



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:21 AM GMT

PDB ID : 2II3  
Title : Crystal structure of a cubic core of the dihydrolipoamide acyltransferase (E2b) component in the branched-chain alpha-ketoacid dehydrogenase complex (BCKDC), Oxidized 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 : 2.17 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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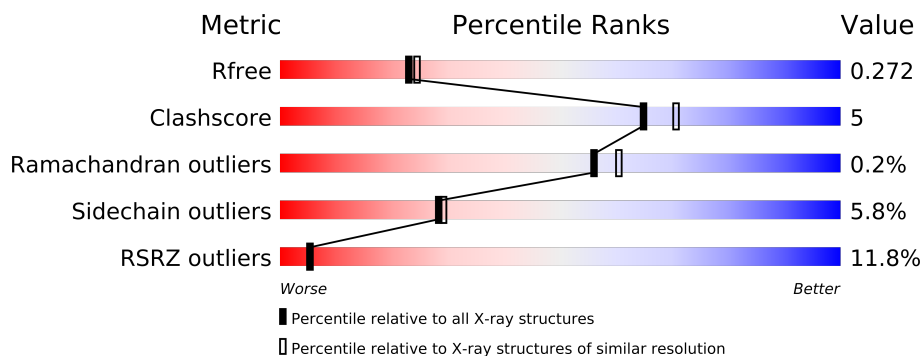
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	262	
1	B	262	
1	C	262	
1	D	262	
1	E	262	
1	F	262	
1	G	262	
1	H	262	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	B	602	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	B	816	-	X
2	ACT	C	814	-	X
2	ACT	E	815	-	X
2	ACT	F	813	-	X
3	CL	H	812	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15647 atoms, of which 0 are hydrogen and 0 are deuterium.

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	2	0
			1814	1164	308	332	10			
1	B	234	Total	C	N	O	S	0	2	0
			1814	1164	308	332	10			
1	C	234	Total	C	N	O	S	0	1	0
			1806	1160	306	330	10			
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	1	0
			1806	1160	306	330	10			
1	F	234	Total	C	N	O	S	0	1	0
			1806	1160	306	330	10			
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	2	0
			1814	1164	308	332	10			

There are 16 discrepancies between the modelled and reference sequences:

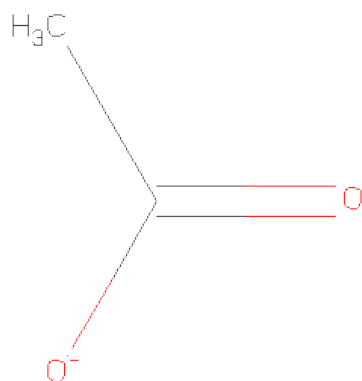
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLY	-	CLONING ARTIFACT	UNP P11181
A	161	HIS	-	CLONING ARTIFACT	UNP P11181
B	160	GLY	-	CLONING ARTIFACT	UNP P11181
B	161	HIS	-	CLONING ARTIFACT	UNP P11181
C	160	GLY	-	CLONING ARTIFACT	UNP P11181
C	161	HIS	-	CLONING ARTIFACT	UNP P11181
D	160	GLY	-	CLONING 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<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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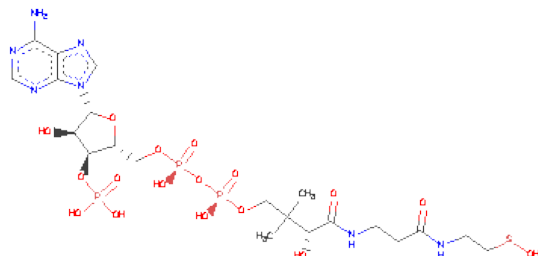
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0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

