



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:46 AM GMT

PDB ID : 2II5  
Title : Crystal structure of a cubic core of the dihydrolipoamide acyltransferase (E2b) component in the branched-chain alpha-ketoacid dehydrogenase complex (BCKDC), Isobutyryl-Coenzyme A-bound form  
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Brautigam, C.A.; Custorio, M.; Chuang, D.T.  
Deposited on : 2006-09-27  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

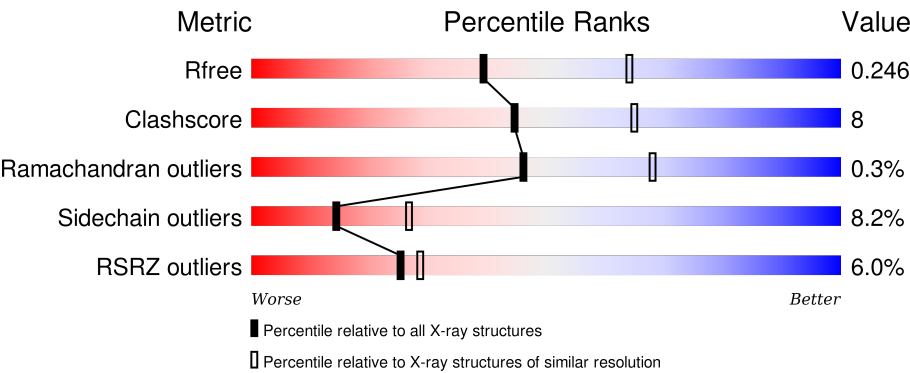
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 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 2.50 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 <sub>free</sub>	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	262	<div><div>3%</div><div>69%18%•11%</div></div>
1	B	262	<div><div>7%</div><div>72%15%•11%</div></div>
1	C	262	<div><div>5%</div><div>72%16%•11%</div></div>
1	D	262	<div><div>5%</div><div>65%24%11%</div></div>
1	E	262	<div><div>5%</div><div>74%13%•11%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	262	
1	G	262	
1	H	262	

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
2	ACT	A	601	-	-	X	-
2	ACT	B	600	-	-	X	-
2	ACT	B	601	-	-	X	-
2	ACT	C	600	-	-	X	-
2	ACT	C	601	-	-	X	-
2	ACT	E	600	-	-	X	-
2	ACT	E	601	-	-	X	X
2	ACT	G	601	-	-	-	X
2	ACT	H	600	-	-	X	-
2	ACT	H	601	-	-	X	-
3	CL	A	803	-	-	X	-
3	CL	A	808	-	-	-	X
3	CL	B	806	-	-	X	-
3	CL	C	802	-	-	-	X
3	CL	D	809	-	-	-	X
3	CL	E	804	-	-	X	-
3	CL	F	805	-	-	-	X
3	CL	H	801	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14899 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 Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	B	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	C	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	D	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	E	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	F	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	G	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	H	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			

There are 16 discrepancies between the modelled and reference sequences:

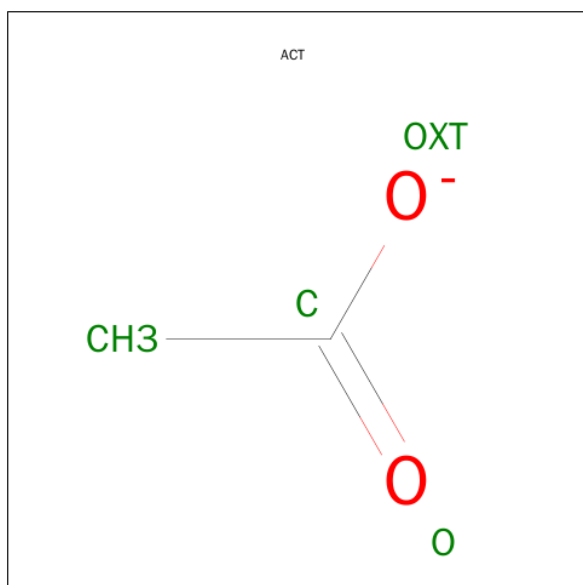
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLY	-	CLONING ARTIFACT	UNP P11181
A	161	HIS	-	CLONING ARTIFACT	UNP P11181
B	160	GLY	-	CLONING ARTIFACT	UNP P11181
B	161	HIS	-	CLONING ARTIFACT	UNP P11181
C	160	GLY	-	CLONING ARTIFACT	UNP P11181
C	161	HIS	-	CLONING ARTIFACT	UNP P11181
D	160	GLY	-	CLONING ARTIFACT	UNP P11181
D	161	HIS	-	CLONING ARTIFACT	UNP P11181
E	160	GLY	-	CLONING ARTIFACT	UNP P11181
E	161	HIS	-	CLONING ARTIFACT	UNP P11181
F	160	GLY	-	CLONING ARTIFACT	UNP P11181
F	161	HIS	-	CLONING ARTIFACT	UNP P11181

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Chain	Residue	Modelled	Actual	Comment	Reference
G	160	GLY	-	CLONING ARTIFACT	UNP P11181
G	161	HIS	-	CLONING ARTIFACT	UNP P11181
H	160	GLY	-	CLONING ARTIFACT	UNP P11181
H	161	HIS	-	CLONING ARTIFACT	UNP P11181

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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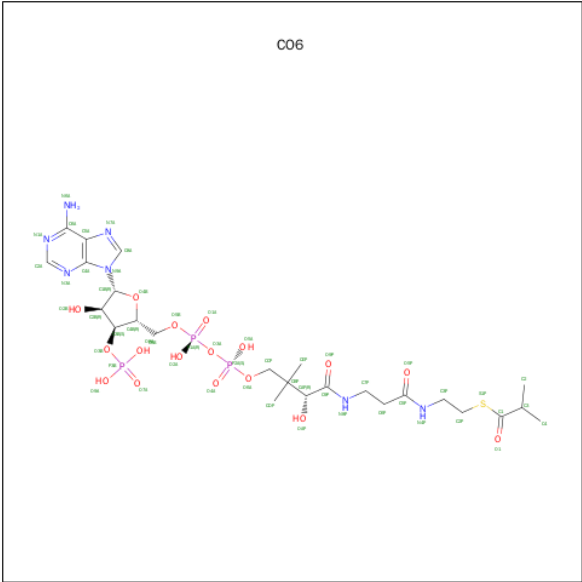
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0
3	E	1	Total Cl 1 1	0	0
3	H	2	Total Cl 2 2	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	2	Total Cl 2 2	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is ISOBUTYRYL-COENZYME A (three-letter code: CO6) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			40	16	6	15	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	19	Total	O	0	0
			19	19		
5	C	14	Total	O	0	0
			14	14		
5	D	19	Total	O	0	0
			19	19		

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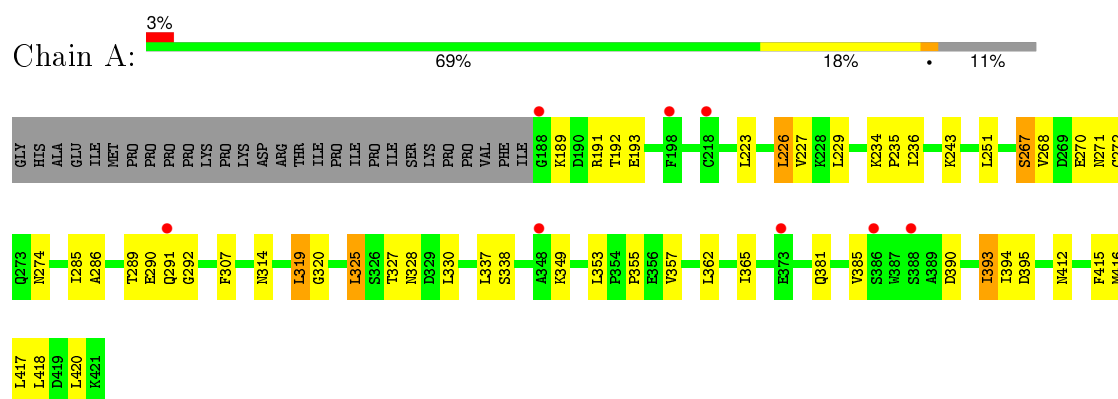
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	20	Total 20	O 20	0	0
5	F	17	Total 17	O 17	0	0
5	G	10	Total 10	O 10	0	0
5	H	27	Total 27	O 27	0	0



