



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:55 AM UTC

PDB ID : 6EUR / pdb_00006eur
Title : Crystal structure of the complex Fe(II)/alpha-ketoglutarate dependent dioxxygenase 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 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

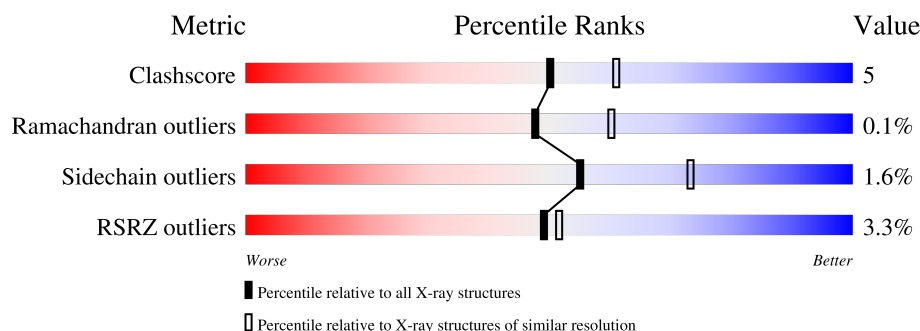
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	372	
1	B	372	
1	C	372	
1	D	372	

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	AKG	A	402	-	X	-	-
3	AKG	C	402	-	X	-	-
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 (CCD ID: 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 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



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

- Molecule 4 is GLYCEROL (CCD ID: 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

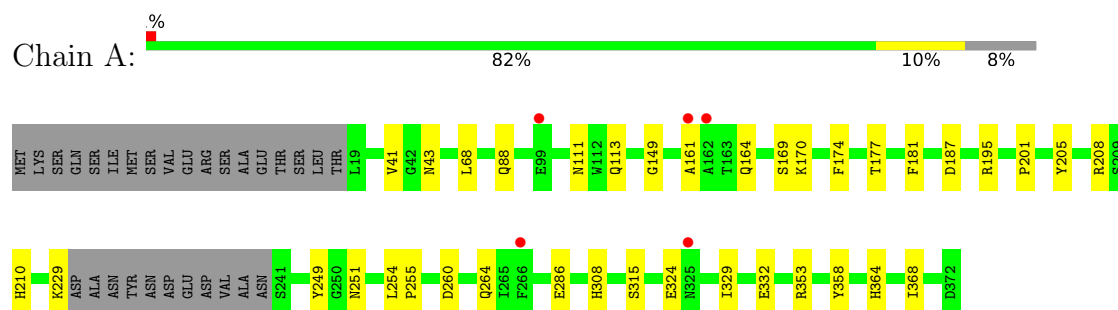
- Molecule 5 is water.

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

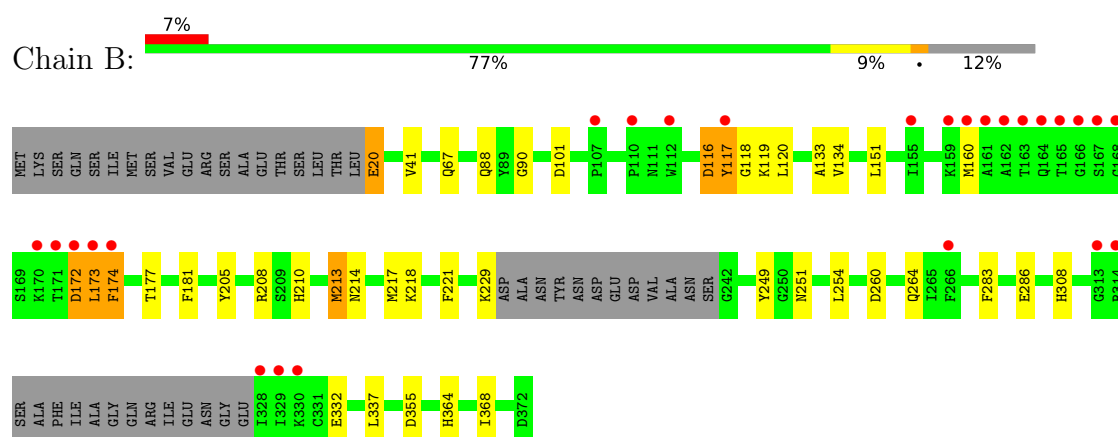
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