- Molecule 4 is OXIDIZED COENZYME A (three-letter code: CAO) (formula:  $C_{21}H_{36}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			49	21	7	17	3	1		
4	B	1	Total	C	N	O	P		0	0
			40	16	6	15	3			
4	C	1	Total	C	N	O	P		0	0
			40	16	6	15	3			
4	D	1	Total	C	N	O	P		0	0
			40	16	6	15	3			
4	E	1	Total	C	N	O	P	S	0	0
			49	21	7	17	3	1		
4	F	1	Total	C	N	O	P		0	0
			40	16	6	15	3			
4	G	1	Total	C	N	O	P	S	0	0
			49	21	7	17	3	1		
4	H	1	Total	C	N	O	P		0	0
			40	16	6	15	3			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	102	Total	O	0	0
			102	102		
5	C	71	Total	O	0	0
			71	71		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	110	Total 110	O 110	0	0
5	E	93	Total 93	O 93	0	0
5	F	105	Total 105	O 105	0	0
5	G	68	Total 68	O 68	0	0
5	H	98	Total 98	O 98	0	0

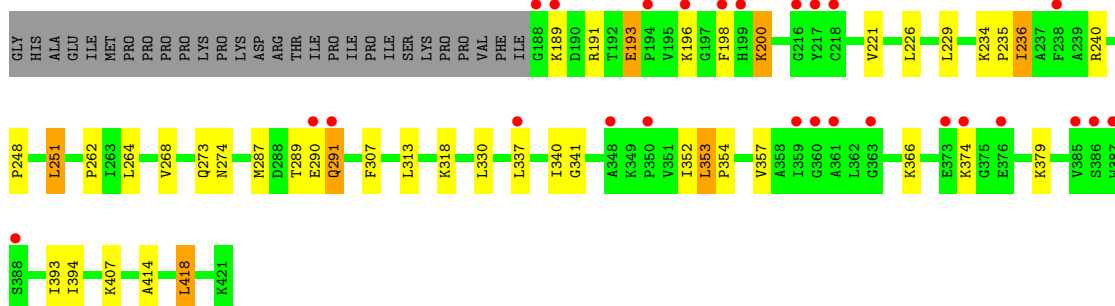


### 3 Residue-property plots

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.

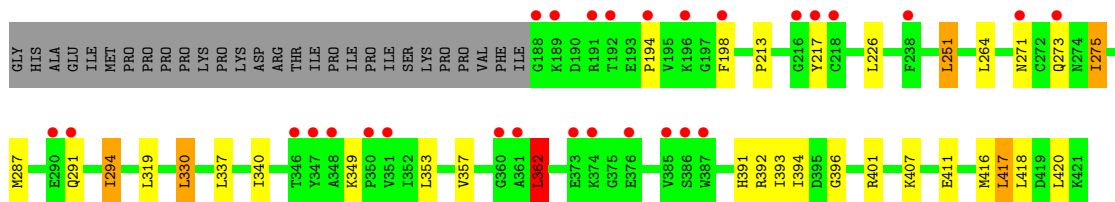
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain A: 



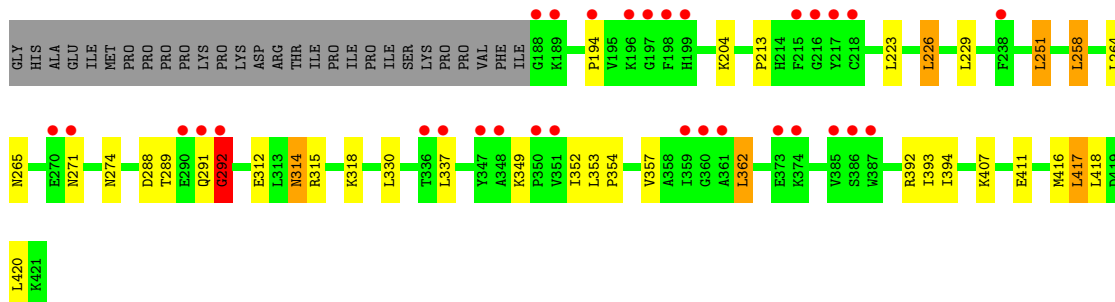
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain B: 