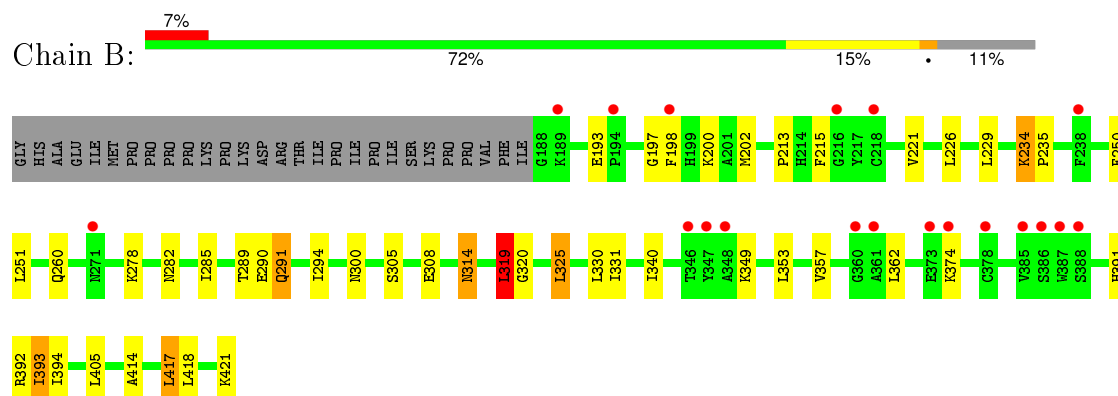
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

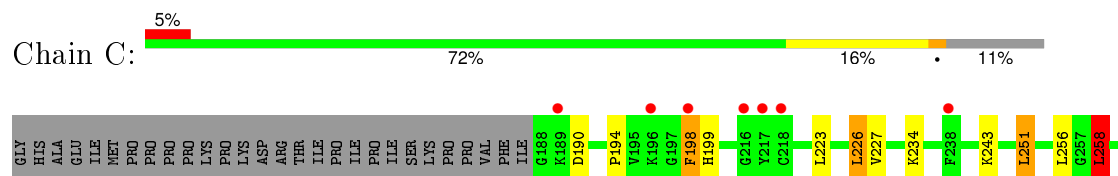
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

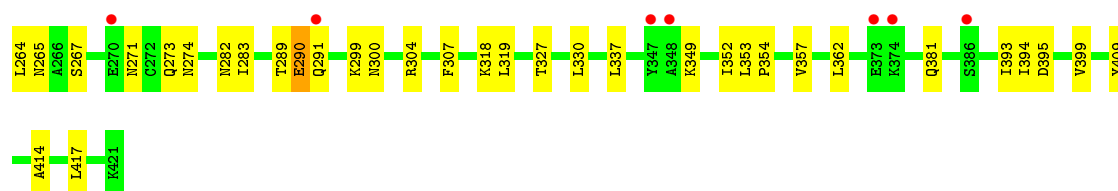


- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

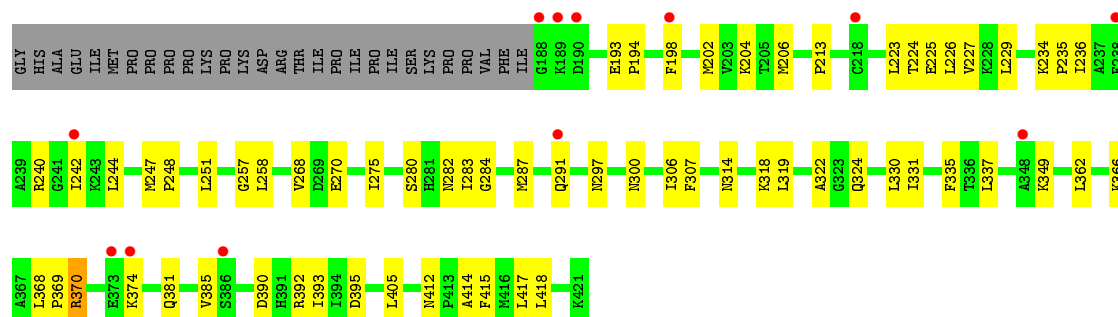


- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

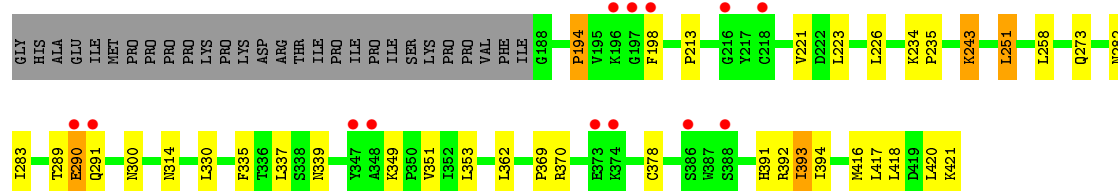
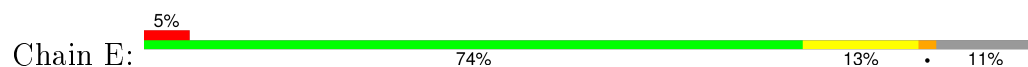




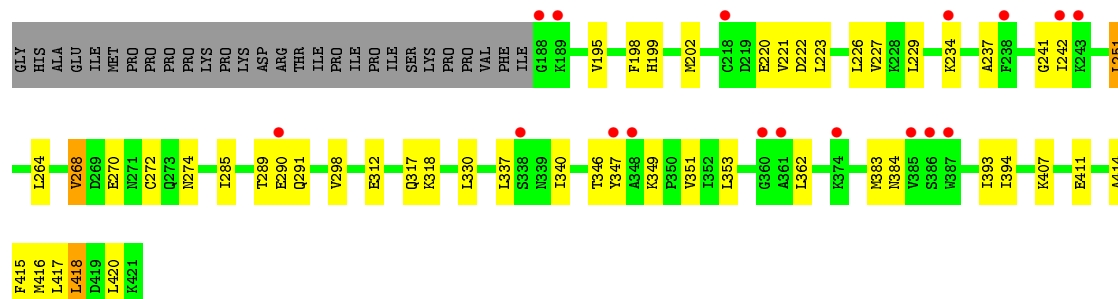
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



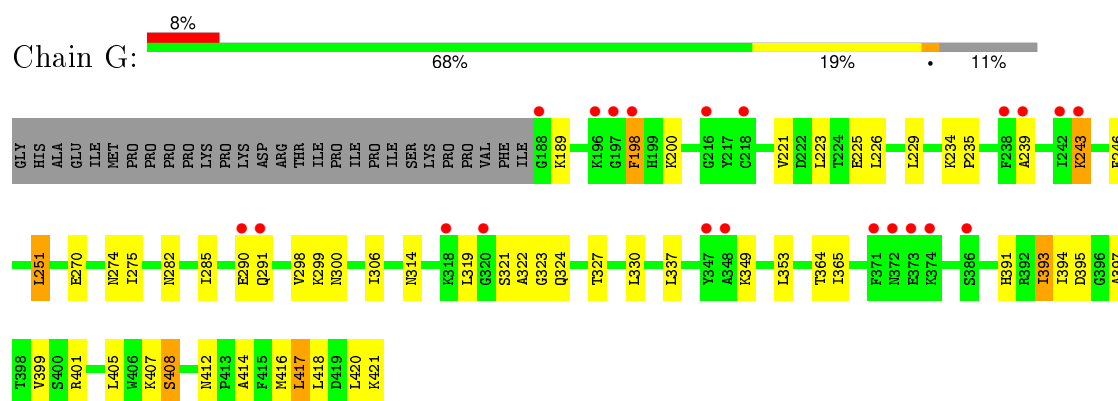
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



