



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:57 AM UTC

PDB ID : 6F2A / pdb_00006f2a
Title : Crystal structure of the complex Fe(II)/alpha-ketoglutarate dependent dioxxygenase 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

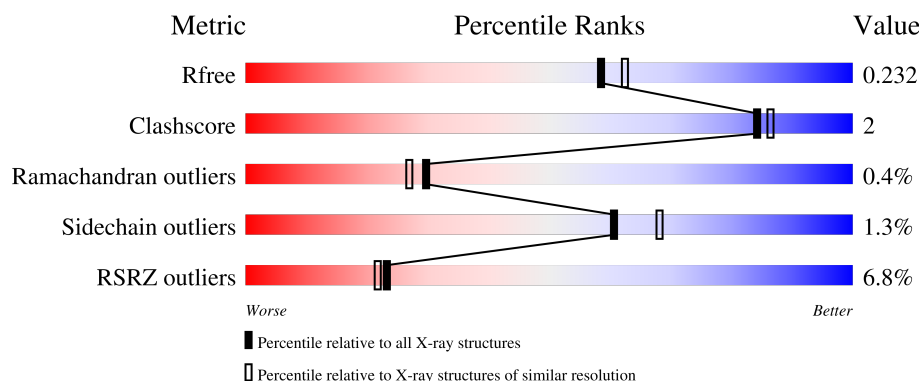
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	6% 82% 8% 9%
1	B	358	5% 83% 7% 9%
1	C	358	8% 84% 7% 9%
1	D	358	6% 84% 6% 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	A	405	-	X	-	-
4	ACY	C	403	-	X	-	-
4	ACY	C	404	-	X	-	-
4	ACY	D	403	-	X	-	-

2 Entry composition

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.

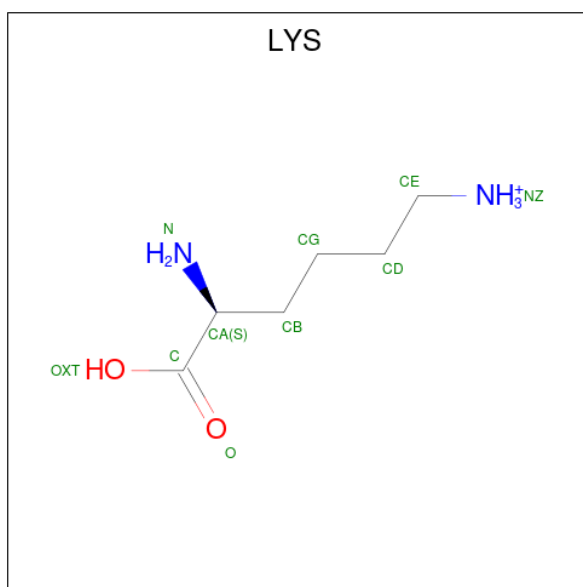
- Molecule 1 is a protein called L-lysine 3-hydroxylase.

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

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

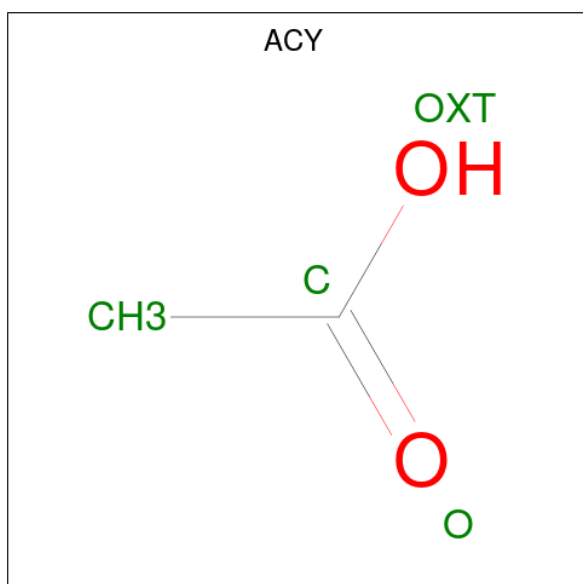
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

