Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 10:12 pm BST

PDB ID	:	6EUR
Title	:	Crystal structure of the complex Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO5 with Fe(II)/alpha-ketoglutarate
Authors	:	Isabet, T.; Stura, E.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on	:	2017-10-31
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

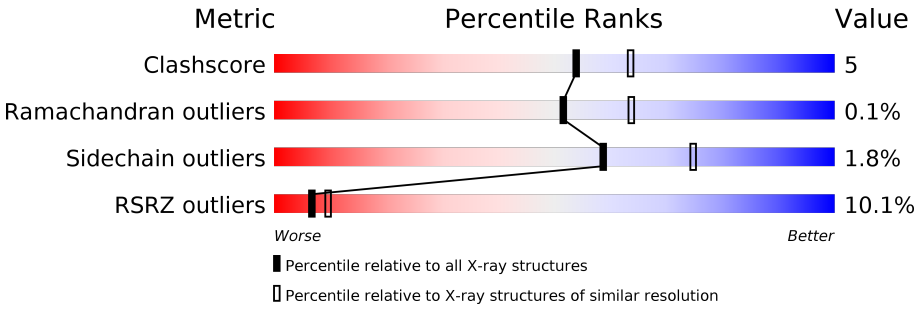
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	4% 83% 9% 8%
1	B	372	13% 79% 8% • 12%
1	C	372	12% 83% 10% 7%
1	D	372	8% 82% 10% • 8%

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	GOL	C	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11695 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.

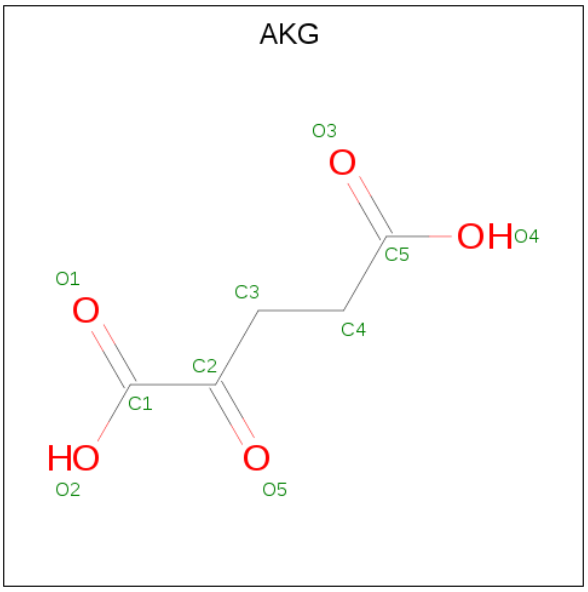
- Molecule 1 is a protein called L-lysine 4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	6	0
			2775	1761	480	522	12			
1	B	328	Total	C	N	O	S	0	18	0
			2662	1695	450	504	13			
1	C	346	Total	C	N	O	S	0	0	0
			2741	1745	468	516	12			
1	D	344	Total	C	N	O	S	0	1	0
			2729	1735	465	517	12			

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

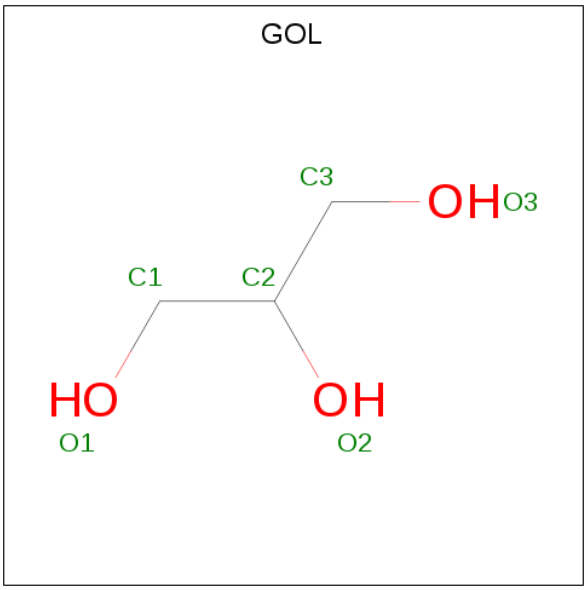
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

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



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

- Molecule 5 is water.