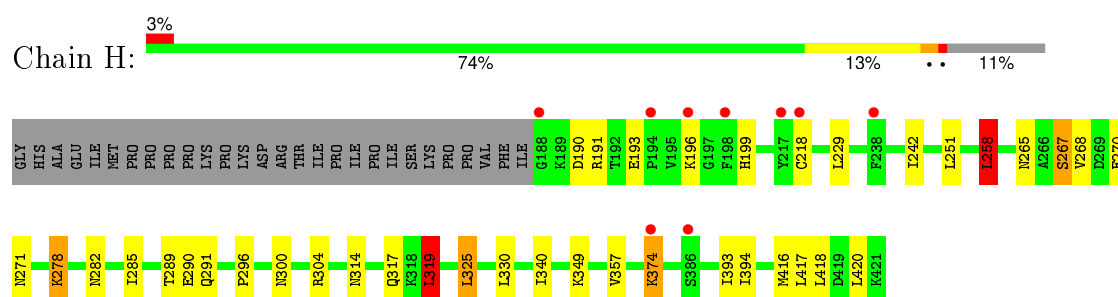
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.77Å 194.77Å 172.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 40.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.50) 99.5 (40.96-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.251 0.196 , 0.246	Depositor DCC
$R_{free}$ test set	4196 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.0	EDS
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 84134 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CO6, ACT

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	0.96	0/1837	0.92	3/2481 (0.1%)
1	B	1.00	0/1837	0.90	3/2481 (0.1%)
1	C	0.93	1/1837 (0.1%)	0.87	3/2481 (0.1%)
1	D	0.91	0/1837	0.89	3/2481 (0.1%)
1	E	0.94	1/1837 (0.1%)	0.90	1/2481 (0.0%)
1	F	0.91	0/1837	0.88	2/2481 (0.1%)
1	G	0.88	0/1837	0.84	0/2481
1	H	0.97	1/1837 (0.1%)	0.92	3/2481 (0.1%)
All	All	0.94	3/14696 (0.0%)	0.89	18/19848 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	378	CYS	CB-SG	-6.39	1.71	1.82
1	H	218	CYS	CB-SG	-5.42	1.73	1.81
1	C	307	PHE	CE2-CZ	5.08	1.47	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	390	ASP	CB-CG-OD1	6.88	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	390	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	395	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	B	417	LEU	CA-CB-CG	5.81	128.65	115.30
1	C	258	LEU	CA-CB-CG	5.75	128.53	115.30
1	H	190	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	202	MET	CG-SD-CE	5.45	108.92	100.20
1	D	202	MET	CG-SD-CE	5.29	108.66	100.20
1	C	190	ASP	CB-CG-OD1	5.23	123.01	118.30
1	H	258	LEU	CB-CG-CD1	5.10	119.67	111.00
1	C	395	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	319	LEU	CA-CB-CG	5.07	126.95	115.30
1	F	362	LEU	CA-CB-CG	-5.05	103.68	115.30
1	F	202	MET	CG-SD-CE	5.04	108.27	100.20
1	H	319	LEU	CA-CB-CG	5.03	126.87	115.30
1	E	362	LEU	CA-CB-CG	-5.03	103.74	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	GLY	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1803	0	1859	31	0
1	B	1803	0	1859	27	0
1	C	1803	0	1859	30	0
1	D	1803	0	1859	35	0
1	E	1803	0	1859	21	0
1	F	1803	0	1859	33	0
1	G	1803	0	1859	28	0
1	H	1803	0	1859	21	0
2	A	8	0	6	2	0
2	B	8	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	6	2	0
2	D	8	0	6	0	0
2	E	8	0	6	3	0
2	F	8	0	6	1	0
2	G	8	0	6	0	0
2	H	8	0	6	3	0
3	A	2	0	0	2	0
3	B	1	0	0	2	0
3	C	1	0	0	1	0
3	D	2	0	0	1	0
3	E	1	0	0	2	0
3	F	1	0	0	1	0
3	G	2	0	0	1	0
3	H	2	0	0	1	0
4	A	31	0	11	1	0
4	B	31	0	11	0	0
4	C	31	0	11	1	0
4	D	31	0	11	2	0
4	E	40	0	21	1	0
4	F	31	0	11	1	0
4	G	31	0	11	2	0
4	H	31	0	11	0	0
5	A	16	0	0	0	0
5	B	19	0	0	1	0
5	C	14	0	0	1	0
5	D	19	0	0	0	0
5	E	20	0	0	1	0
5	F	17	0	0	2	0
5	G	10	0	0	2	0
5	H	27	0	0	0	0
All	All	14899	0	15018	235	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 8.

