Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 05:02 am BST

PDB ID	:	6EXF
Title	:	Crystal structure of the complex Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO5 with Fe(II)/Lysine
Authors	:	Isabet, T.; Stura, E.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on	:	2017-11-08
Resolution	:	1.95 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:

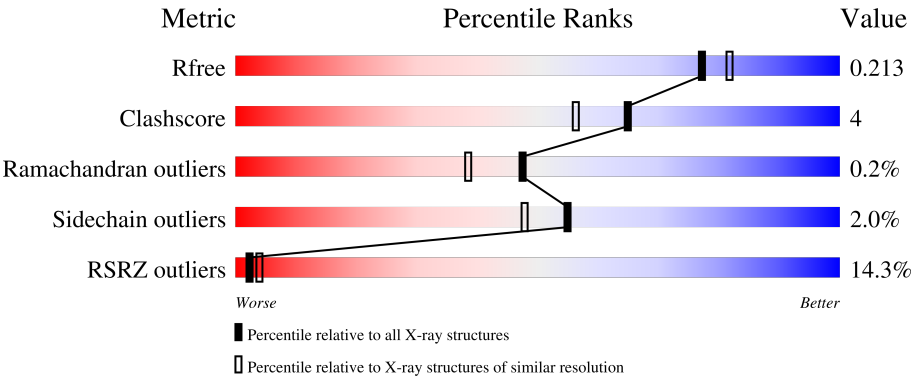
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	372	6% 85% 6% 8%
1	B	372	14% 74% 10% • 15%
1	C	372	20% 84% 11% 5%
1	D	372	12% 85% 8% 7%

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
3	LYS	B	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11784 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.

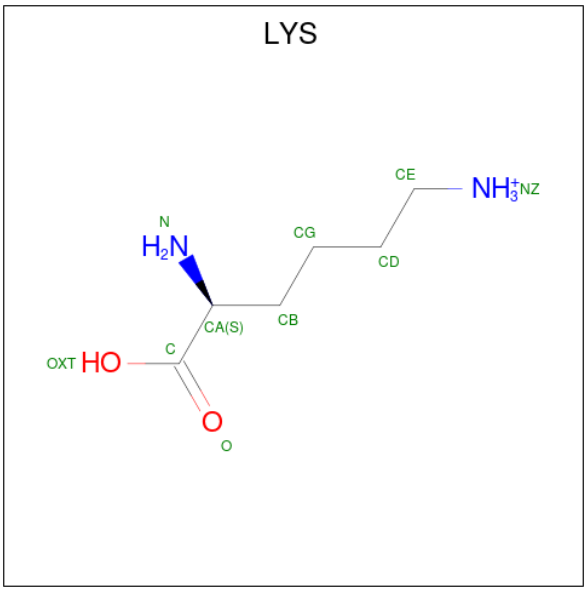
- Molecule 1 is a protein called L-lysine 4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	7	0
			2779	1766	480	520	13			
1	B	315	Total	C	N	O	S	0	5	0
			2548	1623	435	478	12			
1	C	352	Total	C	N	O	S	0	3	0
			2815	1787	481	535	12			
1	D	346	Total	C	N	O	S	0	4	0
			2771	1759	474	526	12			

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

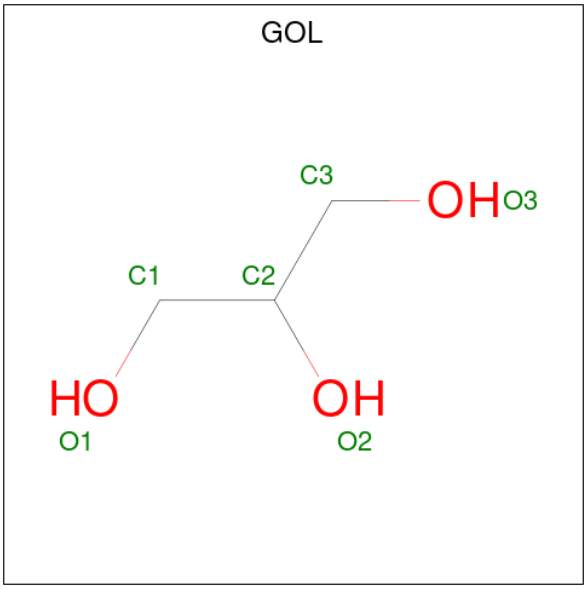
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