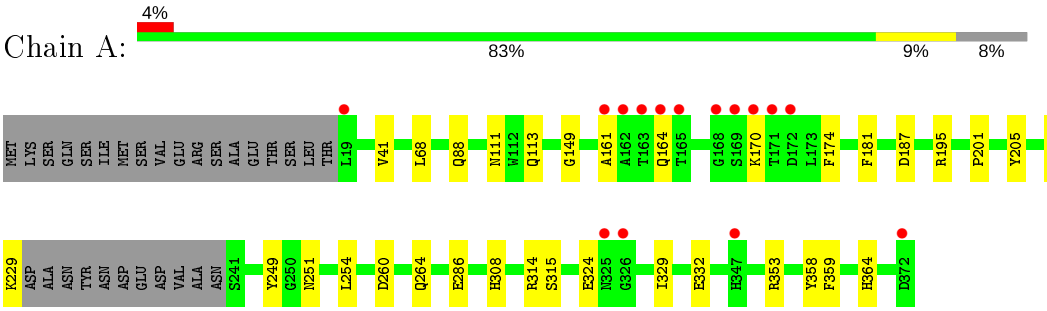
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	223	Total O 224 224	0	1
5	B	153	Total O 153 153	0	0
5	C	152	Total O 152 152	0	0
5	D	155	Total O 155 155	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

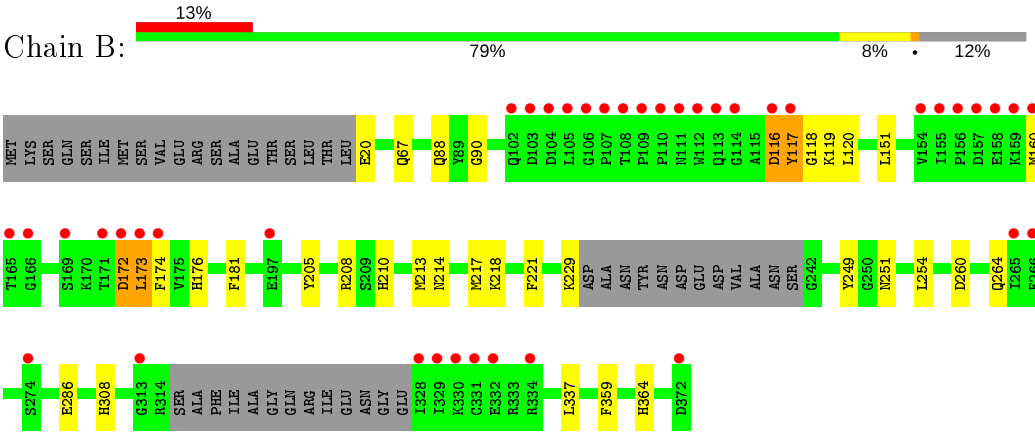
- Molecule 1: L-lysine 4-hydroxylase

Chain A:



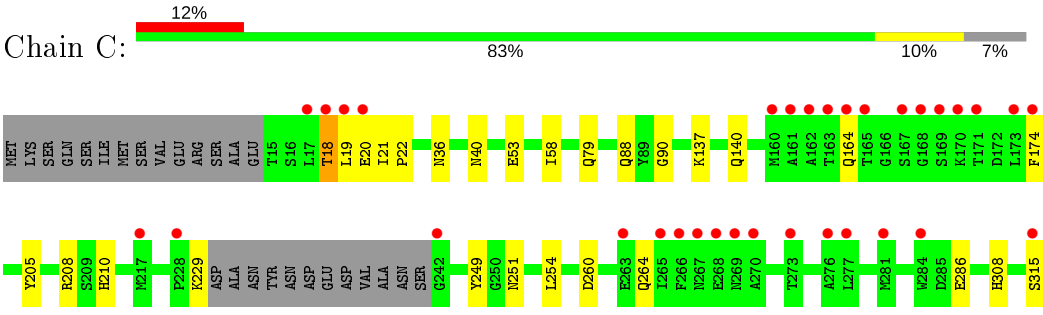
- Molecule 1: L-lysine 4-hydroxylase

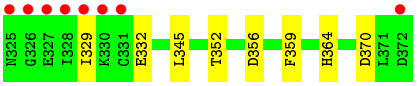
Chain B:



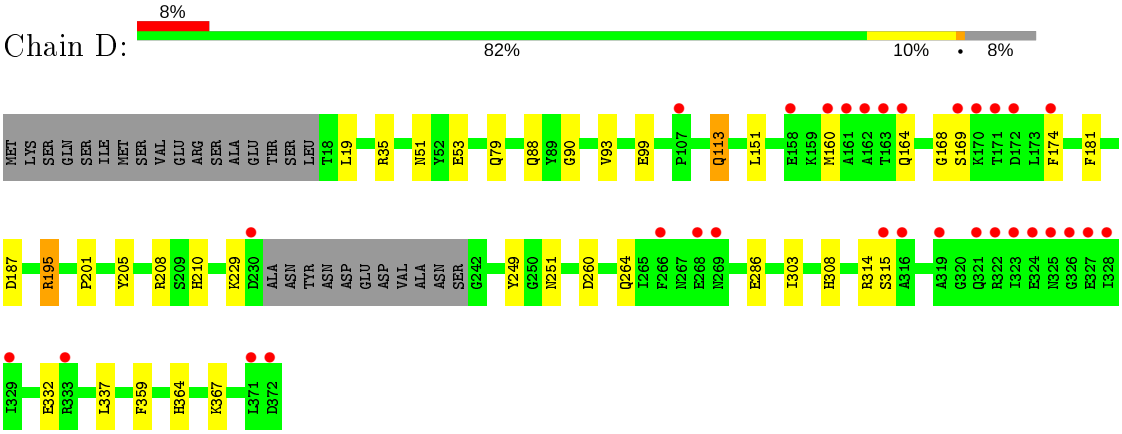
- Molecule 1: L-lysine 4-hydroxylase

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	91.42Å 99.46Å 166.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 2.30 48.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.1 (33.67-2.30) 87.1 (48.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.213 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11695	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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: GOL, AKG, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.52	0/2838	0.68	0/3838
1	B	0.52	0/2723	0.71	1/3689 (0.0%)
1	C	0.49	0/2803	0.68	0/3794
1	D	0.49	0/2791	0.67	0/3780
All	All	0.50	0/11155	0.68	1/15101 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ASP	C-N-CA	6.80	138.70	121.70

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	2775	0	2716	24	0
1	B	2662	0	2576	34	0
1	C	2741	0	2696	33	0
1	D	2729	0	2660	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	24	0	32	4	0
4	B	6	0	8	0	0
4	C	18	0	24	7	0
4	D	12	0	16	0	0
5	A	224	0	0	0	0
5	B	153	0	0	0	0
5	C	152	0	0	2	0
5	D	155	0	0	0	0
All	All	11695	0	10744	116	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 5.