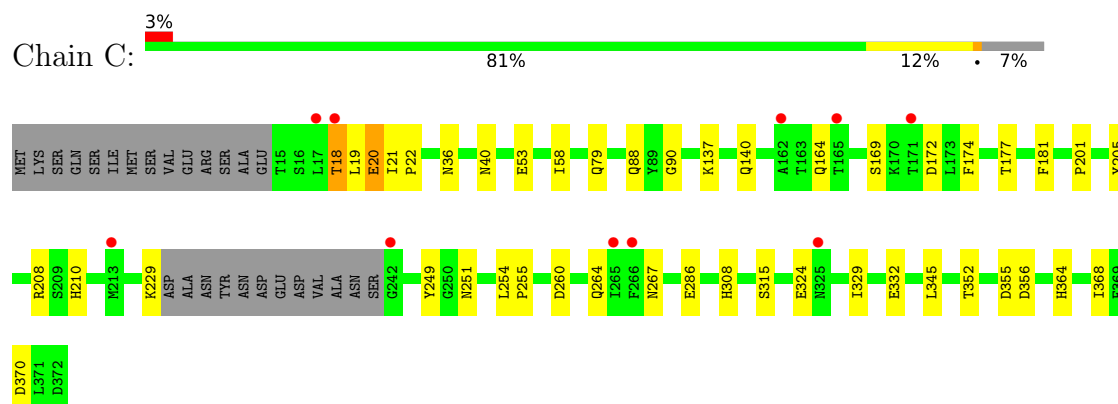
- Molecule 1: L-lysine 4-hydroxylase



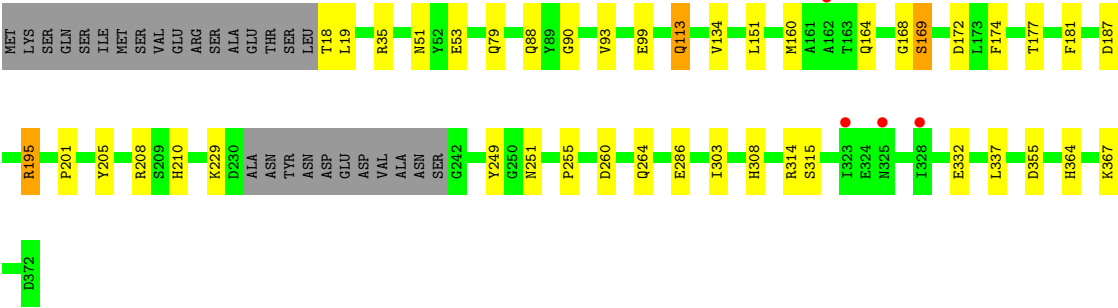
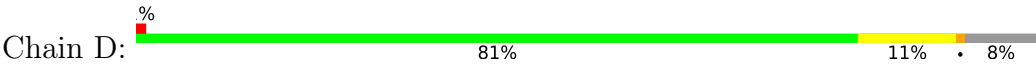
- Molecule 1: L-lysine 4-hydroxylase