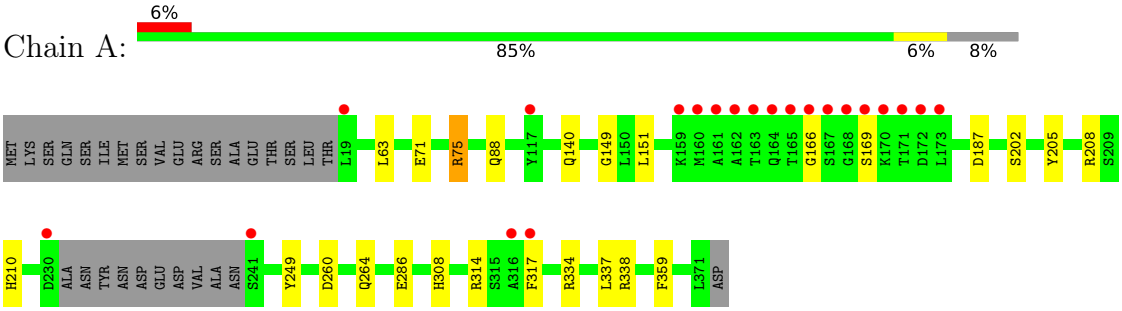
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	270	Total O 270 270	0	0
5	B	164	Total O 164 164	0	0
5	C	176	Total O 176 176	0	0
5	D	195	Total O 195 195	0	0

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.

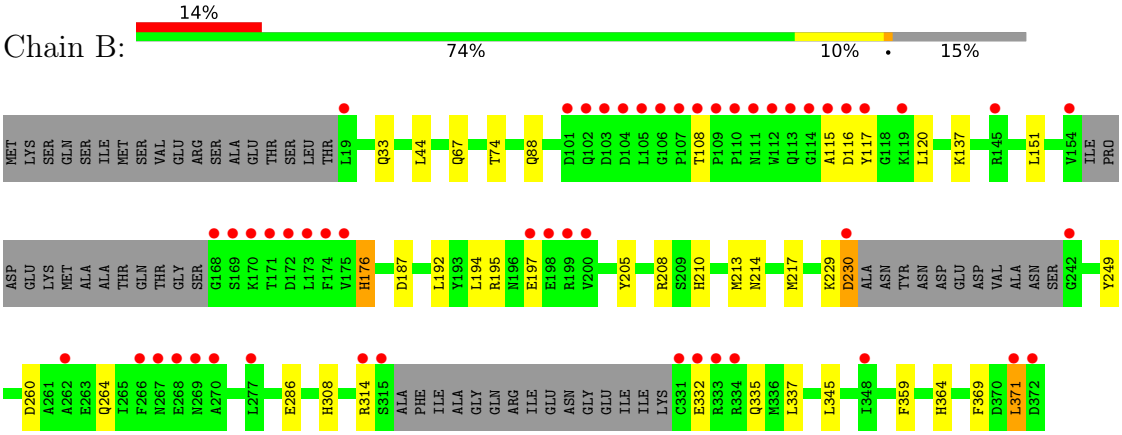
• Molecule 1: L-lysine 4-hydroxylase

Chain A:



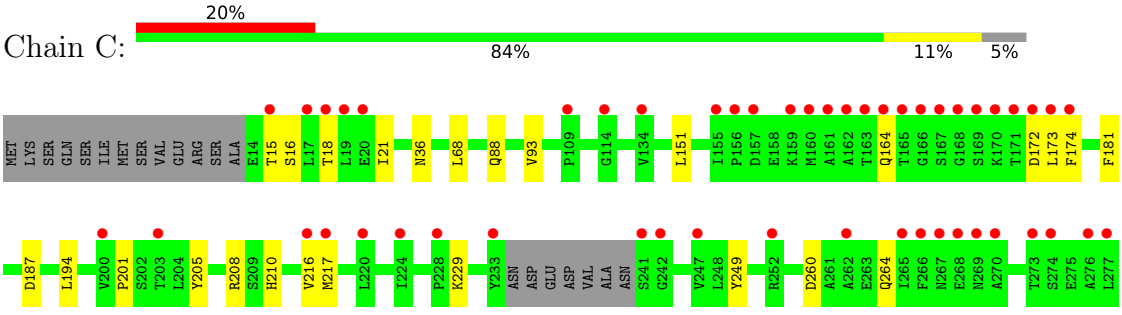
• Molecule 1: L-lysine 4-hydroxylase

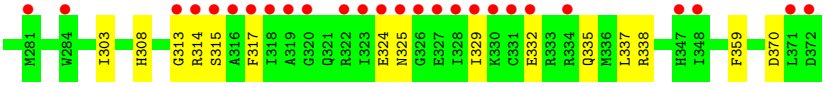
Chain B:



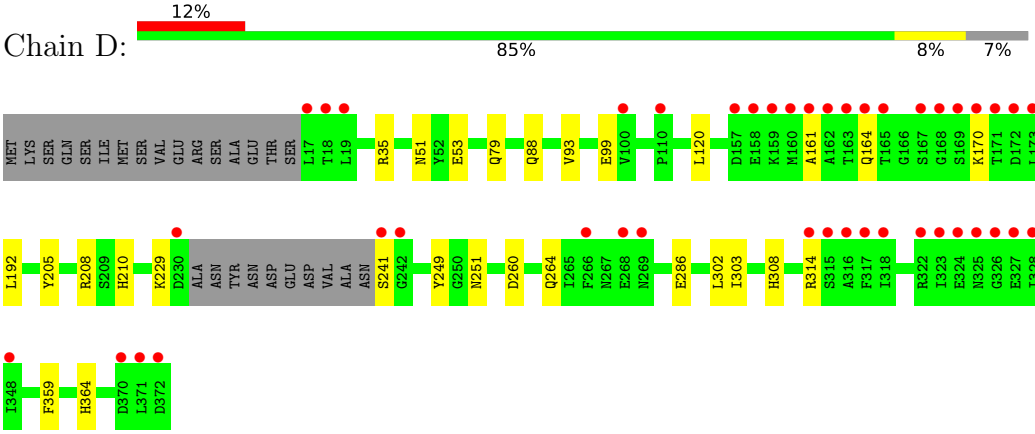
• Molecule 1: L-lysine 4-hydroxylase

Chain C:





- Molecule 1: L-lysine 4-hydroxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.72Å 99.62Å 165.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.55 – 1.95 48.33 – 1.95	Depositor EDS
% Data completeness (in resolution range)	68.8 (28.55-1.95) 68.8 (48.33-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.177 , 0.213 0.177 , 0.213	Depositor DCC
R_{free} test set	3790 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11784	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, GOL

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	0/2842	0.66	0/3844
1	B	0.51	0/2607	0.66	0/3528
1	C	0.49	0/2879	0.65	0/3896
1	D	0.49	0/2833	0.63	0/3833
All	All	0.50	0/11161	0.65	0/15101

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

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	2779	0	2728	21	0
1	B	2548	0	2478	28	0
1	C	2815	0	2748	24	0
1	D	2771	0	2707	19	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	2	0
3	C	10	0	12	1	0
3	D	10	0	12	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	A	270	0	0	0	0
5	B	164	0	0	0	0
5	C	176	0	0	0	0
5	D	195	0	0	0	0
All	All	11784	0	10737	88	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 4.