All (116) 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:88:GLN:HE21	1:D:90:GLY:H	1.19	0.88
1:B:88:GLN:HE21	1:B:90:GLY:H	1.19	0.88
1:C:88:GLN:HE21	1:C:90:GLY:H	1.20	0.87
1:B:251:ASN:HD22	1:B:254:LEU:H	1.26	0.83
1:B:117:TYR:HB2	1:B:120:LEU:HB2	1.61	0.81
1:C:251:ASN:HD22	1:C:254:LEU:H	1.26	0.80
1:A:251:ASN:HD22	1:A:254:LEU:H	1.28	0.77
1:B:172[A]:ASP:HB3	1:B:173[A]:LEU:HA	1.65	0.77
1:B:213:MET:HE2	1:B:221:PHE:CE2	2.28	0.67
1:D:260:ASP:H	1:D:264:GLN:HE21	1.43	0.67
1:D:205:TYR:OH	1:D:210:HIS:HE1	1.77	0.66
1:B:172[A]:ASP:CB	1:B:173[A]:LEU:HA	2.26	0.66
1:B:213:MET:CE	1:B:221:PHE:HE2	2.09	0.65
1:A:205:TYR:OH	1:A:210:HIS:HE1	1.78	0.65
1:C:260:ASP:H	1:C:264:GLN:HE21	1.45	0.65
1:B:260:ASP:H	1:B:264:GLN:HE21	1.44	0.65
1:B:205:TYR:OH	1:B:210:HIS:HE1	1.81	0.64
1:B:213:MET:CE	1:B:221:PHE:CE2	2.81	0.64
1:C:205:TYR:OH	1:C:210:HIS:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLN:HE22	1:C:36:ASN:HB3	1.64	0.63
1:A:164:GLN:HE22	1:A:174:PHE:H	1.46	0.63
1:A:353:ARG:HA	4:A:403:GOL:H32	1.79	0.63
1:C:18:THR:HB	1:C:21:ILE:HD12	1.80	0.62
1:A:260:ASP:H	1:A:264:GLN:HE21	1.47	0.62
1:B:172[A]:ASP:HB3	1:B:173[A]:LEU:CA	2.31	0.61
1:C:58:ILE:HD13	4:C:403:GOL:H32	1.85	0.59
1:D:88:GLN:HE21	1:D:90:GLY:N	1.97	0.59
1:D:164:GLN:HE22	1:D:174:PHE:H	1.49	0.59
1:C:88:GLN:HE21	1:C:90:GLY:N	1.98	0.59
1:C:164:GLN:HE22	1:C:174:PHE:H	1.50	0.58
1:D:113:GLN:H	1:D:113:GLN:HE21	1.52	0.58
1:B:88:GLN:HE21	1:B:90:GLY:N	1.98	0.58
1:B:88:GLN:NE2	1:B:90:GLY:H	1.98	0.57
1:A:353:ARG:HG2	4:A:403:GOL:H11	1.86	0.57
1:D:205:TYR:OH	1:D:210:HIS:CE1	2.57	0.57
1:C:356:ASP:OD2	4:C:403:GOL:H12	2.05	0.57
1:C:88:GLN:NE2	1:C:90:GLY:H	1.99	0.56
1:C:140:GLN:HE21	4:C:403:GOL:H11	1.69	0.56
1:C:324:GLU:HB3	1:C:329:ILE:HD12	1.89	0.55
1:D:88:GLN:NE2	1:D:90:GLY:H	1.98	0.55
1:A:205:TYR:OH	1:A:210:HIS:CE1	2.58	0.54
1:B:213:MET:HE3	1:B:218:LYS:HG2	1.90	0.53
1:A:164:GLN:NE2	1:A:174:PHE:H	2.07	0.53
1:C:201:PRO:HD2	1:C:315:SER:HB2	1.91	0.53
1:B:67:GLN:NE2	1:C:36:ASN:HB3	2.24	0.53
1:B:205:TYR:OH	1:B:210:HIS:CE1	2.61	0.53
1:B:213:MET:HE2	1:B:221:PHE:HE2	1.66	0.52
1:A:210:HIS:HD2	1:A:286:GLU:OE2	1.92	0.52
1:D:249:TYR:OH	1:D:308:HIS:HD2	1.92	0.52
1:D:210:HIS:HD2	1:D:286:GLU:OE2	1.92	0.52
1:C:205:TYR:OH	1:C:210:HIS:CE1	2.61	0.51
1:C:53:GLU:HA	1:C:58:ILE:HD11	1.91	0.51
1:D:93:VAL:HG22	1:D:303:ILE:HG12	1.92	0.51
1:C:332:GLU:HG3	4:C:404:GOL:H31	1.93	0.51
1:D:201:PRO:HD2	1:D:315:SER:HB2	1.93	0.51
1:B:117:TYR:HD1	1:B:118:GLY:HA3	1.74	0.51
1:C:249:TYR:OH	1:C:308:HIS:HD2	1.94	0.50
1:C:140:GLN:NE2	4:C:403:GOL:H11	2.26	0.49
1:A:324:GLU:HB3	1:A:329:ILE:HD12	1.94	0.49