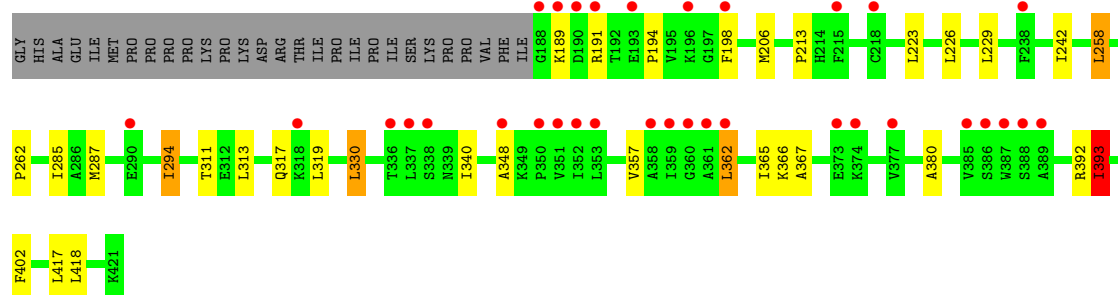
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain C: 



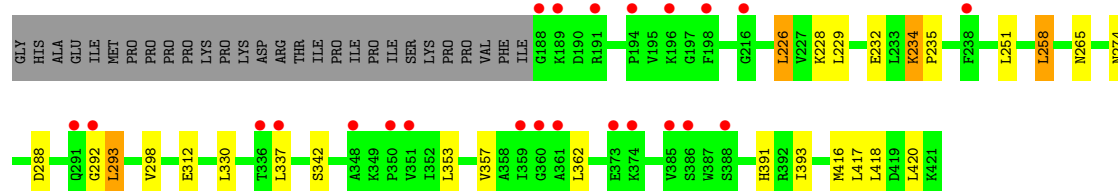
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain D: 



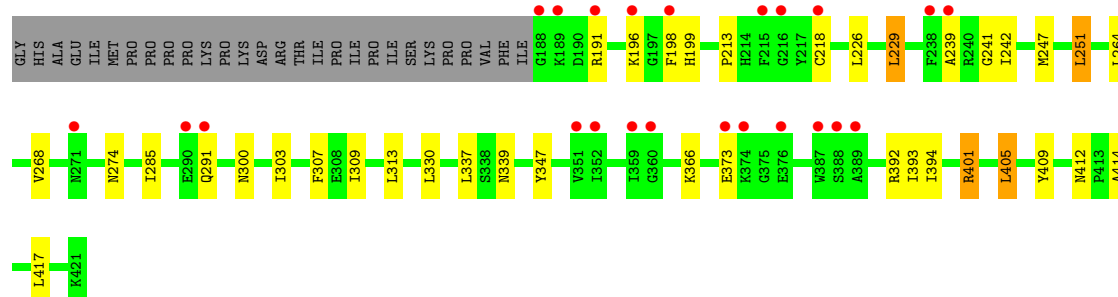
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain E: 



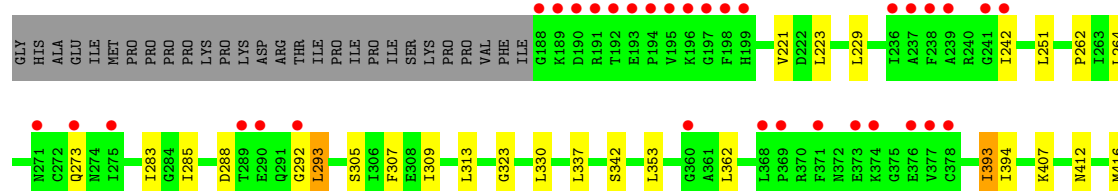
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain F: 