All (88) 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:67:GLN:HE22	1:C:36:ASN:HB3	1.47	0.79
1:D:205:TYR:OH	1:D:210:HIS:HE1	1.78	0.66
1:D:35:ARG:HD3	1:D:99:GLU:HG2	1.78	0.66
1:B:205:TYR:OH	1:B:210:HIS:HE1	1.79	0.66
1:C:205:TYR:OH	1:C:210:HIS:HE1	1.79	0.65
1:A:205:TYR:OH	1:A:210:HIS:HE1	1.80	0.63
1:C:260:ASP:H	1:C:264:GLN:HE21	1.46	0.62
1:A:260:ASP:H	1:A:264:GLN:HE21	1.45	0.62
1:B:176:HIS:CE1	3:B:402:LYS:HD2	2.36	0.61
1:A:166:GLY:H	3:A:403:LYS:HB3	1.69	0.57
1:D:164:GLN:HE22	1:D:174:PHE:H	1.51	0.57
1:B:260:ASP:H	1:B:264:GLN:HE21	1.52	0.57
1:A:249:TYR:OH	1:A:308:HIS:HD2	1.86	0.57
1:B:249:TYR:OH	1:B:308:HIS:HD2	1.88	0.56
1:D:249:TYR:OH	1:D:308:HIS:HD2	1.87	0.56
1:C:201:PRO:HD2	1:C:315:SER:HB2	1.86	0.56
1:D:161:ALA:HB1	1:D:170:LYS:HD3	1.88	0.56
1:D:205:TYR:OH	1:D:210:HIS:CE1	2.60	0.54
1:A:140:GLN:NE2	1:A:149:GLY:H	2.06	0.54
1:C:249:TYR:OH	1:C:308:HIS:HD2	1.91	0.53
1:A:314:ARG:HD2	1:A:317:PHE:HE1	1.73	0.53
1:C:205:TYR:OH	1:C:210:HIS:CE1	2.60	0.52
1:C:181:PHE:CD2	1:C:229:LYS:HA	2.44	0.52
1:A:205:TYR:OH	1:A:210:HIS:CE1	2.60	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TYR:OH	1:B:210:HIS:CE1	2.61	0.52
1:C:216:VAL:HG12	1:C:217:MET:HE1	1.92	0.52
1:C:332:GLU:HG3	4:C:403:GOL:H31	1.91	0.52
1:A:210:HIS:HD2	1:A:286:GLU:OE2	1.93	0.52
1:A:314:ARG:HD2	1:A:317:PHE:CE1	2.45	0.52
1:C:173:LEU:HD23	1:C:313:GLY:HA2	1.91	0.52
1:A:334:ARG:HH12	3:A:402:LYS:HB3	1.75	0.52
1:D:260:ASP:H	1:D:264:GLN:HE21	1.57	0.52
1:B:369:PHE:HB3	1:B:371:LEU:HD13	1.92	0.51
1:A:187:ASP:OD1	1:A:308:HIS:HE1	1.94	0.51
1:A:151:LEU:HD21	1:A:337:LEU:HD13	1.92	0.51
1:D:187:ASP:OD1	1:D:308:HIS:HE1	1.94	0.51
1:B:213[B]:MET:CE	1:B:217:MET:CE	2.88	0.50
1:A:260:ASP:H	1:A:264:GLN:NE2	2.09	0.50
1:B:67:GLN:NE2	1:C:36:ASN:HB3	2.24	0.49
1:B:213[B]:MET:HE2	1:B:217:MET:CE	2.42	0.49
1:C:18:THR:HB	1:C:21:ILE:HD12	1.95	0.49
1:B:44:LEU:HD11	1:C:68:LEU:HD11	1.93	0.49
1:B:187:ASP:OD1	1:B:308:HIS:HE1	1.96	0.48
1:D:210:HIS:HD2	1:D:286:GLU:OE2	1.96	0.47
1:B:195:ARG:HD3	1:B:332:GLU:HB3	1.96	0.47
1:C:314:ARG:HD2	1:C:317:PHE:HE1	1.79	0.47