1:D:164:GLN:NE2	1:D:174:PHE:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:TYR:OH	1:B:308:HIS:HD2	1.96	0.49
1:A:111:ASN:OD1	1:A:113[B]:GLN:HG2	2.13	0.49
1:A:161:ALA:HB1	1:A:170:LYS:HG3	1.95	0.48
1:A:201:PRO:HD2	1:A:315:SER:HB2	1.95	0.48
1:A:249:TYR:OH	1:A:308:HIS:HD2	1.95	0.48
1:B:229:LYS:HD3	1:B:364:HIS:HB2	1.95	0.48
1:A:358:TYR:HB2	4:A:404:GOL:H12	1.96	0.48
1:C:164:GLN:NE2	1:C:174:PHE:H	2.10	0.48
1:B:117:TYR:HB3	1:B:119:LYS:N	2.30	0.47
1:B:116:ASP:HB3	1:B:117:TYR:CG	2.50	0.47
1:C:229:LYS:HD3	1:C:364:HIS:HB2	1.96	0.47
1:C:140:GLN:HE21	4:C:403:GOL:C1	2.27	0.47
1:D:195:ARG:HD3	1:D:332:GLU:HB3	1.97	0.47
1:A:251:ASN:ND2	1:A:254:LEU:H	2.05	0.46
1:D:229:LYS:HD3	1:D:364:HIS:HB2	1.96	0.46
1:B:213:MET:HE1	1:B:221:PHE:CE2	2.50	0.46
1:C:18:THR:HB	1:C:21:ILE:CD1	2.46	0.46
1:C:210:HIS:HD2	1:C:286:GLU:OE2	1.99	0.46
1:B:251:ASN:ND2	1:B:254:LEU:H	2.05	0.46
1:A:229:LYS:HD3	1:A:364:HIS:HB2	1.96	0.46
1:B:260:ASP:H	1:B:264:GLN:NE2	2.13	0.46
1:A:195:ARG:HD3	1:A:332:GLU:HB3	1.98	0.45
1:A:260:ASP:H	1:A:264:GLN:NE2	2.14	0.45
1:B:210:HIS:HD2	1:B:286:GLU:OE2	1.99	0.45
1:B:151:LEU:HD21	1:B:337:LEU:HD13	1.98	0.45
1:C:260:ASP:H	1:C:264:GLN:NE2	2.12	0.44
1:D:160:MET:O	1:D:168:GLY:HA2	2.17	0.44
1:B:181:PHE:HB2	1:B:364:HIS:HD2	1.83	0.44
1:C:20:GLU:O	1:C:22:PRO:HD3	2.17	0.44
1:C:137:LYS:HD3	1:C:345:LEU:HG	1.99	0.43
1:A:181:PHE:HB2	1:A:364:HIS:HD2	1.84	0.43
1:D:51:ASN:HD21	1:D:53:GLU:HB2	1.84	0.43
1:B:214:ASN:OD1	1:B:217[B]:MET:HG2	2.19	0.42
1:B:88:GLN:O	1:B:208:ARG:HG3	2.20	0.42
1:C:88:GLN:O	1:C:208:ARG:HG3	2.18	0.42
1:B:117:TYR:CD1	1:B:118:GLY:HA3	2.54	0.42
1:B:213:MET:HE1	1:B:221:PHE:HE2	1.82	0.42
1:A:88:GLN:O	1:A:208:ARG:HG3	2.19	0.41
1:D:260:ASP:H	1:D:264:GLN:NE2	2.13	0.41
1:B:116:ASP:HB3	1:B:117:TYR:CD2	2.55	0.41
1:D:35:ARG:HD3	1:D:99:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLN:O	1:D:208:ARG:HG3	2.20	0.41
1:D:187:ASP:OD1	1:D:308:HIS:HE1	2.04	0.41
1:C:181:PHE:HB2	1:C:364:HIS:HD2	1.86	0.41
1:C:40:ASN:HB2	5:C:511:HOH:O	2.21	0.41
1:A:149:GLY:HA3	4:A:405:GOL:H11	2.03	0.41
1:A:187:ASP:OD1	1:A:308:HIS:HE1	2.04	0.41
1:C:79:GLN:HG2	5:C:580:HOH:O	2.21	0.41
1:A:41:VAL:HG13	1:A:68:LEU:HD13	2.03	0.41
1:D:151:LEU:HD21	1:D:337:LEU:HD13	2.03	0.41
1:C:352:THR:O	4:C:405:GOL:H31	2.22	0.40
1:D:181:PHE:HB2	1:D:364:HIS:HD2	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	345/372 (93%)	337 (98%)	8 (2%)	0	100 100
1	B	332/372 (89%)	319 (96%)	11 (3%)	2 (1%)	25 31
1	C	342/372 (92%)	336 (98%)	6 (2%)	0	100 100
1	D	341/372 (92%)	332 (97%)	9 (3%)	0	100 100
All	All	1360/1488 (91%)	1324 (97%)	34 (2%)	2 (0%)	51 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174[A]	PHE
1	B	174[B]	PHE