All (235) 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)
2:E:600:ACT:H1	2:E:601:ACT:H3	1.39	1.02
1:F:198:PHE:HE2	1:F:199:HIS:CE1	1.81	0.97
4:F:500:CO6:O4A	4:F:500:CO6:H8	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:ACT:H1	2:A:601:ACT:H2	1.48	0.95
3:A:803:CL:CL	5:B:83:HOH:O	2.23	0.93
1:E:251:LEU:CD1	1:E:337:LEU:HD12	2.00	0.92
1:B:260:GLN:HG3	1:B:405:LEU:HD21	1.51	0.91
2:C:600:ACT:H1	2:C:601:ACT:H3	1.53	0.90
1:B:349:LYS:NZ	3:B:806:CL:CL	2.41	0.90
1:B:260:GLN:HG3	1:B:405:LEU:CD2	2.05	0.86
1:C:299:LYS:O	1:C:304:ARG:NH1	2.10	0.84
1:A:251:LEU:HD12	1:A:337:LEU:HD12	1.58	0.84
1:H:349:LYS:NZ	3:H:801:CL:CL	2.47	0.84
1:G:282:ASN:ND2	1:G:300:ASN:H	1.74	0.83
1:A:251:LEU:HD21	1:A:285:ILE:HD11	1.62	0.82
2:E:600:ACT:H1	2:E:601:ACT:CH3	2.10	0.81
1:C:289:THR:HG22	1:C:291:GLN:H	1.46	0.81
1:C:349:LYS:NZ	3:C:802:CL:CL	2.51	0.80
1:F:198:PHE:CE2	1:F:199:HIS:CE1	2.70	0.80
1:B:319:LEU:HB3	1:B:325:LEU:HD13	1.64	0.80
1:B:320:GLY:HA2	1:B:325:LEU:HD22	1.62	0.79
1:A:319:LEU:HB3	1:A:325:LEU:HD13	1.64	0.79
2:H:600:ACT:H3	2:H:601:ACT:H3	1.63	0.79
1:B:251:LEU:HD21	1:B:285:ILE:HD11	1.63	0.78
1:F:223:LEU:O	1:F:227:VAL:HG23	1.84	0.77
1:A:349:LYS:NZ	3:A:803:CL:CL	2.54	0.77
1:G:282:ASN:HD22	1:G:300:ASN:H	1.32	0.77
1:A:274:ASN:HD22	1:C:194:PRO:HA	1.50	0.77
1:D:227:VAL:HG21	1:D:381:GLN:HG2	1.65	0.77
1:C:393:ILE:HD12	1:C:394:ILE:HG13	1.66	0.76
1:F:393:ILE:CD1	1:F:394:ILE:HG13	2.16	0.76
1:F:264:LEU:HD23	1:F:394:ILE:HD13	1.68	0.75
1:H:191:ARG:NH1	1:H:193:GLU:OE2	2.21	0.73
1:F:393:ILE:HD12	1:F:394:ILE:HG13	1.67	0.73
1:C:198:PHE:HD2	1:C:198:PHE:N	1.86	0.72
1:C:289:THR:HG22	1:C:291:GLN:N	2.04	0.72
1:D:370:ARG:HG2	1:D:370:ARG:HH11	1.55	0.72
3:E:804:CL:CL	5:F:99:HOH:O	2.45	0.71
1:H:393:ILE:HD12	1:H:394:ILE:HG13	1.72	0.71
1:B:289:THR:HG22	1:B:291:GLN:H	1.55	0.70
1:G:416:MET:O	1:G:420:LEU:HG	1.92	0.70
1:F:251:LEU:HD12	1:F:337:LEU:HD12	1.74	0.69
1:C:198:PHE:CD2	1:C:198:PHE:N	2.53	0.69
1:E:349:LYS:NZ	3:E:804:CL:CL	2.63	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ALA:O	1:C:417:LEU:HB2	1.93	0.68
1:A:274:ASN:ND2	1:C:194:PRO:HA	2.09	0.67
1:C:289:THR:C	1:C:291:GLN:H	1.97	0.67
1:A:229:LEU:HD13	1:F:414:ALA:HB1	1.77	0.66
1:A:320:GLY:HA2	1:A:325:LEU:HD22	1.78	0.66
1:B:197:GLY:O	1:B:200:LYS:HB2	1.96	0.66
2:C:600:ACT:CH3	2:C:601:ACT:H3	2.26	0.65
1:D:282:ASN:HD22	1:D:300:ASN:H	1.42	0.64
1:F:414:ALA:O	1:F:417:LEU:HB2	1.97	0.64
2:H:600:ACT:H3	2:H:601:ACT:CH3	2.27	0.64
1:D:282:ASN:ND2	1:D:300:ASN:H	1.96	0.64
1:B:289:THR:HG22	1:B:290:GLU:N	2.13	0.64
3:B:806:CL:CL	5:C:110:HOH:O	2.52	0.63
1:G:251:LEU:HD21	1:G:285:ILE:HD11	1.79	0.63
1:E:243:LYS:H	1:E:314:ASN:HD21	1.44	0.62
1:E:213:PRO:HG2	1:E:392:ARG:HG3	1.80	0.62
1:G:349:LYS:NZ	3:G:812:CL:CL	2.69	0.62
1:D:223:LEU:O	1:D:227:VAL:HG23	1.99	0.62
1:C:264:LEU:HD23	1:C:394:ILE:HD13	1.81	0.62
1:F:349:LYS:NZ	3:F:805:CL:CL	2.69	0.62
1:E:282:ASN:HD22	1:E:300:ASN:H	1.47	0.61
1:D:227:VAL:HG21	1:D:381:GLN:CG	2.30	0.61
1:A:229:LEU:CD1	1:F:414:ALA:HB1	2.31	0.61
4:C:500:CO6:O4A	4:C:500:CO6:H8	2.01	0.61
1:H:319:LEU:HB3	1:H:325:LEU:HD13	1.83	0.61
1:B:314:ASN:HD22	1:B:314:ASN:N	1.99	0.60
1:H:357:VAL:HG21	1:H:394:ILE:HD11	1.83	0.60
1:F:241:GLY:O	1:F:242:ILE:HD13	2.02	0.60
1:A:365:ILE:HG13	4:A:500:CO6:N1A	2.17	0.60
1:D:349:LYS:NZ	3:D:811:CL:CL	2.71	0.60
1:G:393:ILE:HD13	1:G:393:ILE:H	1.67	0.59
1:B:414:ALA:O	1:B:417:LEU:HB2	2.02	0.59
1:E:194:PRO:HA	1:F:274:ASN:HD22	1.66	0.59
1:E:416:MET:O	1:E:420:LEU:HG	2.03	0.59
1:B:305:SER:OG	1:B:308:GLU:HG3	2.02	0.59
1:G:223:LEU:HA	5:G:132:HOH:O	2.02	0.59
1:D:236:ILE:O	1:D:240:ARG:HG3	2.02	0.58
1:D:242:ILE:HG23	1:D:314:ASN:ND2	2.18	0.58
1:F:298:VAL:HG13	1:F:312:GLU:HG2	1.85	0.58
1:H:357:VAL:CG2	1:H:394:ILE:HD11	2.34	0.58
1:E:251:LEU:HD12	1:E:337:LEU:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:ACT:CH3	2:H:601:ACT:H3	2.31	0.57
1:F:416:MET:O	1:F:420:LEU:HG	2.03	0.57
1:F:251:LEU:CD1	1:F:337:LEU:HD12	2.34	0.57
1:H:267:SER:HB2	1:H:278:LYS:HE3	1.87	0.56
1:H:282:ASN:HD22	1:H:300:ASN:H	1.52	0.56
1:G:397:ALA:O	1:G:401:ARG:HG3	2.05	0.56
1:C:223:LEU:HD22	1:C:226:LEU:HD12	1.87	0.56
1:A:267:SER:OG	1:A:355:PRO:HB2	2.06	0.56
1:E:234:LYS:HB2	1:E:235:PRO:HD3	1.88	0.56
1:F:220:GLU:O	1:F:407:LYS:HE3	2.05	0.56
1:E:393:ILE:HD13	1:E:394:ILE:HG13	1.87	0.55
1:C:357:VAL:HG11	1:C:393:ILE:HD11	1.89	0.54
1:C:289:THR:C	1:C:291:GLN:N	2.61	0.54
1:D:370:ARG:HG2	1:D:370:ARG:NH1	2.22	0.54
1:B:289:THR:CG2	1:B:290:GLU:N	2.70	0.54
1:A:307:PHE:HB2	1:F:418:LEU:HD22	1.90	0.54
2:A:601:ACT:O	1:B:391:HIS:NE2	2.40	0.53
1:H:251:LEU:HD21	1:H:285:ILE:HD11	1.89	0.53
1:B:282:ASN:ND2	1:B:300:ASN:H	2.06	0.53
1:C:289:THR:CG2	1:C:290:GLU:N	2.71	0.53
1:E:339:ASN:HB3	4:E:500:CO6:H132	1.91	0.53
1:B:282:ASN:HD22	1:B:300:ASN:H	1.55	0.53
1:F:234:LYS:O	1:F:237:ALA:HB3	2.09	0.53
1:G:405:LEU:O	1:G:408:SER:HB2	2.08	0.53
1:B:213:PRO:HG2	1:B:392:ARG:HG3	1.92	0.53
1:G:251:LEU:CD1	1:G:337:LEU:HD12	2.38	0.52
1:B:250:PHE:CD2	1:B:362:LEU:HD13	2.45	0.51
4:G:500:CO6:O4A	4:G:500:CO6:H8	2.10	0.51
1:G:282:ASN:HD22	1:G:300:ASN:N	2.05	0.51
1:D:268:VAL:HG11	1:D:393:ILE:HG12	1.92	0.51
1:G:282:ASN:ND2	1:G:299:LYS:HA	2.26	0.51
1:H:282:ASN:ND2	1:H:300:ASN:H	2.08	0.51
2:B:600:ACT:H1	2:B:601:ACT:CH3	2.41	0.50
1:H:258:LEU:HG	1:H:265:ASN:HB2	1.93	0.50
1:C:258:LEU:HG	1:C:265:ASN:HB2	1.92	0.50
1:F:351:VAL:O	2:F:600:ACT:OXT	2.28	0.50
1:B:314:ASN:H	1:B:314:ASN:HD22	1.60	0.49
1:A:286:ALA:HB3	1:A:338:SER:HB2	1.94	0.49
1:E:251:LEU:HD11	1:E:337:LEU:HD12	1.88	0.49