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

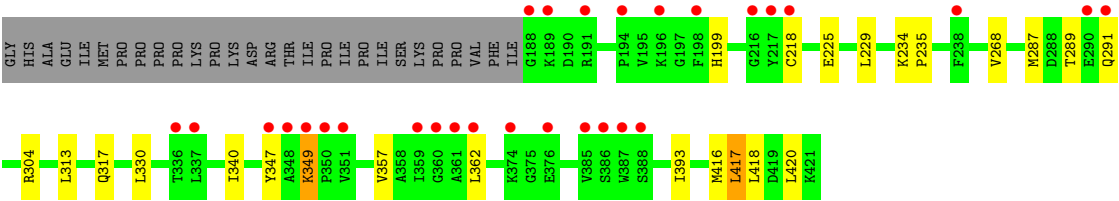
Chain G: 





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

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.91Å 194.91Å 172.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.17 35.31 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.17) 95.7 (35.31-2.17)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.259 0.225 , 0.272	Depositor DCC
$R_{free}$ test set	6243 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.7	EDS
Estimated twinning fraction	0.003 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 123659 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CAO, 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	0.91	1/1851 (0.1%)	0.84	1/2500 (0.0%)
1	B	0.92	1/1851 (0.1%)	0.84	2/2500 (0.1%)
1	C	0.88	1/1843 (0.1%)	0.83	2/2489 (0.1%)
1	D	0.89	0/1837	0.85	2/2481 (0.1%)
1	E	0.86	0/1843	0.85	1/2489 (0.0%)
1	F	0.84	0/1843	0.81	1/2489 (0.0%)
1	G	0.80	0/1837	0.79	1/2481 (0.0%)
1	H	0.92	1/1851 (0.1%)	0.83	2/2500 (0.1%)
All	All	0.88	4/14756 (0.0%)	0.83	12/19929 (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	C	0	2
1	E	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	GLY	N-CA	7.98	1.58	1.46
1	B	217	TYR	CD2-CE2	6.64	1.49	1.39
1	A	189	LYS	CE-NZ	6.60	1.65	1.49
1	H	349	LYS	CE-NZ	5.01	1.61	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	LEU	N-CA-C	-6.51	93.42	111.00
1	H	417	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	417	LEU	CA-CB-CG	5.96	129.00	115.30
1	H	362	LEU	CA-CB-CG	-5.58	102.47	115.30
1	D	362	LEU	CA-CB-CG	-5.52	102.59	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	291	GLN	Peptide
1	C	292	GLY	Peptide
1	E	292	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1814	0	1869	27	0
1	B	1814	0	1869	28	0
1	C	1806	0	1864	17	0
1	D	1803	0	1859	20	0
1	E	1806	0	1864	15	0
1	F	1806	0	1864	26	0
1	G	1803	0	1859	17	0
1	H	1814	0	1869	10	0
2	A	4	0	3	1	0
2	B	16	0	12	0	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0
2	E	8	0	6	2	0
2	F	12	0	9	0	0
2	G	4	0	3	0	0
2	H	12	0	9	2	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	1	0
4	A	49	0	32	3	0
4	B	40	0	21	0	0
4	C	40	0	21	1	0
4	D	40	0	21	6	0
4	E	49	0	32	6	0
4	F	40	0	21	5	0
4	G	49	0	32	3	0
4	H	40	0	21	0	0
5	A	95	0	0	2	0
5	B	102	0	0	2	0
5	C	71	0	0	1	0
5	D	110	0	0	3	0
5	E	93	0	0	2	0
5	F	105	0	0	1	0
5	G	68	0	0	2	0
5	H	98	0	0	2	0
All	All	15647	0	15178	160	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 160 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:293:LEU:HD22	4:E:500:CAO:O1P	1.64	0.98
1:E:288:ASP:OD2	1:F:401:ARG:NH2	2.05	0.89
1:A:229:LEU:CD1	1:F:414:ALA:HB1	2.03	0.89
1:A:229:LEU:HD11	1:F:414:ALA:HB1	1.55	0.88
1:F:251:LEU:HD12	1:F:337:LEU:HD12	1.55	0.86