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	302/322 (94%)	300 (99%)	2 (1%)	84	92
1	B	289/322 (90%)	280 (97%)	9 (3%)	40	55
1	C	299/322 (93%)	295 (99%)	4 (1%)	69	82
1	D	296/322 (92%)	288 (97%)	8 (3%)	44	61
All	All	1186/1288 (92%)	1163 (98%)	23 (2%)	59	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	ARG
1	A	359	PHE
1	B	20	GLU
1	B	117	TYR
1	B	160[A]	MET
1	B	172[A]	ASP
1	B	172[B]	ASP
1	B	173[A]	LEU
1	B	173[B]	LEU
1	B	176	HIS
1	B	359	PHE
1	C	18	THR
1	C	19	LEU
1	C	359	PHE
1	C	370	ASP
1	D	19	LEU
1	D	79	GLN
1	D	113	GLN
1	D	169	SER
1	D	195	ARG
1	D	314	ARG
1	D	359	PHE
1	D	367	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	36	ASN
1	A	164	GLN
1	A	184	ASN
1	A	210	HIS
1	A	226	GLN
1	A	251	ASN
1	A	264	GLN
1	A	298	ASN
1	A	308	HIS
1	B	67	GLN
1	B	88	GLN
1	B	184	ASN
1	B	210	HIS
1	B	226	GLN
1	B	251	ASN
1	B	264	GLN
1	B	298	ASN
1	B	308	HIS
1	C	40	ASN
1	C	88	GLN
1	C	164	GLN
1	C	210	HIS
1	C	251	ASN
1	C	264	GLN
1	C	298	ASN
1	C	308	HIS
1	C	347	HIS
1	D	51	ASN
1	D	88	GLN
1	D	113	GLN
1	D	164	GLN
1	D	210	HIS
1	D	226	GLN
1	D	251	ASN
1	D	264	GLN
1	D	298	ASN
1	D	308	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
4	GOL	A	404	-	5,5,5	0.14	0	5,5,5	0.24	0
3	AKG	B	402	2	3,9,9	0.28	0	4,11,11	0.65	0
4	GOL	A	405	-	5,5,5	0.12	0	5,5,5	0.33	0
4	GOL	C	405	-	5,5,5	0.15	0	5,5,5	0.34	0
4	GOL	D	404	-	5,5,5	0.08	0	5,5,5	0.21	0
3	AKG	C	402	2	3,9,9	0.45	0	4,11,11	0.81	0
4	GOL	A	406	-	5,5,5	0.19	0	5,5,5	0.40	0
3	AKG	A	402	2	3,9,9	0.33	0	4,11,11	0.39	0
4	GOL	B	403	-	5,5,5	0.08	0	5,5,5	0.16	0
4	GOL	C	404	-	5,5,5	0.06	0	5,5,5	0.16	0
4	GOL	C	403	-	5,5,5	0.18	0	5,5,5	0.27	0
3	AKG	D	402	2	3,9,9	0.40	0	4,11,11	0.82	0
4	GOL	A	403	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	D	403	-	5,5,5	0.07	0	5,5,5	0.54	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
4	GOL	A	404	-	-	2/4/4/4	-
3	AKG	B	402	2	-	2/3/9/9	-
4	GOL	A	405	-	-	0/4/4/4	-
4	GOL	C	405	-	-	2/4/4/4	-
4	GOL	D	404	-	-	0/4/4/4	-
3	AKG	C	402	2	-	2/3/9/9	-
4	GOL	A	406	-	-	0/4/4/4	-
3	AKG	A	402	2	-	2/3/9/9	-
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	C	404	-	-	0/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