1:B:108:THR:HG23	1:B:335:GLN:HG3	1.96	0.47
1:A:63:LEU:HD13	1:B:74:THR:HG21	1.97	0.46
1:B:192:LEU:HD23	1:B:337:LEU:HD12	1.98	0.46
1:D:192:LEU:HB2	1:D:302:LEU:HD12	1.97	0.46
1:C:338:ARG:HH12	3:C:402:LYS:HB2	1.80	0.46
1:C:151:LEU:HD21	1:C:337:LEU:HD13	1.97	0.46
1:D:229:LYS:HE2	1:D:364:HIS:HB2	1.98	0.46
1:B:229:LYS:HE2	1:B:364:HIS:HB2	1.98	0.46
1:C:314:ARG:HD2	1:C:317:PHE:CE1	2.51	0.46
1:B:213[B]:MET:CE	1:B:217:MET:HE2	2.46	0.46
1:C:187:ASP:OD1	1:C:308:HIS:HE1	1.98	0.46
1:B:151:LEU:HD21	1:B:337:LEU:HD13	1.98	0.45
1:A:338:ARG:HH12	3:A:403:LYS:HD3	1.81	0.45
1:B:210:HIS:HD2	1:B:286:GLU:OE2	2.01	0.44
1:C:164:GLN:HE22	1:C:174:PHE:H	1.65	0.43
1:B:230:ASP:HB2	3:B:402:LYS:HE3	2.00	0.43
1:C:173:LEU:HB2	1:C:314:ARG:NH2	2.34	0.43
1:B:249:TYR:OH	1:B:308:HIS:CD2	2.71	0.43
1:A:75:ARG:HH21	1:A:75:ARG:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:GLU:HB2	1:C:329:ILE:HD12	2.01	0.42
1:D:88:GLN:O	1:D:208:ARG:HG3	2.18	0.42
1:A:334:ARG:HH12	3:A:402:LYS:CB	2.33	0.42
1:B:213[B]:MET:HE2	1:B:217:MET:HE1	2.01	0.42
1:C:93:VAL:HG22	1:C:303:ILE:HG12	2.01	0.42
1:D:93:VAL:HG22	1:D:303:ILE:HG12	2.02	0.42
1:A:249:TYR:OH	1:A:308:HIS:CD2	2.70	0.42
1:B:194:LEU:HD11	1:B:337:LEU:HD11	2.01	0.42
1:B:197:GLU:HG3	1:B:332:GLU:HB2	2.02	0.42
1:C:194:LEU:HD12	1:C:335:GLN:HG2	2.00	0.42
1:B:117:TYR:HA	1:B:120:LEU:HB2	2.01	0.41
1:B:137:LYS:HD3	1:B:345:LEU:HG	2.01	0.41
1:A:314:ARG:HG2	1:A:314:ARG:HH11	1.86	0.41
1:D:249:TYR:OH	1:D:308:HIS:CD2	2.70	0.41
1:B:88:GLN:O	1:B:208:ARG:HG3	2.20	0.41
1:A:88:GLN:O	1:A:208:ARG:HG3	2.20	0.41
1:A:166:GLY:N	3:A:403:LYS:HB3	2.34	0.40
1:C:88:GLN:O	1:C:208:ARG:HG3	2.21	0.40
1:D:51:ASN:HD21	1:D:53:GLU:HB2	1.86	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	346/372 (93%)	341 (99%)	5 (1%)	0	100	100
1	B	312/372 (84%)	303 (97%)	7 (2%)	2 (1%)	25	14
1	C	351/372 (94%)	341 (97%)	9 (3%)	1 (0%)	41	30
1	D	346/372 (93%)	339 (98%)	7 (2%)	0	100	100
All	All	1355/1488 (91%)	1324 (98%)	28 (2%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ALA
1	B	371	LEU
1	C	325	ASN