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	234/262 (89%)	225 (96%)	7 (3%)	2 (1%)	25	20
1	B	234/262 (89%)	229 (98%)	5 (2%)	0	100	100
1	C	233/262 (89%)	224 (96%)	8 (3%)	1 (0%)	43	44
1	D	232/262 (88%)	224 (97%)	8 (3%)	0	100	100
1	E	233/262 (89%)	227 (97%)	6 (3%)	0	100	100
1	F	233/262 (89%)	224 (96%)	8 (3%)	1 (0%)	43	44
1	G	232/262 (88%)	223 (96%)	9 (4%)	0	100	100
1	H	234/262 (89%)	225 (96%)	9 (4%)	0	100	100
All	All	1865/2096 (89%)	1801 (97%)	60 (3%)	4 (0%)	56	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLU
1	A	291	GLN
1	F	239	ALA
1	C	292	GLY

### 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	198/222 (89%)	182 (92%)	16 (8%)	17	15
1	B	198/222 (89%)	186 (94%)	12 (6%)	26	26
1	C	197/222 (89%)	185 (94%)	12 (6%)	26	26
1	D	196/222 (88%)	183 (93%)	13 (7%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	197/222 (89%)	189 (96%)	8 (4%)	41	47
1	F	197/222 (89%)	184 (93%)	13 (7%)	24	23
1	G	196/222 (88%)	187 (95%)	9 (5%)	37	41
1	H	198/222 (89%)	190 (96%)	8 (4%)	42	48
All	All	1577/1776 (89%)	1486 (94%)	91 (6%)	28	29