3	AKG	D	402	2	-	2/3/9/9	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	D	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	GOL	O1-C1-C2-C3
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3
3	B	402	AKG	C1-C2-C3-C4
3	A	402	AKG	C1-C2-C3-C4
3	D	402	AKG	C1-C2-C3-C4
3	C	402	AKG	C1-C2-C3-C4
4	A	404	GOL	O1-C1-C2-O2
3	B	402	AKG	O5-C2-C3-C4
3	C	402	AKG	O5-C2-C3-C4
3	A	402	AKG	O5-C2-C3-C4
3	D	402	AKG	O5-C2-C3-C4
4	C	405	GOL	O1-C1-C2-O2
4	C	405	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	1	0
4	A	405	GOL	1	0
4	C	405	GOL	1	0
4	C	404	GOL	1	0
4	C	403	GOL	5	0
4	A	403	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.00	15 (4%) 34 41	28, 45, 78, 112	0
1	B	328/372 (88%)	0.78	48 (14%) 2 3	30, 54, 117, 158	9 (2%)
1	C	346/372 (93%)	0.60	44 (12%) 3 5	31, 58, 107, 139	0
1	D	344/372 (92%)	0.37	31 (9%) 9 12	31, 55, 123, 173	0
All	All	1361/1488 (91%)	0.44	138 (10%) 7 9	28, 52, 111, 173	9 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	14.7
1	B	165[A]	THR	14.2
1	B	330	LYS	11.0
1	C	162	ALA	9.7
1	D	162	ALA	9.6
1	B	164[A]	GLN	9.5
1	B	159	LYS	9.0
1	B	331	CYS	9.0
1	D	324	GLU	8.6
1	D	372	ASP	7.7
1	B	328	ILE	7.7
1	A	162	ALA	7.7
1	D	323	ILE	7.1
1	C	160	MET	6.8
1	D	161	ALA	6.7
1	C	324	GLU	6.6
1	C	165	THR	6.6
1	D	163	THR	6.4
1	D	325	ASN	6.4
1	B	173[A]	LEU	6.3
1	C	325	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	171	THR	5.7
1	C	327	GLU	5.7
1	B	117	TYR	5.7
1	B	174[A]	PHE	5.6
1	C	266	PHE	5.5
1	C	328	ILE	5.5
1	B	155	ILE	5.2
1	A	163	THR	5.2
1	D	371	LEU	5.1
1	C	323	ILE	5.1
1	C	163	THR	5.0
1	B	266	PHE	5.0
1	C	268	GLU	4.8
1	B	103	ASP	4.7
1	B	108	THR	4.7
1	D	328	ILE	4.5
1	C	173	LEU	4.5
1	B	268	GLU	4.4
1	C	270	ALA	4.4
1	B	270	ALA	4.4
1	B	107	PRO	4.3
1	B	160[A]	MET	4.3
1	C	161	ALA	4.3
1	B	112	TRP	4.3
1	A	325	ASN	4.2
1	B	110	PRO	4.2
1	C	164	GLN	4.2
1	B	109	PRO	4.1
1	D	322	ARG	4.1
1	B	162[A]	ALA	4.1
1	C	372	ASP	4.1
1	B	158	GLU	4.0
1	B	171[A]	THR	4.0
1	D	174	PHE	4.0
1	C	316	ALA	4.0
1	C	276	ALA	3.9
1	D	164	GLN	3.9
1	D	266	PHE	3.8
1	C	265	ILE	3.8
1	D	327	GLU	3.7
1	C	18	THR	3.7
1	B	156	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	315	SER	3.7
1	C	169	SER	3.6
1	D	171	THR	3.6
1	B	106	GLY	3.6