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	303/322 (94%)	298 (98%)	5 (2%)	60	55
1	B	279/322 (87%)	270 (97%)	9 (3%)	39	27
1	C	307/322 (95%)	302 (98%)	5 (2%)	62	58
1	D	302/322 (94%)	297 (98%)	5 (2%)	60	55
All	All	1191/1288 (92%)	1167 (98%)	24 (2%)	55	48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	75	ARG
1	A	169	SER
1	A	202	SER
1	A	359	PHE
1	B	33[A]	GLN
1	B	33[B]	GLN
1	B	116	ASP
1	B	176	HIS
1	B	214[A]	ASN
1	B	214[B]	ASN
1	B	230	ASP
1	B	314	ARG
1	B	359	PHE
1	C	15	THR
1	C	16	SER
1	C	172	ASP

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Mol	Chain	Res	Type
1	C	359	PHE
1	C	370	ASP
1	D	79	GLN
1	D	120	LEU
1	D	241	SER
1	D	314	ARG
1	D	359	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	33	GLN
1	A	36	ASN
1	A	67	GLN
1	A	140	GLN
1	A	184	ASN
1	A	210	HIS
1	A	264	GLN
1	A	308	HIS
1	B	67	GLN
1	B	184	ASN
1	B	210	HIS
1	B	264	GLN
1	B	308	HIS
1	C	40	ASN
1	C	164	GLN
1	C	210	HIS
1	C	226	GLN
1	C	264	GLN
1	C	308	HIS
1	D	51	ASN
1	D	164	GLN
1	D	184	ASN
1	D	210	HIS
1	D	251	ASN
1	D	264	GLN
1	D	308	HIS

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	D	402	-	8,9,9	0.80	0	9,10,10	0.79	0
3	LYS	A	402	-	8,9,9	0.79	0	9,10,10	0.75	0
4	GOL	D	403	-	5,5,5	0.05	0	5,5,5	0.13	0
4	GOL	C	403	-	5,5,5	0.04	0	5,5,5	0.13	0
3	LYS	B	402	-	8,9,9	0.80	0	9,10,10	0.65	0
3	LYS	A	403	-	8,9,9	0.95	0	9,10,10	1.13	0
3	LYS	C	402	-	8,9,9	0.77	0	9,10,10	0.71	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	D	402	-	-	6/9/9/9	-
3	LYS	A	402	-	-	6/9/9/9	-
4	GOL	D	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	403	-	-	0/4/4/4	-
3	LYS	B	402	-	-	8/9/9/9	-
3	LYS	A	403	-	-	3/9/9/9	-
3	LYS	C	402	-	-	5/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	LYS	O-C-CA-N
3	A	403	LYS	C-CA-CB-CG
3	B	402	LYS	O-C-CA-N
3	B	402	LYS	N-CA-CB-CG
3	C	402	LYS	O-C-CA-N
3	D	402	LYS	O-C-CA-N
3	D	402	LYS	N-CA-CB-CG
3	D	402	LYS	C-CA-CB-CG
3	B	402	LYS	OXT-C-CA-N
3	A	402	LYS	OXT-C-CA-N
3	C	402	LYS	OXT-C-CA-N
3	A	402	LYS	CA-CB-CG-CD
3	B	402	LYS	CE-CD-CG-CB
3	D	402	LYS	OXT-C-CA-N
3	C	402	LYS	CE-CD-CG-CB
3	D	402	LYS	CG-CD-CE-NZ
3	B	402	LYS	CA-CB-CG-CD
3	B	402	LYS	C-CA-CB-CG
3	D	402	LYS	CA-CB-CG-CD
3	C	402	LYS	OXT-C-CA-CB
3	A	403	LYS	N-CA-CB-CG
3	A	402	LYS	O-C-CA-CB
3	C	402	LYS	O-C-CA-CB
3	A	402	LYS	OXT-C-CA-CB
3	B	402	LYS	OXT-C-CA-CB
3	B	402	LYS	O-C-CA-CB
3	A	403	LYS	CA-CB-CG-CD
3	A	402	LYS	CE-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	LYS	2	0
4	C	403	GOL	1	0
3	B	402	LYS	2	0
3	A	403	LYS	3	0
3	C	402	LYS	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^{th} 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	343/372 (92%)	0.37	21 (6%) 21 29	31, 47, 83, 118	11 (3%)
1	B	315/372 (84%)	1.12	51 (16%) 1 2	33, 54, 110, 129	0
1	C	352/372 (94%)	1.26	76 (21%) 0 1	36, 58, 107, 140	4 (1%)
1	D	346/372 (93%)	0.82	46 (13%) 3 5	33, 56, 124, 194	0
All	All	1356/1488 (91%)	0.89	194 (14%) 2 4	31, 54, 107, 194	15 (1%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	ALA	11.5
1	D	161	ALA	11.2
1	B	331	CYS	11.1
1	D	162	ALA	10.9
1	C	323	ILE	10.2
1	C	171	THR	10.2
1	B	103	ASP	8.9
1	C	328	ILE	8.9
1	B	173	LEU	8.5
1	C	161	ALA	8.4
1	D	163	THR	8.2
1	B	116	ASP	8.2
1	B	114	GLY	8.1
1	B	106	GLY	8.0
1	D	171	THR	7.9
1	D	371	LEU	7.9
1	C	242	GLY	7.8
1	B	117	TYR	7.8
1	D	17	LEU	7.6
1	C	327	GLU	7.5
1	C	241	SER	7.5