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	ARG
1	D	393	ILE
1	H	268	VAL
1	D	198	PHE
1	D	319	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN
1	E	273	GLN
1	G	381	GLN
1	C	381	GLN
1	H	291	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 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	CAO	A	500	-	51,51,51	1.15	5 (9%)	75,76,76	1.82	12 (16%)
2	ACT	A	600	-	1,3,3	1.95	0	0,3,3	0.00	-
4	CAO	B	500	-	41,42,51	0.89	2 (4%)	64,66,76	1.92	13 (20%)
2	ACT	B	600	-	1,3,3	2.74	1 (100%)	0,3,3	0.00	-
2	ACT	B	601	-	1,3,3	1.74	0	0,3,3	0.00	-
2	ACT	B	602	-	1,3,3	3.00	1 (100%)	0,3,3	0.00	-
2	ACT	B	816	-	1,3,3	1.47	0	0,3,3	0.00	-
4	CAO	C	500	-	41,42,51	0.95	3 (7%)	64,66,76	1.73	12 (18%)
2	ACT	C	600	-	1,3,3	1.92	0	0,3,3	0.00	-
2	ACT	C	601	-	1,3,3	0.85	0	0,3,3	0.00	-
2	ACT	C	814	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-
4	CAO	D	500	-	41,42,51	1.01	3 (7%)	64,66,76	2.28	16 (25%)
2	ACT	D	600	-	1,3,3	1.44	0	0,3,3	0.00	-
2	ACT	D	601	-	1,3,3	2.80	1 (100%)	0,3,3	0.00	-
2	ACT	D	602	-	1,3,3	0.98	0	0,3,3	0.00	-
4	CAO	E	500	-	51,51,51	1.12	6 (11%)	75,76,76	2.08	12 (16%)
2	ACT	E	600	-	1,3,3	0.89	0	0,3,3	0.00	-
2	ACT	E	815	-	1,3,3	1.95	0	0,3,3	0.00	-
4	CAO	F	500	-	41,42,51	1.04	2 (4%)	64,66,76	1.95	14 (21%)
2	ACT	F	600	-	1,3,3	1.59	0	0,3,3	0.00	-
2	ACT	F	601	-	1,3,3	1.29	0	0,3,3	0.00	-
2	ACT	F	813	-	1,3,3	1.86	0	0,3,3	0.00	-
4	CAO	G	500	-	51,51,51	1.03	4 (7%)	75,76,76	1.99	16 (21%)
2	ACT	G	600	-	1,3,3	0.83	0	0,3,3	0.00	-
4	CAO	H	500	-	41,42,51	0.98	2 (4%)	64,66,76	1.99	18 (28%)
2	ACT	H	600	-	1,3,3	1.60	0	0,3,3	0.00	-
2	ACT	H	601	-	1,3,3	1.49	0	0,3,3	0.00	-
2	ACT	H	602	-	1,3,3	0.15	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	CAO	A	500	-	-	0/48/65/65	0/1/3/3
2	ACT	A	600	-	-	0/0/0/0	0/0/0/0
4	CAO	B	500	-	1/1/10/13	0/38/54/65	0/1/3/3
2	ACT	B	600	-	-	0/0/0/0	0/0/0/0
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0
2	ACT	B	602	-	-	0/0/0/0	0/0/0/0
2	ACT	B	816	-	-	0/0/0/0	0/0/0/0
4	CAO	C	500	-	-	0/38/54/65	0/1/3/3
2	ACT	C	600	-	-	0/0/0/0	0/0/0/0
2	ACT	C	601	-	-	0/0/0/0	0/0/0/0
2	ACT	C	814	-	-	0/0/0/0	0/0/0/0
4	CAO	D	500	-	-	0/38/54/65	0/1/3/3
2	ACT	D	600	-	-	0/0/0/0	0/0/0/0
2	ACT	D	601	-	-	0/0/0/0	0/0/0/0
2	ACT	D	602	-	-	0/0/0/0	0/0/0/0
4	CAO	E	500	-	-	0/48/65/65	0/1/3/3
2	ACT	E	600	-	-	0/0/0/0	0/0/0/0
2	ACT	E	815	-	-	0/0/0/0	0/0/0/0
4	CAO	F	500	-	1/1/10/13	0/38/54/65	0/1/3/3
2	ACT	F	600	-	-	0/0/0/0	0/0/0/0
2	ACT	F	601	-	-	0/0/0/0	0/0/0/0
2	ACT	F	813	-	-	0/0/0/0	0/0/0/0
4	CAO	G	500	-	-	0/48/65/65	0/1/3/3
2	ACT	G	600	-	-	0/0/0/0	0/0/0/0
4	CAO	H	500	-	1/1/10/13	1/38/54/65	0/1/3/3
2	ACT	H	600	-	-	0/0/0/0	0/0/0/0
2	ACT	H	601	-	-	0/0/0/0	0/0/0/0
2	ACT	H	602	-	-	0/0/0/0	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	CAO	O1P-S1P	3.53	1.77	1.62
4	A	500	CAO	C5A-C4A	3.41	1.48	1.40
4	G	500	CAO	O1P-S1P	3.22	1.76	1.62
4	B	500	CAO	C5A-C4A	3.12	1.47	1.40
4	E	500	CAO	O1P-S1P	3.10	1.75	1.62

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	500	CAO	O4B-C1B-N9A	10.51	118.22	108.44
4	D	500	CAO	O4B-C1B-N9A	9.57	117.34	108.44
4	G	500	CAO	N3A-C2A-N1A	-8.42	121.67	128.71
4	B	500	CAO	N3A-C2A-N1A	-7.96	122.05	128.71
4	D	500	CAO	N3A-C2A-N1A	-7.21	122.68	128.71

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	500	CAO	C2B
4	F	500	CAO	CAP
4	H	500	CAO	CAP

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	500	CAO	OAP-CAP-C9P-N8P

There are no ring outliers.