- Molecule 1: L-lysine 4-hydroxylase



● Molecule 1: L-lysine 4-hydroxylase



4 Data and refinement statistics

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 33.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.1 (33.67-2.30) 87.1 (33.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.87	0/2838	1.28	6/3838 (0.2%)
1	B	0.86	4/2723 (0.1%)	1.33	15/3689 (0.4%)
1	C	0.85	0/2803	1.30	7/3794 (0.2%)
1	D	0.84	1/2791 (0.0%)	1.28	8/3780 (0.2%)
All	All	0.85	5/11155 (0.0%)	1.30	36/15101 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	MET	SD-CE	-6.65	1.62	1.79
1	B	134	VAL	CA-C	5.79	1.57	1.52
1	B	20	GLU	C-N	5.69	1.39	1.33
1	B	116	ASP	CA-C	5.48	1.60	1.52
1	D	134	VAL	CA-C	5.29	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CA-C-N	9.45	138.70	121.70
1	B	116	ASP	C-N-CA	9.45	138.70	121.70
1	A	169	SER	CA-C-N	7.13	130.79	120.38
1	A	169	SER	C-N-CA	7.13	130.79	120.38
1	D	177	THR	N-CA-C	-6.31	100.28	110.32
1	C	355	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	177	THR	N-CA-C	-6.04	100.72	110.32
1	C	177	THR	N-CA-C	-6.00	100.79	110.32
1	B	177	THR	N-CA-C	-5.70	102.04	110.48
1	B	355	ASP	CA-CB-CG	5.70	118.30	112.60
1	D	355	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	169	SER	CA-C-N	5.43	128.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	SER	C-N-CA	5.43	128.30	120.38
1	B	133	ALA	CA-C-N	5.38	123.63	120.24
1	B	133	ALA	C-N-CA	5.38	123.63	120.24
1	A	43	ASN	CA-C-N	5.34	127.38	120.44
1	A	43	ASN	C-N-CA	5.34	127.38	120.44
1	C	267	ASN	CA-CB-CG	5.34	117.94	112.60
1	D	172	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	255	PRO	N-CA-C	5.29	119.00	111.13
1	B	117	TYR	CA-C-N	5.24	131.13	121.70
1	B	117	TYR	C-N-CA	5.24	131.13	121.70
1	C	172	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	101	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	41	VAL	CA-C-N	5.12	125.62	119.94
1	B	41	VAL	C-N-CA	5.12	125.62	119.94
1	D	169	SER	CA-C-N	5.11	128.85	120.63
1	D	169	SER	C-N-CA	5.11	128.85	120.63
1	C	255	PRO	N-CA-C	5.10	118.73	111.13
1	B	174[A]	PHE	CA-C-N	-5.06	113.27	122.43
1	B	174[A]	PHE	C-N-CA	-5.06	113.27	122.43
1	B	174[B]	PHE	CA-C-N	-5.06	113.27	122.43
1	B	174[B]	PHE	C-N-CA	-5.06	113.27	122.43
1	A	255	PRO	N-CA-C	5.06	118.66	111.13
1	D	18	THR	CA-C-N	5.04	128.25	121.05
1	D	18	THR	C-N-CA	5.04	128.25	121.05

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
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:213:MET:HE1	1:B:221:PHE:CE2	2.10	0.86
1:B:213:MET:HE1	1:B:221:PHE:HE2	1.35	0.86
1:B:251:ASN:HD22	1:B:254:LEU:H	1.26	0.83
1:B:213:MET:HE3	1:B:218:LYS:HG2	1.60	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:TYR:OH	1:C:210:HIS:HE1	1.81	0.63
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:213:MET:CE	1:B:221:PHE:CE2	2.81	0.61
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:213:MET:CE	1:B:221:PHE:HE2	2.09	0.57
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: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: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:B:213:MET:HE3	1:B:218:LYS:CG	2.38	0.50
1:C:140:GLN:NE2	4:C:403:GOL:H11	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:140:GLN:HE21	4:C:403:GOL:C1	2.27	0.47
1:C:229:LYS:HD3	1:C:364:HIS:HB2	1.96	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: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:B:217[B]:MET:HE1	1:B:283:PHE:CE1	2.51	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HD3	1:D:99:GLU:HG2	2.02	0.41
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	27
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%)	48	60

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

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%)	301 (100%)	1 (0%)	86	93
1	B	289/322 (90%)	281 (97%)	8 (3%)	38	56
1	C	299/322 (93%)	294 (98%)	5 (2%)	53	72
1	D	296/322 (92%)	289 (98%)	7 (2%)	43	62
All	All	1186/1288 (92%)	1165 (98%)	21 (2%)	55	70

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

Mol	Chain	Res	Type
1	A	368	ILE
1	B	20	GLU
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	332	GLU
1	B	368	ILE
1	C	18	THR
1	C	19	LEU
1	C	20	GLU
1	C	368	ILE
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	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	43	ASN
1	A	79	GLN
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	308	HIS
1	A	335	GLN
1	B	67	GLN
1	B	79	GLN
1	B	88	GLN
1	B	164[A]	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	B	347	HIS
1	C	43	ASN
1	C	88	GLN
1	C	164	GLN
1	C	184	ASN
1	C	210	HIS
1	C	226	GLN
1	C	251	ASN
1	C	264	GLN
1	C	298	ASN
1	C	308	HIS
1	D	40	ASN
1	D	51	ASN
1	D	79	GLN
1	D	88	GLN
1	D	113	GLN
1	D	164	GLN
1	D	184	ASN
1	D	210	HIS
1	D	226	GLN
1	D	251	ASN