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Mol	Chain	Res	Type	RSRZ
1	C	160	MET	7.4
1	B	112	TRP	7.1
1	D	174	PHE	7.0
1	D	170	LYS	6.9
1	C	325	ASN	6.9
1	C	165	THR	6.8
1	B	110	PRO	6.8
1	C	329	ILE	6.7
1	B	169	SER	6.6
1	D	164	GLN	6.6
1	C	316	ALA	6.5
1	D	325	ASN	6.5
1	A	171	THR	6.5
1	C	372	ASP	6.4
1	C	317	PHE	6.4
1	C	167	SER	6.3
1	C	168	GLY	6.2
1	B	107	PRO	6.2
1	D	328	ILE	6.2
1	D	372	ASP	6.0
1	C	326	GLY	6.0
1	C	173	LEU	5.9
1	B	230	ASP	5.8
1	A	162	ALA	5.8
1	A	163	THR	5.8
1	C	268	GLU	5.8
1	B	333	ARG	5.7
1	D	316	ALA	5.6
1	B	268	GLU	5.6
1	D	172	ASP	5.4
1	B	109	PRO	5.4
1	A	173	LEU	5.4
1	B	108	THR	5.3
1	B	105	LEU	5.3
1	B	266	PHE	5.2
1	C	324	GLU	5.2
1	B	104	ASP	5.2
1	C	318	ILE	5.2
1	C	277	LEU	5.2
1	C	169	SER	5.2
1	B	168	GLY	5.2
1	D	169	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	163	THR	5.1
1	A	161	ALA	5.1
1	A	19	LEU	5.1
1	B	174	PHE	5.1
1	B	270	ALA	5.1
1	C	315	SER	4.9
1	D	18	THR	4.8
1	D	323	ILE	4.7
1	C	170	LYS	4.7
1	C	18	THR	4.7
1	C	330	LYS	4.6
1	B	19	LEU	4.6
1	C	266	PHE	4.6
1	D	266	PHE	4.6
1	D	173	LEU	4.4
1	C	270	ALA	4.4
1	D	315	SER	4.4
1	B	111	ASN	4.3
1	D	160	MET	4.3
1	B	314	ARG	4.3
1	D	317	PHE	4.2
1	C	281	MET	4.2
1	B	154	VAL	4.2
1	B	315	SER	4.2
1	D	168	GLY	4.1
1	C	109	PRO	4.0
1	B	332	GLU	4.0
1	D	165	THR	4.0
1	D	242	GLY	4.0
1	A	316	ALA	4.0
1	C	19	LEU	4.0
1	B	115	ALA	4.0
1	A	168	GLY	3.9
1	C	166	GLY	3.9
1	C	174	PHE	3.9
1	C	172	ASP	3.9
1	D	268	GLU	3.8
1	C	156	PRO	3.8
1	B	102	GLN	3.8
1	C	269	ASN	3.7
1	B	200	VAL	3.7
1	B	113	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	158	GLU	3.6
1	C	233	TYR	3.6
1	B	171	THR	3.6
1	D	230	ASP	3.6
1	D	318	ILE	3.6
1	D	110	PRO	3.5
1	C	313	GLY	3.4
1	B	334	ARG	3.4
1	A	164	GLN	3.4
1	D	241	SER	3.4
1	A	172	ASP	3.4
1	D	329	ILE	3.4
1	A	166	GLY	3.4
1	B	269	ASN	3.3
1	C	164	GLN	3.3
1	C	274	SER	3.3
1	C	265	ILE	3.3
1	C	15	THR	3.3
1	A	117	TYR	3.2