1	B	114	GLY	3.6
1	D	268	GLU	3.6
1	B	113	GLN	3.5
1	B	267	ASN	3.5
1	C	269	ASN	3.4
1	C	326	GLY	3.4
1	B	102	GLN	3.4
1	C	330	LYS	3.4
1	C	242	GLY	3.4
1	A	168	GLY	3.3
1	A	372	ASP	3.3
1	B	157	ASP	3.3
1	B	332	GLU	3.3
1	A	170	LYS	3.2
1	C	19	LEU	3.2
1	B	161[A]	ALA	3.2
1	C	284	TRP	3.2
1	C	329	ILE	3.1
1	C	281	MET	3.1
1	D	158	GLU	3.1
1	A	164	GLN	3.0
1	A	171	THR	3.0
1	C	20	GLU	3.0
1	C	174	PHE	3.0
1	D	160	MET	3.0
1	B	104	ASP	3.0
1	C	168	GLY	2.9
1	B	334	ARG	2.9
1	B	116	ASP	2.9
1	D	269	ASN	2.9
1	B	105	LEU	2.9
1	D	316	ALA	2.9
1	B	197	GLU	2.8
1	C	263	GLU	2.8
1	C	277	LEU	2.8
1	B	265	ILE	2.8
1	B	269	ASN	2.8
1	D	319	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	170	LYS	2.7
1	C	17	LEU	2.7
1	B	313	GLY	2.7
1	D	107	PRO	2.6
1	B	111	ASN	2.6
1	A	169	SER	2.6
1	A	161	ALA	2.6
1	D	321	GLN	2.6
1	D	326	GLY	2.5
1	A	19	LEU	2.5
1	D	230	ASP	2.5
1	B	372	ASP	2.4
1	A	347[A]	HIS	2.4
1	D	329	ILE	2.4
1	B	172[A]	ASP	2.4
1	A	165	THR	2.4
1	B	154	VAL	2.4
1	C	331	CYS	2.3
1	D	170	LYS	2.3
1	C	267	ASN	2.3
1	A	172	ASP	2.2
1	C	167	SER	2.2
1	D	315	SER	2.2
1	B	166[A]	GLY	2.2
1	C	228	PRO	2.1
1	A	326	GLY	2.1
1	B	274	SER	2.1
1	D	169	SER	2.1
1	D	172	ASP	2.0
1	D	333	ARG	2.0
1	B	169[A]	SER	2.0
1	C	217	MET	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 carbohydrates 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, 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
4	GOL	A	405	6/6	0.69	0.26	92,93,93,93	0
4	GOL	D	404	6/6	0.74	0.22	92,98,99,99	0
4	GOL	C	405	6/6	0.77	0.23	64,71,73,73	0
4	GOL	D	403	6/6	0.79	0.30	89,91,92,95	0
3	AKG	B	402	10/10	0.84	0.35	93,96,99,101	0
4	GOL	B	403	6/6	0.84	0.18	85,87,89,91	0
4	GOL	A	406	6/6	0.84	0.18	46,53,54,55	0
4	GOL	A	403	6/6	0.86	0.20	76,76,78,81	0
3	AKG	C	402	10/10	0.89	0.34	82,83,84,84	0
4	GOL	C	404	6/6	0.90	0.27	78,83,86,88	0
3	AKG	D	402	10/10	0.92	0.21	80,86,91,91	0
4	GOL	C	403	6/6	0.92	0.15	54,62,63,65	0
3	AKG	A	402	10/10	0.94	0.12	60,65,71,74	0
4	GOL	A	404	6/6	0.95	0.14	63,66,67,70	0
2	FE	D	401	1/1	0.99	0.10	61,61,61,61	0
2	FE	C	401	1/1	0.99	0.12	58,58,58,58	0
2	FE	B	401	1/1	0.99	0.11	51,51,51,51	0
2	FE	A	401	1/1	0.99	0.11	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.