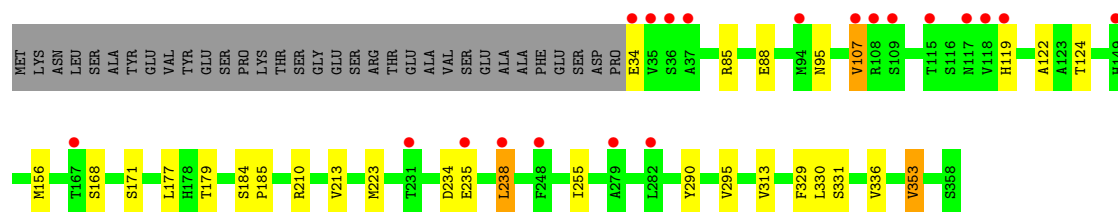
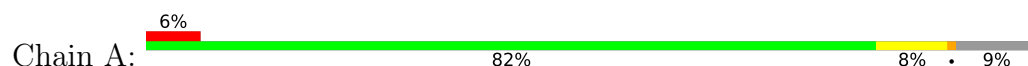
- Molecule 6 is water.

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

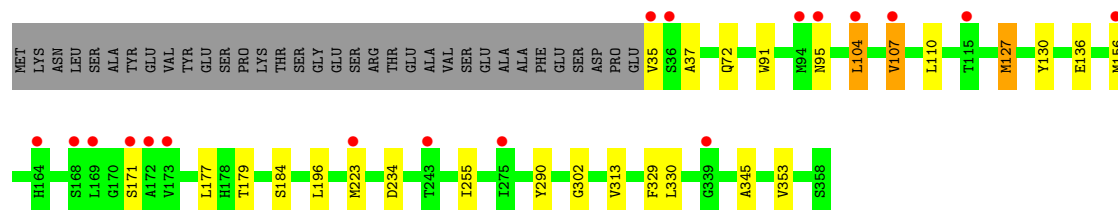
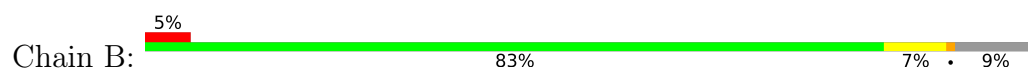
3 Residue-property plots [i](#)

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.

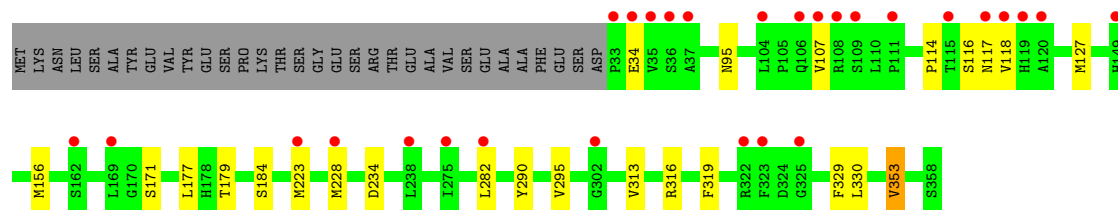
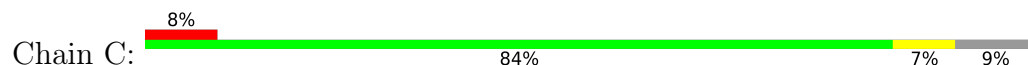
- Molecule 1: L-lysine 3-hydroxylase