1:D:213:PRO:HG2	1:D:392:ARG:HG3	1.94	0.49
1:F:251:LEU:HD21	1:F:285:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:HG13	1:D:307:PHE:CE1	2.48	0.49
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.94	0.49
1:A:243:LYS:H	1:A:314:ASN:HD21	1.61	0.49
1:A:268:VAL:HG13	1:A:272:CYS:HA	1.94	0.48
1:D:414:ALA:O	1:D:417:LEU:HB2	2.14	0.48
1:C:289:THR:HG22	1:C:290:GLU:N	2.28	0.48
1:C:282:ASN:HD22	1:C:300:ASN:H	1.61	0.48
1:G:365:ILE:HG13	4:G:500:CO6:N1A	2.29	0.48
1:H:242:ILE:HG23	1:H:314:ASN:ND2	2.29	0.48
4:D:500:CO6:P2A	4:D:500:CO6:H5'1	2.54	0.47
1:H:416:MET:O	1:H:420:LEU:HG	2.14	0.47
1:C:227:VAL:HG21	1:C:381:GLN:HG3	1.96	0.47
1:C:251:LEU:HD12	1:C:283:ILE:HG21	1.96	0.47
1:B:234:LYS:N	1:B:235:PRO:HD2	2.28	0.47
1:D:257:GLY:HA2	1:D:405:LEU:HD23	1.96	0.47
1:H:270:GLU:HA	1:H:270:GLU:OE1	2.14	0.47
1:D:206:MET:HG3	1:E:391:HIS:O	2.13	0.47
1:D:251:LEU:HD23	1:D:337:LEU:HD12	1.96	0.47
1:D:275:ILE:HD11	1:F:195:VAL:HG22	1.96	0.47
1:C:198:PHE:H	1:C:198:PHE:HD2	1.37	0.47
1:A:357:VAL:HB	1:A:394:ILE:HD11	1.97	0.47
1:A:229:LEU:HD12	1:A:229:LEU:O	2.16	0.46
1:B:340:ILE:HG12	1:B:362:LEU:O	2.15	0.46
1:G:234:LYS:HB2	1:G:235:PRO:HD3	1.98	0.46
1:G:322:ALA:O	1:G:324:GLN:HG2	2.16	0.46
1:A:192:THR:HG22	1:A:193:GLU:N	2.31	0.46
1:A:191:ARG:HD2	1:A:193:GLU:OE2	2.16	0.46
1:A:223:LEU:HD22	1:A:226:LEU:HD12	1.97	0.46
1:E:251:LEU:CD1	1:E:337:LEU:CD1	2.84	0.46
1:A:227:VAL:HG21	1:A:381:GLN:HG2	1.97	0.46
1:F:268:VAL:HG21	1:F:393:ILE:HG12	1.99	0.45
1:G:243:LYS:H	1:G:314:ASN:HD21	1.63	0.45
1:G:414:ALA:O	1:G:417:LEU:HB2	2.17	0.45
1:E:351:VAL:O	2:E:600:ACT:O	2.34	0.45
1:A:357:VAL:HG11	1:A:393:ILE:HD11	1.99	0.45
1:A:234:LYS:N	1:A:235:PRO:CD	2.79	0.45
1:F:393:ILE:HD13	1:F:394:ILE:HG13	1.94	0.45
1:A:289:THR:C	1:A:291:GLN:H	2.19	0.44
1:B:215:PHE:HB2	1:B:391:HIS:HD2	1.82	0.44
1:B:193:GLU:O	1:C:274:ASN:HA	2.18	0.44
1:H:268:VAL:HG21	1:H:393:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:ACT:CH3	2:B:601:ACT:H2	2.47	0.44
1:F:221:VAL:HG12	1:F:383:MET:O	2.18	0.44
1:G:251:LEU:HD12	1:G:251:LEU:HA	1.72	0.44
1:G:323:GLY:HA2	5:G:121:HOH:O	2.16	0.44
1:D:234:LYS:O	1:D:235:PRO:C	2.56	0.44
1:F:222:ASP:O	1:F:411:GLU:HG2	2.17	0.44
1:C:256:LEU:HB3	1:C:409:TYR:CE2	2.53	0.44
1:D:244:LEU:HD12	1:D:248:PRO:HG2	2.00	0.44
1:G:282:ASN:HA	1:G:298:VAL:O	2.18	0.43
1:F:349:LYS:O	1:F:349:LYS:HD3	2.18	0.43
1:E:223:LEU:HA	5:E:106:HOH:O	2.17	0.43
1:C:352:ILE:O	1:C:354:PRO:HD3	2.18	0.43
1:G:221:VAL:HG13	1:G:407:LYS:HG3	2.00	0.43
1:B:393:ILE:HD12	1:B:394:ILE:HG13	2.00	0.43
1:E:282:ASN:ND2	1:E:300:ASN:H	2.12	0.43
1:G:198:PHE:HD1	1:G:291:GLN:HB2	1.83	0.43
1:F:415:PHE:CD1	1:F:415:PHE:N	2.85	0.43
1:D:415:PHE:CD1	1:D:415:PHE:N	2.86	0.43
1:H:374:LYS:H	1:H:374:LYS:HD2	1.84	0.43
1:D:229:LEU:O	1:D:229:LEU:HD12	2.18	0.43
1:H:289:THR:C	1:H:291:GLN:H	2.22	0.43
1:D:247:MET:O	1:D:251:LEU:HG	2.18	0.43
1:B:357:VAL:HB	1:B:394:ILE:HD11	1.99	0.43
1:A:417:LEU:O	1:A:418:LEU:C	2.57	0.43
1:A:319:LEU:CB	1:A:325:LEU:HD13	2.42	0.42
1:A:415:PHE:CD1	1:A:415:PHE:N	2.87	0.42
1:H:285:ILE:O	1:H:296:PRO:HD2	2.18	0.42
1:F:340:ILE:HD13	1:F:340:ILE:HG21	1.73	0.42
1:D:284:GLY:HA2	1:D:297:ASN:HA	2.02	0.42
1:H:300:ASN:O	1:H:304:ARG:HG2	2.19	0.42
1:F:229:LEU:C	1:F:229:LEU:HD23	2.40	0.42
1:A:362:LEU:HD23	1:A:385:VAL:HG23	2.00	0.42
1:D:385:VAL:HG13	1:D:385:VAL:O	2.18	0.42
4:D:500:CO6:H5'1	4:D:500:CO6:O6A	2.20	0.42
1:D:270:GLU:OE1	1:D:270:GLU:HA	2.19	0.42
1:E:283:ILE:HA	1:E:335:PHE:O	2.20	0.42
1:C:299:LYS:HB2	1:C:304:ARG:HH12	1.84	0.42
1:C:282:ASN:ND2	1:C:299:LYS:HA	2.35	0.42
1:C:198:PHE:HD1	1:C:291:GLN:HB3	1.85	0.42
1:D:415:PHE:HD1	1:D:415:PHE:N	2.18	0.42
1:H:196:LYS:O	1:H:199:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:THR:C	1:F:291:GLN:N	2.72	0.42
1:E:289:THR:C	1:E:291:GLN:N	2.73	0.41
1:D:283:ILE:HA	1:D:335:PHE:O	2.20	0.41
1:A:416:MET:O	1:A:420:LEU:HG	2.19	0.41
1:E:251:LEU:HA	1:E:251:LEU:HD12	1.79	0.41
1:G:393:ILE:HD13	1:G:393:ILE:N	2.33	0.41
1:G:393:ILE:CD1	1:G:394:ILE:HD12	2.51	0.41
1:G:226:LEU:HD23	1:G:246:PHE:HD1	1.86	0.41
1:B:391:HIS:ND1	1:B:391:HIS:O	2.54	0.41
1:E:369:PRO:O	1:E:370:ARG:HG2	2.21	0.41
1:D:224:THR:HA	1:D:381:GLN:HB2	2.03	0.41
1:D:193:GLU:HA	1:D:194:PRO:HD2	1.91	0.41
1:G:391:HIS:CE1	1:G:395:ASP:HA	2.56	0.41
1:F:346:THR:OG1	1:F:347:TYR:N	2.51	0.41
1:G:282:ASN:HD22	1:G:299:LYS:HA	1.85	0.41
1:C:198:PHE:CE2	1:C:199:HIS:CE1	3.09	0.41
1:D:368:LEU:HA	1:D:369:PRO:HD3	1.88	0.41
1:F:384:ASN:HB2	5:F:17:HOH:O	2.20	0.41
1:D:322:ALA:CB	1:D:324:GLN:HG3	2.50	0.41
1:D:390:ASP:OD2	1:D:392:ARG:NH2	2.32	0.40
1:D:280:SER:HB3	1:D:282:ASN:HD21	1.85	0.40
1:G:393:ILE:CD1	1:G:393:ILE:H	2.33	0.40
1:H:374:LYS:H	1:H:374:LYS:CD	2.35	0.40
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.95	0.40
1:D:280:SER:HB3	1:D:282:ASN:ND2	2.36	0.40
1:B:314:ASN:ND2	1:B:314:ASN:H	2.18	0.40
1:C:251:LEU:HD13	1:C:337:LEU:HD12	2.02	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	232/262 (88%)	220 (95%)	12 (5%)	0	100	100
1	B	232/262 (88%)	222 (96%)	10 (4%)	0	100	100
1	C	232/262 (88%)	222 (96%)	9 (4%)	1 (0%)	39	61
1	D	232/262 (88%)	217 (94%)	15 (6%)	0	100	100
1	E	232/262 (88%)	223 (96%)	7 (3%)	2 (1%)	21	37
1	F	232/262 (88%)	218 (94%)	13 (6%)	1 (0%)	39	61
1	G	232/262 (88%)	218 (94%)	13 (6%)	1 (0%)	39	61
1	H	232/262 (88%)	224 (97%)	7 (3%)	1 (0%)	39	61
All	All	1856/2096 (88%)	1764 (95%)	86 (5%)	6 (0%)	46	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	GLU
1	F	272	CYS
1	G	239	ALA
1	H	290	GLU
1	E	194	PRO
1	E	290	GLU