1	B	267	ASN	3.2
1	A	317	PHE	3.1
1	B	198	GLU	3.0
1	D	324	GLU	3.0
1	C	347[A]	HIS	3.0
1	D	19	LEU	3.0
1	D	326	GLY	3.0
1	A	165	THR	3.0
1	B	170	LYS	3.0
1	C	157	ASP	3.0
1	C	284	TRP	3.0
1	C	159	LYS	3.0
1	A	230	ASP	2.9
1	C	331	CYS	2.9
1	A	160	MET	2.9
1	D	159	LYS	2.9
1	B	197	GLU	2.9
1	C	17	LEU	2.9
1	C	322	ARG	2.9
1	A	159	LYS	2.8
1	D	314	ARG	2.8
1	C	134	VAL	2.8
1	A	170	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	314	ARG	2.7
1	C	262	ALA	2.7
1	D	322	ARG	2.7
1	B	145	ARG	2.7
1	C	247	VAL	2.7
1	D	269	ASN	2.6
1	B	372	ASP	2.6
1	C	320	GLY	2.6
1	C	155	ILE	2.6
1	C	203	THR	2.6
1	A	169	SER	2.6
1	D	370	ASP	2.5
1	C	228	PRO	2.5
1	C	217	MET	2.5
1	C	252	ARG	2.5
1	B	172	ASP	2.4
1	B	262	ALA	2.4
1	D	157	ASP	2.4
1	C	20	GLU	2.4
1	B	371	LEU	2.3
1	D	167	SER	2.3
1	C	332	GLU	2.3
1	C	200	VAL	2.3
1	C	216	VAL	2.3
1	C	371	LEU	2.3
1	C	114	GLY	2.2
1	B	277	LEU	2.2
1	B	348	ILE	2.2
1	C	267	ASN	2.2
1	D	348	ILE	2.2
1	A	167	SER	2.2
1	B	101	ASP	2.1
1	A	241	SER	2.1
1	D	100	VAL	2.1
1	D	345	LEU	2.1
1	C	334	ARG	2.1
1	B	175	VAL	2.1
1	B	242	GLY	2.1
1	C	276	ALA	2.1
1	B	119	LYS	2.1
1	B	199	ARG	2.1
1	C	319	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	327	GLU	2.1
1	C	224	ILE	2.1
1	C	220	LEU	2.1
1	C	348	ILE	2.0
1	C	273	THR	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, 95^{th} 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	C	402	10/10	0.58	0.27	101,110,125,130	0
3	LYS	A	402	10/10	0.63	0.34	95,100,107,130	0
3	LYS	A	403	10/10	0.71	0.27	67,93,114,115	0
3	LYS	B	402	10/10	0.74	0.52	76,100,124,125	0
3	LYS	D	402	10/10	0.79	0.35	73,86,113,140	0
4	GOL	D	403	6/6	0.85	0.17	88,89,90,91	0
4	GOL	C	403	6/6	0.88	0.30	102,103,104,106	0
2	FE	D	401	1/1	0.97	0.10	70,70,70,70	0
2	FE	A	401	1/1	0.99	0.11	55,55,55,55	0
2	FE	C	401	1/1	0.99	0.12	70,70,70,70	0
2	FE	B	401	1/1	1.00	0.12	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.