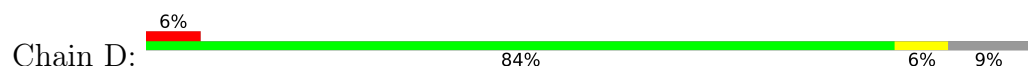
- Molecule 1: L-lysine 3-hydroxylase

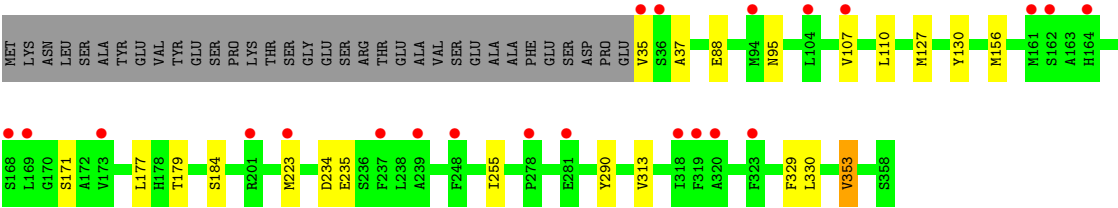


- Molecule 1: L-lysine 3-hydroxylase



- Molecule 1: L-lysine 3-hydroxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.94Å 67.02Å 110.75Å 107.48° 102.76° 93.74°	Depositor
Resolution (Å)	20.16 – 2.00 20.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.16-2.00) 98.2 (20.16-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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	0.86	0/2580	1.19	8/3504 (0.2%)
1	B	0.83	0/2583	1.19	5/3506 (0.1%)
1	C	0.85	0/2568	1.21	9/3489 (0.3%)
1	D	0.83	0/2554	1.20	7/3468 (0.2%)
All	All	0.84	0/10285	1.20	29/13967 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	PHE	CA-CB-CG	8.50	122.30	113.80
1	B	329	PHE	CA-CB-CG	8.16	121.96	113.80
1	D	95	ASN	CA-CB-CG	7.52	120.12	112.60
1	A	329	PHE	CA-CB-CG	7.21	121.01	113.80
1	C	95	ASN	CA-CB-CG	7.15	119.75	112.60
1	C	329	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	95	ASN	CA-CB-CG	6.64	119.24	112.60
1	D	179	THR	N-CA-C	-6.62	98.83	109.96
1	A	107	VAL	CB-CA-C	6.35	118.51	111.08
1	D	353	VAL	N-CA-CB	6.30	118.00	110.95
1	C	179	THR	N-CA-C	-6.26	100.31	110.20
1	B	179	THR	N-CA-C	-6.14	99.65	109.96
1	A	179	THR	N-CA-C	-6.10	99.72	109.96
1	C	117	ASN	CA-C-N	6.02	132.80	121.97
1	C	117	ASN	C-N-CA	6.02	132.80	121.97
1	C	353	VAL	N-CA-CB	5.95	117.61	110.95
1	A	353	VAL	N-CA-CB	5.89	117.54	110.95
1	A	234	ASP	CA-CB-CG	5.64	118.25	112.60
1	C	234	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	184	SER	N-CA-C	5.53	117.64	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	255	ILE	N-CA-C	-5.42	106.41	111.45
1	B	234	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	255	ILE	N-CA-C	-5.36	105.90	111.58
1	C	184	SER	N-CA-C	5.22	117.20	109.62
1	A	184	SER	N-CA-C	5.21	117.18	109.62
1	D	184	SER	N-CA-C	5.12	117.04	109.62
1	A	255	ILE	N-CA-C	-5.09	106.18	111.58
1	C	319	PHE	CA-CB-CG	5.06	118.86	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	15	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10848	0	9956	46	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 (46) 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:223[B]:MET:HG3	1:C:228:MET:HE1	1.71	0.72
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: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:223[B]:MET:CG	1:C:228:MET:HE1	2.33	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[A]:MET:HE2	1:C:282:LEU:HD22	1.95	0.48
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:156[A]:MET:HE1	1:A:168:SER:HB2	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	36	35
1	B	327/358 (91%)	324 (99%)	2 (1%)	1 (0%)	36	35
1	C	326/358 (91%)	322 (99%)	2 (1%)	2 (1%)	21	17
1	D	323/358 (90%)	321 (99%)	1 (0%)	1 (0%)	36	35
All	All	1303/1432 (91%)	1290 (99%)	8 (1%)	5 (0%)	30	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	VAL
1	B	171	SER

