PRO:HD2	6:A:503:HOH:O	2.15	0.46
1:B:127[B]:MET:HA	1:B:130:TYR:CD2	2.51	0.45
1:A:119:HIS:HD2	6:C:526:HOH:O	1.99	0.44
1:B:110:LEU:HD11	1:B:196:LEU:HD23	1.99	0.44
4:C:404:ACY:H2	1:D:88:GLU:HA	2.00	0.44
1:D:127:MET:HA	1:D:130:TYR:CD2	2.53	0.43
1:C:114:PRO:HB2	1:C:116:SER:O	2.18	0.43
1:C:223[B]:MET:HG3	1:C:228:MET:HE2	1.98	0.43
1:C:316:ARG:HD3	6:C:608:HOH:O	2.19	0.43
1:B:345:ALA:HB1	1:B:353:VAL:HG13	2.02	0.42
1:A:156[A]:MET:HB2	1:A:330:LEU:HB2	2.02	0.42
1:A:210:ARG:HA	1:A:213:VAL:HG22	2.02	0.42
1:D:107:VAL:CG1	1:D:110:LEU:HD13	2.49	0.42
1:A:85[B]:ARG:HH11	1:A:88:GLU:HG3	1.83	0.41
1:B:127[A]:MET:HA	1:B:130:TYR:CD2	2.55	0.41
1:B:72:GLN:HA	1:B:136:GLU:HB3	2.03	0.41
1:A:156[B]:MET:SD	1:A:330:LEU:HD12	2.61	0.40
1:A:336:VAL:HG11	5:A:406:CL:CL	2.58	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	327/358 (91%)	323 (99%)	3 (1%)	1 (0%)	41	37
1	B	327/358 (91%)	324 (99%)	2 (1%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	326/358 (91%)	322 (99%)	2 (1%)	2 (1%)	25	19
1	D	323/358 (90%)	321 (99%)	1 (0%)	1 (0%)	41	37
All	All	1303/1432 (91%)	1290 (99%)	8 (1%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	VAL
1	B	171	SER
1	C	171	SER
1	A	171	SER
1	D	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	266/293 (91%)	260 (98%)	6 (2%)	50	53
1	B	267/293 (91%)	261 (98%)	6 (2%)	52	55
1	C	266/293 (91%)	263 (99%)	3 (1%)	73	78
1	D	264/293 (90%)	261 (99%)	3 (1%)	73	78
All	All	1063/1172 (91%)	1045 (98%)	18 (2%)	62	65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	VAL
1	A	124	THR
1	A	223	MET
1	A	238	LEU
1	A	329	PHE
1	A	353	VAL
1	B	104	LEU

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Mol	Chain	Res	Type
1	B	127[A]	MET
1	B	127[B]	MET
1	B	223	MET
1	B	310	ARG
1	B	329	PHE
1	C	34	GLU
1	C	341	ARG
1	C	353	VAL
1	D	223	MET
1	D	235	GLU
1	D	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	269	GLN
1	A	283	GLN
1	A	344	HIS
1	B	283	GLN
1	C	283	GLN
1	D	269	GLN
1	D	283	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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	LYS	A	403	-	8,9,9	0.77	0	9,10,10	0.81	0
3	LYS	B	402	-	8,9,9	0.82	0	9,10,10	0.66	0
4	ACY	C	404	-	3,3,3	1.91	1 (33%)	3,3,3	2.44	2 (66%)
3	LYS	D	402	2	8,9,9	0.80	0	9,10,10	0.73	0
4	ACY	A	405	-	3,3,3	1.70	0	3,3,3	2.89	2 (66%)
3	LYS	C	402	-	8,9,9	0.63	0	9,10,10	0.72	0
4	ACY	A	404	-	3,3,3	0.48	0	3,3,3	1.18	0
4	ACY	D	403	-	3,3,3	1.96	2 (66%)	3,3,3	2.36	2 (66%)
3	LYS	A	402	2	8,9,9	0.74	0	9,10,10	0.74	0
4	ACY	C	403	-	3,3,3	1.94	1 (33%)	3,3,3	2.34	2 (66%)

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	LYS	A	403	-	-	5/9/9/9	-
3	LYS	B	402	-	-	0/9/9/9	-
3	LYS	D	402	2	-	0/9/9/9	-
3	LYS	C	402	-	-	0/9/9/9	-
3	LYS	A	402	2	-	0/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	ACY	O-C	2.94	1.35	1.22
4	C	404	ACY	O-C	2.62	1.34	1.22
4	D	403	ACY	O-C	2.43	1.33	1.22
4	D	403	ACY	OXT-C	-2.17	1.20	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	405	ACY	O-C-CH3	-3.70	107.93	122.33
4	A	405	ACY	OXT-C-CH3	3.35	129.04	115.18
4	C	404	ACY	OXT-C-CH3	3.14	128.14	115.18
4	D	403	ACY	OXT-C-CH3	3.11	128.04	115.18