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Mol	Chain	Res	Type
1	D	264	GLN
1	D	298	ASN
1	D	308	HIS
1	D	347	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	403	-	5,5,5	0.19	0	5,5,5	0.26	0
3	AKG	C	402	2	9,9,9	1.88	4 (44%)	11,11,11	3.36	4 (36%)
4	GOL	A	406	-	5,5,5	0.20	0	5,5,5	0.42	0
4	GOL	C	404	-	5,5,5	0.07	0	5,5,5	0.15	0
4	GOL	C	405	-	5,5,5	0.15	0	5,5,5	0.35	0
4	GOL	D	404	-	5,5,5	0.09	0	5,5,5	0.20	0
4	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.14	0
4	GOL	A	404	-	5,5,5	0.14	0	5,5,5	0.24	0
4	GOL	A	403	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	A	405	-	5,5,5	0.12	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	B	402	2	9,9,9	0.30	0	11,11,11	1.26	2 (18%)
3	AKG	A	402	2	9,9,9	2.00	4 (44%)	11,11,11	2.99	5 (45%)
3	AKG	D	402	2	9,9,9	0.24	0	11,11,11	1.18	2 (18%)
4	GOL	D	403	-	5,5,5	0.07	0	5,5,5	0.56	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	C	403	-	-	0/4/4/4	-
3	AKG	C	402	2	-	6/9/9/9	-
4	GOL	A	406	-	-	0/4/4/4	-
4	GOL	C	404	-	-	0/4/4/4	-
4	GOL	C	405	-	-	1/4/4/4	-
4	GOL	D	404	-	-	0/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-
3	AKG	B	402	2	-	5/9/9/9	-
3	AKG	A	402	2	-	3/9/9/9	-
3	AKG	D	402	2	-	1/9/9/9	-
4	GOL	D	403	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AKG	O1-C1	3.31	1.30	1.22
3	A	402	AKG	O3-C5	3.16	1.32	1.22
3	C	402	AKG	O3-C5	3.10	1.32	1.22
3	C	402	AKG	O1-C1	2.95	1.29	1.22
3	A	402	AKG	O2-C1	-2.76	1.23	1.30
3	C	402	AKG	O2-C1	-2.73	1.23	1.30
3	A	402	AKG	O4-C5	-2.66	1.22	1.30
3	C	402	AKG	O4-C5	-2.33	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	AKG	O1-C1-C2	-8.85	110.80	121.81
3	A	402	AKG	O1-C1-C2	-7.80	112.11	121.81
3	C	402	AKG	O2-C1-C2	4.72	126.67	113.59
3	A	402	AKG	O2-C1-C2	4.26	125.39	113.59
3	B	402	AKG	O1-C1-C2	3.41	126.06	121.81
3	C	402	AKG	O4-C5-C4	3.16	123.98	114.00
3	C	402	AKG	O3-C5-C4	-3.15	113.10	123.09
3	D	402	AKG	O1-C1-C2	3.09	125.65	121.81
3	A	402	AKG	O3-C5-C4	-2.80	114.20	123.09
3	A	402	AKG	O4-C5-C4	2.57	122.13	114.00
3	B	402	AKG	C3-C2-C1	2.16	119.53	115.86
3	A	402	AKG	C3-C2-C1	2.10	119.44	115.86
3	D	402	AKG	C3-C2-C1	2.09	119.41	115.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	AKG	C1-C2-C3-C4
3	B	402	AKG	O2-C1-C2-C3
3	B	402	AKG	C1-C2-C3-C4
3	C	402	AKG	O1-C1-C2-C3
3	C	402	AKG	O2-C1-C2-O5
3	C	402	AKG	O2-C1-C2-C3
3	C	402	AKG	C1-C2-C3-C4
3	D	402	AKG	C1-C2-C3-C4
4	A	404	GOL	O1-C1-C2-C3
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2
4	C	405	GOL	O1-C1-C2-O2
3	C	402	AKG	O1-C1-C2-O5
3	B	402	AKG	O1-C1-C2-C3
3	C	402	AKG	O5-C2-C3-C4
3	B	402	AKG	O1-C1-C2-O5
3	B	402	AKG	C2-C3-C4-C5
3	A	402	AKG	C3-C4-C5-O3
3	A	402	AKG	C3-C4-C5-O4