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Mol	Chain	Res	Type
1	C	171	SER
1	A	171	SER
1	D	171	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	266/293 (91%)	261 (98%)	5 (2%)	50	56
1	B	267/293 (91%)	260 (97%)	7 (3%)	40	44
1	C	266/293 (91%)	265 (100%)	1 (0%)	84	89
1	D	264/293 (90%)	261 (99%)	3 (1%)	65	73
All	All	1063/1172 (91%)	1047 (98%)	16 (2%)	61	64

All (16) 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	353	VAL
1	B	95[A]	ASN
1	B	95[B]	ASN
1	B	104	LEU
1	B	107	VAL
1	B	127[A]	MET
1	B	127[B]	MET
1	B	223	MET
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 (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	154	GLN
1	A	269	GLN
1	A	344	HIS
1	B	131	GLN
1	B	154	GLN
1	B	344	HIS
1	C	154	GLN
1	C	283	GLN
1	C	344	HIS
1	D	131	GLN
1	D	154	GLN
1	D	181	GLN
1	D	269	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 oligosaccharides 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	402	2	8,9,9	0.77	0	7,10,10	0.34	0
3	LYS	C	402	-	8,9,9	0.65	0	7,10,10	0.28	0
3	LYS	B	402	-	8,9,9	0.84	0	7,10,10	0.36	0
4	ACY	A	404	-	3,3,3	0.49	0	3,3,3	1.10	0
3	LYS	A	403	-	8,9,9	0.80	0	7,10,10	0.39	0
4	ACY	C	404	-	3,3,3	2.01	1 (33%)	3,3,3	2.40	2 (66%)
4	ACY	D	403	-	3,3,3	2.06	2 (66%)	3,3,3	2.33	2 (66%)
4	ACY	A	405	-	3,3,3	1.81	1 (33%)	3,3,3	2.82	2 (66%)
4	ACY	C	403	-	3,3,3	2.04	1 (33%)	3,3,3	2.30	2 (66%)
3	LYS	D	402	2	8,9,9	0.82	0	7,10,10	0.36	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	LYS	A	402	2	-	0/9/9/9	-
3	LYS	C	402	-	-	0/9/9/9	-
3	LYS	B	402	-	-	0/9/9/9	-
3	LYS	A	403	-	-	5/9/9/9	-
3	LYS	D	402	2	-	0/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	ACY	O-C	3.11	1.35	1.22
4	C	404	ACY	O-C	2.77	1.34	1.22
4	D	403	ACY	O-C	2.57	1.33	1.22
4	D	403	ACY	OXT-C	-2.27	1.20	1.30
4	A	405	ACY	O-C	2.09	1.31	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	ACY	O-C-CH3	-3.56	107.93	122.53
4	A	405	ACY	OXT-C-CH3	3.34	129.04	115.05
4	C	404	ACY	OXT-C-CH3	3.12	128.14	115.05
4	D	403	ACY	OXT-C-CH3	3.10	128.04	115.05
4	C	403	ACY	OXT-C-CH3	3.09	128.02	115.05
4	C	404	ACY	O-C-CH3	-2.71	111.43	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	ACY	O-C-CH3	-2.50	112.28	122.53
4	C	403	ACY	O-C-CH3	-2.41	112.64	122.53