### 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	196/222 (88%)	181 (92%)	15 (8%)	16	30
1	B	196/222 (88%)	178 (91%)	18 (9%)	11	21
1	C	196/222 (88%)	180 (92%)	16 (8%)	14	27
1	D	196/222 (88%)	178 (91%)	18 (9%)	11	21
1	E	196/222 (88%)	182 (93%)	14 (7%)	18	34
1	F	196/222 (88%)	186 (95%)	10 (5%)	29	52
1	G	196/222 (88%)	171 (87%)	25 (13%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	196/222 (88%)	183 (93%)	13 (7%)	21	38
All	All	1568/1776 (88%)	1439 (92%)	129 (8%)	14	27

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	226	LEU
1	A	236	ILE
1	A	267	SER
1	A	270	GLU
1	A	271	ASN
1	A	290	GLU
1	A	319	LEU
1	A	325	LEU
1	A	327	THR
1	A	328	ASN
1	A	330	LEU
1	A	353	LEU
1	A	393	ILE
1	A	412	ASN
1	B	198	PHE
1	B	221	VAL
1	B	226	LEU
1	B	229	LEU
1	B	234	LYS
1	B	278	LYS
1	B	291	GLN
1	B	294	ILE
1	B	314	ASN
1	B	319	LEU
1	B	325	LEU
1	B	330	LEU
1	B	331	ILE
1	B	353	LEU
1	B	374	LYS
1	B	393	ILE
1	B	418	LEU
1	B	421	LYS
1	C	198	PHE
1	C	226	LEU
1	C	234	LYS

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Mol	Chain	Res	Type
1	C	243	LYS
1	C	251	LEU
1	C	258	LEU
1	C	267	SER
1	C	271	ASN
1	C	273	GLN
1	C	318	LYS
1	C	319	LEU
1	C	327	THR
1	C	330	LEU
1	C	353	LEU
1	C	362	LEU
1	C	399	VAL
1	D	198	PHE
1	D	204	LYS
1	D	225	GLU
1	D	226	LEU
1	D	258	LEU
1	D	287	MET
1	D	291	GLN
1	D	306	ILE
1	D	318	LYS
1	D	319	LEU
1	D	330	LEU
1	D	331	ILE
1	D	362	LEU
1	D	366	LYS
1	D	370	ARG
1	D	374	LYS
1	D	412	ASN
1	D	418	LEU
1	E	198	PHE
1	E	221	VAL
1	E	226	LEU
1	E	243	LYS
1	E	251	LEU
1	E	258	LEU
1	E	273	GLN
1	E	290	GLU
1	E	330	LEU
1	E	353	LEU
1	E	393	ILE

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Mol	Chain	Res	Type
1	E	417	LEU
1	E	418	LEU
1	E	421	LYS
1	F	226	LEU
1	F	251	LEU
1	F	268	VAL
1	F	270	GLU
1	F	290	GLU
1	F	317	GLN
1	F	318	LYS
1	F	330	LEU
1	F	353	LEU
1	F	418	LEU
1	G	189	LYS
1	G	198	PHE
1	G	200	LYS
1	G	225	GLU
1	G	229	LEU
1	G	243	LYS
1	G	251	LEU
1	G	270	GLU
1	G	274	ASN
1	G	275	ILE
1	G	290	GLU
1	G	306	ILE
1	G	319	LEU
1	G	321	SER
1	G	327	THR
1	G	330	LEU
1	G	353	LEU
1	G	364	THR
1	G	393	ILE
1	G	399	VAL
1	G	408	SER
1	G	412	ASN
1	G	417	LEU
1	G	418	LEU
1	G	421	LYS
1	H	229	LEU
1	H	258	LEU
1	H	267	SER
1	H	271	ASN

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Mol	Chain	Res	Type
1	H	278	LYS
1	H	317	GLN
1	H	319	LEU
1	H	325	LEU
1	H	330	LEU
1	H	340	ILE
1	H	374	LYS
1	H	417	LEU
1	H	418	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	291	GLN
1	A	314	ASN
1	A	328	ASN
1	A	381	GLN
1	B	282	ASN
1	B	314	ASN
1	B	381	GLN
1	C	271	ASN
1	C	282	ASN
1	D	282	ASN
1	D	314	ASN
1	E	282	ASN
1	E	314	ASN
1	F	274	ASN
1	G	282	ASN
1	G	314	ASN
1	G	372	ASN
1	G	381	GLN
1	G	384	ASN
1	H	274	ASN
1	H	282	ASN
1	H	314	ASN
1	H	381	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	CO6	A	500	-	26,33,55	1.31	4 (15%)	33,52,82	2.20	3 (9%)
2	ACT	A	600	-	1,3,3	2.10	1 (100%)	0,3,3	0.00	-
2	ACT	A	601	-	1,3,3	2.81	1 (100%)	0,3,3	0.00	-
4	CO6	B	500	-	26,33,55	1.15	4 (15%)	33,52,82	2.57	6 (18%)
2	ACT	B	600	-	1,3,3	1.62	0	0,3,3	0.00	-
2	ACT	B	601	-	1,3,3	0.26	0	0,3,3	0.00	-
4	CO6	C	500	-	26,33,55	1.09	3 (11%)	33,52,82	2.62	5 (15%)
2	ACT	C	600	-	1,3,3	1.30	0	0,3,3	0.00	-
2	ACT	C	601	-	1,3,3	1.57	0	0,3,3	0.00	-
4	CO6	D	500	-	26,33,55	1.20	3 (11%)	33,52,82	2.39	4 (12%)
2	ACT	D	600	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
2	ACT	D	601	-	1,3,3	1.21	0	0,3,3	0.00	-
4	CO6	E	500	-	32,42,55	2.01	3 (9%)	40,66,82	2.64	8 (20%)
2	ACT	E	600	-	1,3,3	1.64	0	0,3,3	0.00	-
2	ACT	E	601	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-
4	CO6	F	500	-	26,33,55	1.16	3 (11%)	33,52,82	2.27	4 (12%)
2	ACT	F	600	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
2	ACT	F	601	-	1,3,3	1.25	0	0,3,3	0.00	-
4	CO6	G	500	-	26,33,55	1.20	3 (11%)	33,52,82	2.72	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	G	600	-	1,3,3	2.27	1 (100%)	0,3,3	0.00	-
2	ACT	G	601	-	1,3,3	1.34	0	0,3,3	0.00	-
4	CO6	H	500	-	26,33,55	1.12	3 (11%)	33,52,82	2.69	7 (21%)
2	ACT	H	600	-	1,3,3	0.71	0	0,3,3	0.00	-
2	ACT	H	601	-	1,3,3	0.16	0	0,3,3	0.00	-