## 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%)	0.57	26 (11%) 6 6	31, 37, 50, 64	0
1	B	234/262 (89%)	0.45	28 (11%) 5 5	30, 37, 49, 63	0
1	C	234/262 (89%)	0.63	31 (13%) 4 4	30, 37, 49, 68	0
1	D	234/262 (89%)	0.56	33 (14%) 3 3	31, 37, 47, 60	0
1	E	234/262 (89%)	0.57	23 (9%) 8 8	31, 37, 51, 62	0
1	F	234/262 (89%)	0.48	23 (9%) 8 8	31, 37, 48, 61	0
1	G	234/262 (89%)	0.63	33 (14%) 3 3	29, 37, 50, 59	0
1	H	234/262 (89%)	0.58	29 (12%) 5 5	31, 36, 50, 61	0
All	All	1872/2096 (89%)	0.56	226 (12%) 5 5	29, 37, 49, 68	0

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	PHE	7.7
1	A	198	PHE	7.1
1	E	198	PHE	6.8
1	F	188	GLY	6.5
1	G	238	PHE	6.2

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

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

### 6.3 Carbohydrates ⓘ

There are no 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	H	812	1/1	0.15	35.50	52,52,52,52	1
2	ACT	E	815	4/4	0.28	6.71	49,52,52,54	0
2	ACT	B	816	4/4	0.25	6.26	60,61,61,62	0
2	ACT	B	602	4/4	0.23	4.19	40,41,43,43	0
2	ACT	C	814	4/4	0.27	3.89	58,59,59,60	0
2	ACT	F	813	4/4	0.20	3.20	60,61,61,61	0
3	CL	C	807	1/1	0.16	1.98	62,62,62,62	0
2	ACT	H	602	4/4	0.24	1.84	74,75,75,75	0
3	CL	G	811	1/1	0.21	1.46	69,69,69,69	0
3	CL	A	802	1/1	0.25	1.31	67,67,67,67	0
3	CL	C	803	1/1	0.26	0.91	62,62,62,62	0
3	CL	F	804	1/1	0.20	0.35	63,63,63,63	0
3	CL	B	801	1/1	0.19	0.02	63,63,63,63	0
3	CL	H	809	1/1	0.18	-0.18	58,58,58,58	0
2	ACT	C	601	4/4	0.13	-0.19	37,39,39,40	0
4	CAO	F	500	40/49	0.12	-0.26	47,64,81,82	0
2	ACT	D	602	4/4	0.13	-0.47	65,65,65,65	0
4	CAO	D	500	40/49	0.12	-0.53	51,62,68,71	0
4	CAO	C	500	40/49	0.12	-0.54	41,54,61,61	0
2	ACT	A	600	4/4	0.16	-0.59	42,43,43,44	0
2	ACT	E	600	4/4	0.17	-0.59	39,40,40,41	0
4	CAO	H	500	40/49	0.13	-0.60	35,54,62,64	0
3	CL	D	805	1/1	0.15	-0.60	59,59,59,59	0
2	ACT	H	601	4/4	0.13	-0.71	33,35,36,37	0
2	ACT	G	600	4/4	0.12	-0.76	42,42,42,43	0
4	CAO	B	500	40/49	0.11	-0.80	44,55,63,64	0
3	CL	E	806	1/1	0.12	-0.82	68,68,68,68	0
4	CAO	A	500	49/49	0.11	-0.90	37,48,56,56	0
4	CAO	G	500	49/49	0.10	-0.90	45,54,64,66	0
2	ACT	F	601	4/4	0.07	-1.08	30,32,32,33	0
2	ACT	C	600	4/4	0.12	-1.10	39,40,40,40	0
2	ACT	B	601	4/4	0.08	-1.15	34,36,36,37	0
2	ACT	F	600	4/4	0.12	-1.16	33,33,34,35	0
2	ACT	D	600	4/4	0.15	-1.17	38,38,39,40	0
2	ACT	H	600	4/4	0.12	-1.24	34,34,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	B	600	4/4	0.13	-1.25	34,34,35,35	0
4	CAO	E	500	49/49	0.09	-1.46	32,43,50,52	0
2	ACT	D	601	4/4	0.07	-1.91	29,30,31,32	0
3	CL	F	808	1/1	0.06	-2.72	66,66,66,66	0
3	CL	G	810	1/1	0.09	-18.33	66,66,66,66	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.