4	C	403	ACY	OXT-C-CH3	3.11	128.02	115.18
4	C	404	ACY	O-C-CH3	-2.80	111.43	122.33
4	D	403	ACY	O-C-CH3	-2.58	112.28	122.33
4	C	403	ACY	O-C-CH3	-2.49	112.64	122.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	LYS	O-C-CA-N
3	A	403	LYS	OXT-C-CA-N
3	A	403	LYS	CE-CD-CG-CB
3	A	403	LYS	OXT-C-CA-CB
3	A	403	LYS	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	ACY	1	0
4	A	404	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 (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, 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	325/358 (90%)	0.00	11 (3%)	45	44	29, 44, 69, 95	0
1	B	324/358 (90%)	0.45	30 (9%)	8	8	34, 53, 80, 99	0
1	C	326/358 (91%)	0.11	13 (3%)	38	37	32, 47, 74, 101	0
1	D	324/358 (90%)	0.38	22 (6%)	17	16	34, 51, 77, 108	0
All	All	1299/1432 (90%)	0.24	76 (5%)	22	21	29, 49, 77, 108	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	SER	9.6
1	D	35	VAL	7.7
1	C	36	SER	6.3
1	B	164	HIS	5.8
1	B	172	ALA	5.7
1	D	239	ALA	5.5
1	A	35	VAL	5.5
1	C	33	PRO	5.2
1	B	173	VAL	5.1
1	B	36	SER	5.0
1	B	161	MET	4.5
1	D	36	SER	4.4
1	C	107	VAL	4.4
1	B	171	SER	4.3
1	D	173	VAL	4.2
1	B	277	ALA	4.1
1	D	323	PHE	4.0
1	D	164	HIS	3.9
1	D	241	GLY	3.7
1	D	172	ALA	3.7
1	A	34	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	240	GLU	3.6
1	D	278	PRO	3.4
1	D	162	SER	3.3
1	C	240	GLU	3.3
1	D	201	ARG	3.3
1	C	35	VAL	3.3
1	D	161	MET	3.2
1	B	278	PRO	3.2
1	D	318	ILE	3.2
1	B	323	PHE	3.2
1	D	160	ALA	3.2
1	B	321	PRO	3.1
1	B	166	GLN	3.0
1	B	239	ALA	3.0
1	B	318	ILE	3.0
1	C	34	GLU	3.0
1	B	162	SER	2.9
1	B	243	THR	2.9
1	C	109	SER	2.8
1	C	108	ARG	2.7
1	A	37	ALA	2.7
1	A	104	LEU	2.7
1	B	115	THR	2.7
1	C	302	GLY	2.7
1	A	238	LEU	2.7
1	B	95[A]	ASN	2.6
1	D	321	PRO	2.6
1	C	118	VAL	2.5
1	C	325	GLY	2.5
1	B	168	SER	2.5
1	B	248	PHE	2.5
1	A	118	VAL	2.4
1	B	281	GLU	2.4
1	B	35	VAL	2.4
1	C	200	PRO	2.4
1	B	322	ARG	2.3
1	B	275	ILE	2.3
1	D	82	VAL	2.3
1	D	170	GLY	2.3
1	D	240	GLU	2.3
1	A	107	VAL	2.3
1	A	108	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	152	THR	2.2
1	B	121	VAL	2.2
1	A	119	HIS	2.2
1	B	273	ARG	2.2
1	B	320	ALA	2.2
1	D	80	SER	2.2
1	D	248	PHE	2.1
1	D	281	GLU	2.1
1	B	40	VAL	2.1
1	B	167	THR	2.1
1	C	37	ALA	2.1
1	B	165	SER	2.0
1	A	282	LEU	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 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, 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	B-factors(Å^2)	Q<0.9
3	LYS	A	403	10/10	0.73	0.27	84,98,115,117	0
2	FE2	C	401	1/1	0.78	0.14	99,99,99,99	0
3	LYS	A	402	10/10	0.79	0.17	47,52,59,59	0
2	FE2	D	401	1/1	0.83	0.07	112,112,112,112	0
4	ACY	C	404	4/4	0.83	0.18	52,56,58,58	0
3	LYS	D	402	10/10	0.84	0.15	48,66,73,76	0
2	FE2	A	401	1/1	0.84	0.25	104,104,104,104	0
4	ACY	C	403	4/4	0.86	0.15	74,76,76,77	0
3	LYS	B	402	10/10	0.86	0.24	57,67,74,76	0
3	LYS	C	402	10/10	0.88	0.12	49,51,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	B	401	1/1	0.89	0.13	107,107,107,107	0
5	CL	A	406	1/1	0.89	0.23	70,70,70,70	0
4	ACY	D	403	4/4	0.92	0.15	39,45,46,49	0
4	ACY	A	404	4/4	0.93	0.17	46,47,47,50	0
4	ACY	A	405	4/4	0.97	0.12	36,39,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.