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	GOL	5	0
4	C	404	GOL	1	0
4	C	405	GOL	1	0
4	A	404	GOL	1	0
4	A	403	GOL	2	0
4	A	405	GOL	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	343/372 (92%)	-0.19	5 (1%) 72 73	18, 44, 78, 112	6 (1%)
1	B	328/372 (88%)	0.33	26 (7%) 18 20	19, 52, 117, 158	19 (5%)
1	C	346/372 (93%)	0.20	10 (2%) 53 56	31, 58, 107, 139	0
1	D	344/372 (92%)	0.06	4 (1%) 76 77	22, 55, 123, 173	1 (0%)
All	All	1361/1488 (91%)	0.10	45 (3%) 49 51	18, 52, 109, 173	26 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166[A]	GLY	5.7
1	B	173[A]	LEU	5.7
1	B	163[A]	THR	4.5
1	B	160[A]	MET	4.4
1	B	162[A]	ALA	4.4
1	C	17	LEU	3.9
1	C	162	ALA	3.7
1	D	162	ALA	3.6
1	B	174[A]	PHE	3.5
1	B	172[A]	ASP	3.5
1	B	171[A]	THR	3.4
1	D	323	ILE	3.4
1	B	165[A]	THR	3.3
1	C	325	ASN	3.2
1	B	167[A]	SER	3.2
1	B	164[A]	GLN	3.2
1	B	161[A]	ALA	3.1
1	B	329	ILE	3.1
1	C	266	PHE	3.1
1	C	165	THR	2.9
1	D	325	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLY	2.8
1	B	159	LYS	2.8
1	B	168[A]	GLY	2.8
1	D	328	ILE	2.7
1	B	117	TYR	2.7
1	C	171	THR	2.7
1	B	170[A]	LYS	2.6
1	B	266	PHE	2.6
1	C	18	THR	2.6
1	B	330	LYS	2.5
1	B	328	ILE	2.5
1	A	325	ASN	2.4
1	B	155	ILE	2.3
1	A	162	ALA	2.3
1	C	242	GLY	2.3
1	C	213	MET	2.3
1	B	314	ARG	2.3
1	B	112	TRP	2.2
1	C	265	ILE	2.2
1	A	161	ALA	2.2
1	B	107	PRO	2.1
1	A	99	GLU	2.0
1	A	266	PHE	2.0
1	B	110	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	GOL	A	405	6/6	0.65	0.18	92,93,93,93	0
4	GOL	D	404	6/6	0.69	0.20	92,98,99,99	0
4	GOL	D	403	6/6	0.73	0.18	89,91,92,95	0
4	GOL	C	405	6/6	0.85	0.14	64,71,73,73	0
3	AKG	B	402	10/10	0.86	0.16	93,96,99,101	0
4	GOL	B	403	6/6	0.86	0.15	85,87,89,91	0
4	GOL	C	404	6/6	0.86	0.11	78,83,86,88	0
3	AKG	C	402	10/10	0.87	0.14	82,83,84,84	0
3	AKG	D	402	10/10	0.87	0.15	80,86,91,91	0
4	GOL	A	403	6/6	0.88	0.12	76,76,78,81	0
4	GOL	A	406	6/6	0.89	0.12	46,53,54,55	0
4	GOL	A	404	6/6	0.91	0.10	63,66,67,70	0
4	GOL	C	403	6/6	0.91	0.11	54,62,63,65	0
3	AKG	A	402	10/10	0.95	0.10	60,65,71,74	0
2	FE	C	401	1/1	0.99	0.05	58,58,58,58	0
2	FE	D	401	1/1	0.99	0.04	61,61,61,61	0
2	FE	A	401	1/1	0.99	0.03	50,50,50,50	0
2	FE	B	401	1/1	0.99	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.