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	CO6	A	500	-	-	0/17/37/71	0/3/3/3
2	ACT	A	600	-	-	0/0/0/0	0/0/0/0
2	ACT	A	601	-	-	0/0/0/0	0/0/0/0
4	CO6	B	500	-	-	0/17/37/71	0/3/3/3
2	ACT	B	600	-	-	0/0/0/0	0/0/0/0
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0
4	CO6	C	500	-	-	0/17/37/71	0/3/3/3
2	ACT	C	600	-	-	0/0/0/0	0/0/0/0
2	ACT	C	601	-	-	0/0/0/0	0/0/0/0
4	CO6	D	500	-	-	0/17/37/71	0/3/3/3
2	ACT	D	600	-	-	0/0/0/0	0/0/0/0
2	ACT	D	601	-	-	0/0/0/0	0/0/0/0
4	CO6	E	500	-	-	0/33/54/71	0/3/3/3
2	ACT	E	600	-	-	0/0/0/0	0/0/0/0
2	ACT	E	601	-	-	0/0/0/0	0/0/0/0
4	CO6	F	500	-	-	0/17/37/71	0/3/3/3
2	ACT	F	600	-	-	0/0/0/0	0/0/0/0
2	ACT	F	601	-	-	0/0/0/0	0/0/0/0
4	CO6	G	500	-	-	0/17/37/71	0/3/3/3
2	ACT	G	600	-	-	0/0/0/0	0/0/0/0
2	ACT	G	601	-	-	0/0/0/0	0/0/0/0
4	CO6	H	500	-	-	0/17/37/71	0/3/3/3
2	ACT	H	600	-	-	0/0/0/0	0/0/0/0
2	ACT	H	601	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	CO6	O4B-C1B	2.00	1.43	1.41
2	A	600	ACT	CH3-C	2.10	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	CO6	C2A-N1A	2.11	1.37	1.33
4	D	500	CO6	P2A-O6A	2.13	1.62	1.54
4	F	500	CO6	P2A-O6A	2.14	1.62	1.54
4	A	500	CO6	C6A-N6A	2.17	1.41	1.34
4	G	500	CO6	C2A-N1A	2.22	1.38	1.33
2	E	601	ACT	CH3-C	2.25	1.51	1.48
4	H	500	CO6	C2A-N1A	2.26	1.38	1.33
4	C	500	CO6	P2A-O6A	2.27	1.62	1.54
2	G	600	ACT	CH3-C	2.27	1.52	1.48
4	E	500	CO6	C2A-N1A	2.27	1.38	1.33
4	C	500	CO6	C2A-N1A	2.30	1.38	1.33
2	D	600	ACT	CH3-C	2.34	1.52	1.48
2	F	600	ACT	CH3-C	2.34	1.52	1.48
4	H	500	CO6	P2A-O6A	2.49	1.63	1.54
4	F	500	CO6	C2A-N1A	2.49	1.38	1.33
4	G	500	CO6	P2A-O6A	2.54	1.63	1.54
4	D	500	CO6	C2A-N1A	2.60	1.38	1.33
4	A	500	CO6	C2A-N1A	2.72	1.39	1.33
2	A	601	ACT	CH3-C	2.81	1.52	1.48
4	B	500	CO6	P2A-O6A	2.86	1.65	1.54
4	A	500	CO6	P2A-O6A	2.86	1.65	1.54
4	C	500	CO6	C2A-N3A	2.99	1.37	1.32
4	H	500	CO6	C2A-N3A	3.18	1.37	1.32
4	B	500	CO6	C2A-N3A	3.23	1.37	1.32
4	G	500	CO6	C2A-N3A	3.50	1.38	1.32
4	E	500	CO6	C2A-N3A	3.56	1.38	1.32
4	A	500	CO6	C2A-N3A	3.67	1.38	1.32
4	D	500	CO6	C2A-N3A	3.87	1.39	1.32
4	F	500	CO6	C2A-N3A	3.99	1.39	1.32
4	E	500	CO6	O9P-C9P	9.87	1.42	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	500	CO6	N3A-C2A-N1A	-13.70	118.41	128.89
4	E	500	CO6	N3A-C2A-N1A	-13.37	118.66	128.89
4	H	500	CO6	N3A-C2A-N1A	-13.15	118.82	128.89
4	C	500	CO6	N3A-C2A-N1A	-13.12	118.85	128.89
4	B	500	CO6	N3A-C2A-N1A	-12.26	119.50	128.89
4	F	500	CO6	N3A-C2A-N1A	-11.64	119.98	128.89
4	A	500	CO6	N3A-C2A-N1A	-11.23	120.29	128.89
4	D	500	CO6	N3A-C2A-N1A	-11.19	120.32	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	CO6	P1A-O3A-P2A	-4.38	118.00	132.67
4	H	500	CO6	P1A-O3A-P2A	-4.16	118.70	132.67
4	G	500	CO6	P1A-O3A-P2A	-3.64	120.45	132.67
4	E	500	CO6	C1B-N9A-C4A	-3.33	121.92	126.94
4	E	500	CO6	CDP-CBP-CCP	-3.17	104.39	108.50
4	E	500	CO6	O9P-C9P-N8P	-3.10	118.49	123.08
4	C	500	CO6	C2B-C1B-N9A	-3.08	109.58	114.29
4	F	500	CO6	C1B-N9A-C4A	-2.75	122.79	126.94
4	C	500	CO6	P1A-O3A-P2A	-2.75	123.45	132.67
4	B	500	CO6	C2B-C1B-N9A	-2.69	110.19	114.29
4	E	500	CO6	P2A-O3A-P1A	-2.39	126.03	132.73
4	H	500	CO6	C1B-N9A-C4A	-2.37	123.37	126.94
4	D	500	CO6	O3B-C3B-C4B	-2.28	101.04	109.99
4	H	500	CO6	O3B-C3B-C2B	-2.28	102.66	111.51
4	H	500	CO6	O3B-C3B-C4B	-2.27	101.07	109.99
4	G	500	CO6	C2B-C1B-N9A	-2.17	110.97	114.29
4	B	500	CO6	C1B-N9A-C4A	-2.09	123.78	126.94
4	A	500	CO6	O3B-C3B-C2B	-2.01	103.71	111.51
4	D	500	CO6	O3A-P1A-O5B	2.08	108.45	102.94
4	C	500	CO6	C2A-N1A-C6A	2.09	122.51	118.77
4	F	500	CO6	O3A-P1A-O5B	2.10	108.50	102.94
4	A	500	CO6	O4B-C1B-N9A	2.10	112.50	108.10
4	H	500	CO6	N6A-C6A-N1A	2.16	123.84	119.20
4	B	500	CO6	O4B-C1B-N9A	2.18	112.66	108.10
4	H	500	CO6	P3B-O3B-C3B	2.22	126.89	121.56
4	G	500	CO6	O4B-C1B-N9A	2.25	112.81	108.10
4	C	500	CO6	O4B-C1B-N9A	2.31	112.94	108.10
4	E	500	CO6	O3A-P2A-O6A	2.37	109.22	102.94
4	E	500	CO6	O4B-C1B-N9A	2.57	113.48	108.10
4	B	500	CO6	O5A-P2A-O3A	2.75	117.57	105.09
4	F	500	CO6	O4B-C1B-N9A	2.91	114.19	108.10
4	E	500	CO6	O6A-CCP-CBP	4.40	117.63	110.55
4	D	500	CO6	P3B-O3B-C3B	4.55	132.47	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	CO6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ACT	1	0
2	A	601	ACT	2	0
2	B	600	ACT	2	0
2	B	601	ACT	2	0
4	C	500	CO6	1	0
2	C	600	ACT	2	0
2	C	601	ACT	2	0
4	D	500	CO6	2	0
4	E	500	CO6	1	0
2	E	600	ACT	3	0
2	E	601	ACT	2	0
4	F	500	CO6	1	0
2	F	600	ACT	1	0
4	G	500	CO6	2	0
2	H	600	ACT	3	0