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	A	404	ACY	1	0
4	C	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/358 (90%)	0.52	20 (6%) 26 25	17, 44, 69, 95	4 (1%)
1	B	324/358 (90%)	0.68	18 (5%) 30 29	21, 52, 80, 99	5 (1%)
1	C	326/358 (91%)	0.65	28 (8%) 16 15	20, 47, 74, 101	2 (0%)
1	D	324/358 (90%)	0.64	22 (6%) 23 22	20, 51, 77, 108	1 (0%)
All	All	1299/1432 (90%)	0.62	88 (6%) 23 22	17, 49, 77, 108	12 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	SER	6.8
1	D	35	VAL	5.8
1	A	35	VAL	5.6
1	C	36	SER	5.1
1	C	33	PRO	4.8
1	C	323	PHE	4.3
1	C	37	ALA	4.2
1	B	35	VAL	4.0
1	C	35	VAL	4.0
1	D	239	ALA	3.9
1	B	95[A]	ASN	3.9
1	B	243	THR	3.9
1	A	238	LEU	3.8
1	A	37	ALA	3.8
1	C	107	VAL	3.8
1	B	173	VAL	3.5
1	B	172	ALA	3.5
1	B	164	HIS	3.5
1	B	36	SER	3.5
1	A	107	VAL	3.3
1	C	108	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	119	HIS	3.3
1	D	162	SER	3.1
1	B	94[A]	MET	3.1
1	C	228	MET	3.1
1	A	118	VAL	3.0
1	A	115	THR	2.9
1	A	149[A]	HIS	2.9
1	C	118	VAL	2.8
1	A	34	GLU	2.8
1	B	168	SER	2.8
1	D	168	SER	2.8
1	D	248	PHE	2.8
1	D	223	MET	2.8
1	C	275	ILE	2.8
1	A	282	LEU	2.7
1	B	169	LEU	2.7
1	C	104	LEU	2.7
1	D	173	VAL	2.7
1	D	107	VAL	2.6
1	A	109	SER	2.6
1	C	322	ARG	2.6
1	C	119	HIS	2.6
1	C	169	LEU	2.5
1	C	223[A]	MET	2.5
1	A	231	THR	2.5
1	B	171	SER	2.5
1	D	104	LEU	2.5
1	A	94	MET	2.5
1	C	162	SER	2.5
1	D	278	PRO	2.5
1	C	325	GLY	2.5
1	A	235	GLU	2.4
1	B	223	MET	2.4
1	D	201	ARG	2.4
1	C	106	GLN	2.4
1	C	111	PRO	2.4
1	D	169	LEU	2.4
1	D	237	PHE	2.4
1	D	94	MET	2.4
1	C	115	THR	2.4
1	C	120	ALA	2.3
1	B	107	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	34	GLU	2.3
1	B	156	MET	2.3
1	A	167	THR	2.3
1	D	164	HIS	2.3
1	D	320	ALA	2.3
1	C	302	GLY	2.3
1	C	109	SER	2.2
1	A	117	ASN	2.2
1	B	275	ILE	2.2
1	B	104	LEU	2.2
1	C	149	HIS	2.2
1	A	108	ARG	2.2
1	B	115	THR	2.2
1	B	339	GLY	2.1
1	A	279	ALA	2.1
1	C	117	ASN	2.1
1	D	318	ILE	2.1
1	A	248	PHE	2.1
1	D	323	PHE	2.1
1	D	161	MET	2.1
1	D	319	PHE	2.1
1	D	281	GLU	2.0
1	D	36	SER	2.0
1	C	238	LEU	2.0
1	C	282	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	LYS	A	403	10/10	0.68	0.22	84,98,115,117	0
3	LYS	A	402	10/10	0.74	0.15	47,52,59,59	0
4	ACY	C	403	4/4	0.77	0.19	74,76,76,77	0
4	ACY	C	404	4/4	0.80	0.21	52,56,58,58	0
3	LYS	B	402	10/10	0.82	0.14	57,67,74,76	0
2	FE2	C	401	1/1	0.83	0.17	99,99,99,99	0
3	LYS	D	402	10/10	0.83	0.14	48,66,73,76	0
2	FE2	D	401	1/1	0.84	0.16	112,112,112,112	0
4	ACY	D	403	4/4	0.84	0.15	39,45,46,49	0
3	LYS	C	402	10/10	0.85	0.13	49,51,52,54	0
5	CL	A	406	1/1	0.86	0.16	70,70,70,70	0
2	FE2	A	401	1/1	0.91	0.20	104,104,104,104	0
4	ACY	A	405	4/4	0.91	0.10	36,39,40,42	0
2	FE2	B	401	1/1	0.91	0.11	107,107,107,107	0
4	ACY	A	404	4/4	0.92	0.14	46,47,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.