2	H	601	ACT	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	234/262 (89%)	0.03	8 (3%) 49 54	34, 47, 69, 76	0
1	B	234/262 (89%)	0.14	19 (8%) 15 16	35, 44, 67, 74	0
1	C	234/262 (89%)	0.05	14 (5%) 25 28	36, 48, 69, 79	0
1	D	234/262 (89%)	0.05	12 (5%) 32 36	36, 47, 67, 77	0
1	E	234/262 (89%)	0.13	13 (5%) 28 31	35, 47, 71, 79	0
1	F	234/262 (89%)	0.22	17 (7%) 18 20	37, 49, 70, 76	0
1	G	234/262 (89%)	0.35	21 (8%) 12 12	43, 54, 74, 83	0
1	H	234/262 (89%)	-0.02	9 (3%) 44 49	32, 44, 68, 74	0
All	All	1872/2096 (89%)	0.12	113 (6%) 25 28	32, 48, 70, 83	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	188	GLY	5.5
1	G	373	GLU	5.1
1	E	198	PHE	4.9
1	G	198	PHE	4.9
1	D	188	GLY	4.3
1	G	291	GLN	4.2
1	F	238	PHE	4.0
1	D	189	LYS	3.8
1	B	386	SER	3.6
1	D	238	PHE	3.6
1	E	196	LYS	3.5
1	H	198	PHE	3.4
1	G	188	GLY	3.4
1	F	242	ILE	3.3
1	E	290	GLU	3.3
1	A	188	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	373	GLU	3.2
1	D	190	ASP	3.2
1	F	189	LYS	3.1
1	G	238	PHE	3.0
1	B	348	ALA	3.0
1	F	218	CYS	3.0
1	H	188	GLY	2.9
1	A	198	PHE	2.9
1	G	374	LYS	2.9
1	B	374	LYS	2.9
1	G	290	GLU	2.9
1	E	348	ALA	2.8
1	F	243	LYS	2.8
1	F	386	SER	2.8
1	G	242	ILE	2.8
1	G	196	LYS	2.8
1	E	218	CYS	2.8
1	E	373	GLU	2.8
1	D	218	CYS	2.8
1	H	196	LYS	2.8
1	D	242	ILE	2.7
1	A	348	ALA	2.7
1	B	347	TYR	2.7
1	C	196	LYS	2.7
1	G	318	LYS	2.7
1	C	238	PHE	2.6
1	G	320	GLY	2.6
1	A	386	SER	2.6
1	H	218	CYS	2.6
1	E	291	GLN	2.5
1	B	361	ALA	2.5
1	B	218	CYS	2.5
1	B	189	LYS	2.5
1	G	348	ALA	2.5
1	H	374	LYS	2.5
1	B	216	GLY	2.5
1	D	291	GLN	2.5
1	C	374	LYS	2.4
1	G	372	ASN	2.4
1	B	198	PHE	2.4
1	C	270	GLU	2.4
1	D	348	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	346	THR	2.4
1	C	218	CYS	2.4
1	E	347	TYR	2.4
1	E	374	LYS	2.4
1	B	238	PHE	2.4
1	E	197	GLY	2.4
1	H	238	PHE	2.4
1	C	348	ALA	2.4
1	G	216	GLY	2.3
1	E	386	SER	2.3
1	F	348	ALA	2.3
1	F	385	VAL	2.3
1	F	360	GLY	2.3
1	F	374	LYS	2.3
1	E	388	SER	2.3
1	F	290	GLU	2.2
1	C	347	TYR	2.2
1	D	386	SER	2.2
1	D	373	GLU	2.2
1	B	385	VAL	2.2
1	F	234	LYS	2.2
1	F	387	TRP	2.2
1	H	194	PRO	2.2
1	G	243	LYS	2.2
1	F	347	TYR	2.2
1	F	361	ALA	2.2
1	B	387	TRP	2.2
1	C	386	SER	2.1
1	C	217	TYR	2.1
1	C	198	PHE	2.1
1	D	198	PHE	2.1
1	B	271	ASN	2.1
1	A	218	CYS	2.1
1	B	388	SER	2.1
1	G	386	SER	2.1
1	H	217	TYR	2.1
1	G	371	PHE	2.1
1	B	378	CYS	2.1
1	H	386	SER	2.1
1	G	347	TYR	2.1
1	A	291	GLN	2.1
1	C	216	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	197	GLY	2.1
1	D	374	LYS	2.1
1	G	218	CYS	2.1
1	B	194	PRO	2.1
1	B	360	GLY	2.1
1	C	373	GLU	2.1
1	C	189	LYS	2.1
1	C	291	GLN	2.0
1	A	373	GLU	2.0
1	E	216	GLY	2.0
1	F	338	SER	2.0
1	G	239	ALA	2.0
1	A	388	SER	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	D	809	1/1	0.95	0.34	8.21	77,77,77,77	0
2	ACT	G	601	4/4	0.85	0.31	6.28	76,76,76,77	0
3	CL	F	805	1/1	0.97	0.39	2.96	69,69,69,69	0
2	ACT	E	601	4/4	0.83	0.23	2.57	65,66,66,67	0
3	CL	H	801	1/1	0.96	0.27	2.54	66,66,66,66	0
3	CL	C	802	1/1	0.96	0.28	2.18	59,59,59,59	0
3	CL	A	808	1/1	0.95	0.22	2.09	69,69,69,69	0
2	ACT	D	600	4/4	0.94	0.24	1.74	55,56,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	803	1/1	0.97	0.27	1.63	65,65,65,65	0
3	CL	B	806	1/1	0.95	0.24	1.34	69,69,69,69	0
2	ACT	A	601	4/4	0.86	0.19	1.18	57,58,58,58	0
3	CL	E	804	1/1	0.99	0.26	1.11	62,62,62,62	0
2	ACT	C	601	4/4	0.94	0.17	1.08	59,60,60,61	0
3	CL	G	812	1/1	0.99	0.25	0.98	75,75,75,75	0
3	CL	D	811	1/1	0.96	0.23	0.88	67,67,67,67	0
2	ACT	F	601	4/4	0.97	0.18	0.85	50,51,51,51	0
2	ACT	B	601	4/4	0.95	0.17	0.67	51,53,54,54	0
4	CO6	A	500	31/53	0.90	0.16	0.36	81,94,112,113	0
2	ACT	D	601	4/4	0.98	0.15	0.11	49,49,49,49	0
2	ACT	G	600	4/4	0.97	0.16	-0.03	43,44,45,46	0
4	CO6	E	500	40/53	0.90	0.16	-0.07	67,82,96,97	0
2	ACT	F	600	4/4	0.97	0.16	-0.22	43,43,44,45	0
2	ACT	H	601	4/4	0.95	0.13	-0.25	46,47,47,48	0
4	CO6	D	500	31/53	0.85	0.14	-0.36	91,101,117,117	0
4	CO6	F	500	31/53	0.86	0.16	-0.42	73,92,110,112	0
4	CO6	H	500	31/53	0.89	0.14	-0.69	79,89,106,107	0
2	ACT	B	600	4/4	0.99	0.14	-0.70	43,46,46,47	0
4	CO6	G	500	31/53	0.92	0.13	-0.78	80,94,105,106	0
4	CO6	C	500	31/53	0.90	0.12	-0.84	88,99,112,113	0
4	CO6	B	500	31/53	0.91	0.12	-0.91	81,94,109,111	0
2	ACT	H	600	4/4	0.97	0.12	-1.18	45,46,46,46	0
2	ACT	A	600	4/4	0.98	0.11	-1.35	48,48,49,49	0
2	ACT	C	600	4/4	0.98	0.11	-1.36	45,46,46,46	0
2	ACT	E	600	4/4	0.98	0.11	-1.59	43,44,44,44	0
3	CL	G	807	1/1	0.94	0.39	-	91,91,91,91	1
3	CL	H	810	1/1	0.67	0.27	-	73,73,73,73	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.