wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:46 AM GMT

PDB ID	:	2II4
Title	:	Crystal structure of a cubic core of the dihydrolipoamide acyltransferase (E2b) component in the branched-chain alpha-ketoacid dehydrogenase complex (BCKDC), 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	:	2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

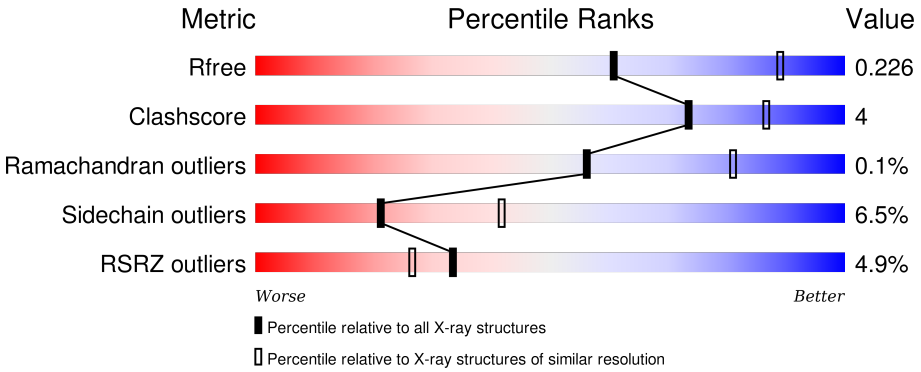
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.59 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	3% 71% 16% • 11%
1	B	262	3% 74% 13% • 11%
1	C	262	3% 76% 12% • 11%
1	D	262	3% 78% 11% • 11%
1	E	262	3% 77% 11% • 11%

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Mol	Chain	Length	Quality of chain
1	F	262	4% 76% 12% • 11%
1	G	262	8% 77% 11% • 11%
1	H	262	6% 77% 11% 11%

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	CL	E	806	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15112 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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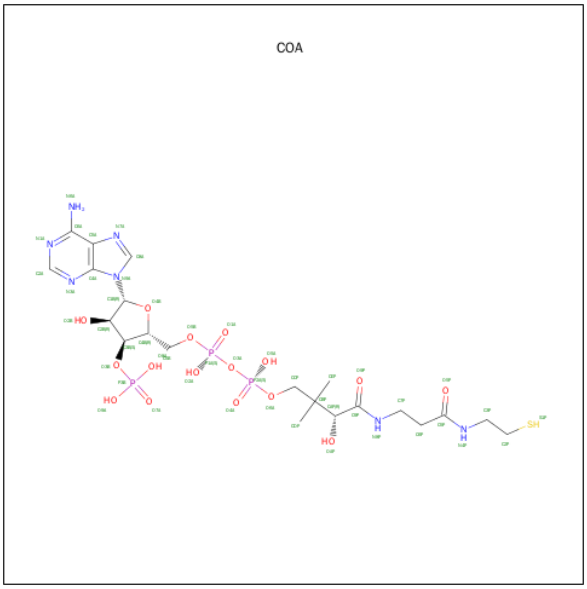
Chain	Residue	Modelled	Actual	Comment	Reference
G	160	GLY	-	CLONING ARTIFACT	UNP P11181
G	161	HIS	-	CLONING ARTIFACT	UNP P11181
H	160	GLY	-	CLONING ARTIFACT	UNP P11181
H	161	HIS	-	CLONING ARTIFACT	UNP P11181

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

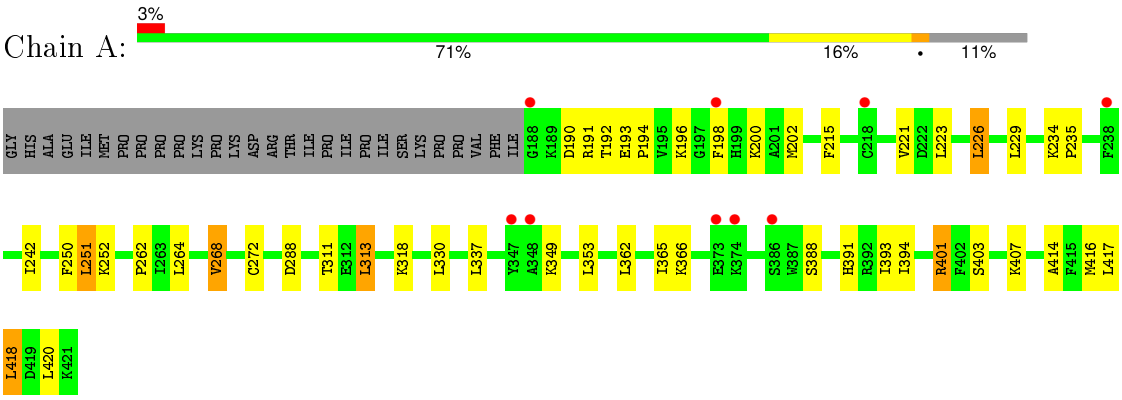
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	34	Total	O	0	0
			34	34		
4	C	37	Total	O	0	0
			37	37		
4	D	33	Total	O	0	0
			33	33		
4	E	39	Total	O	0	0
			39	39		
4	F	36	Total	O	0	0
			36	36		
4	G	26	Total	O	0	0
			26	26		
4	H	41	Total	O	0	0
			41	41		

3 Residue-property plots (i)

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

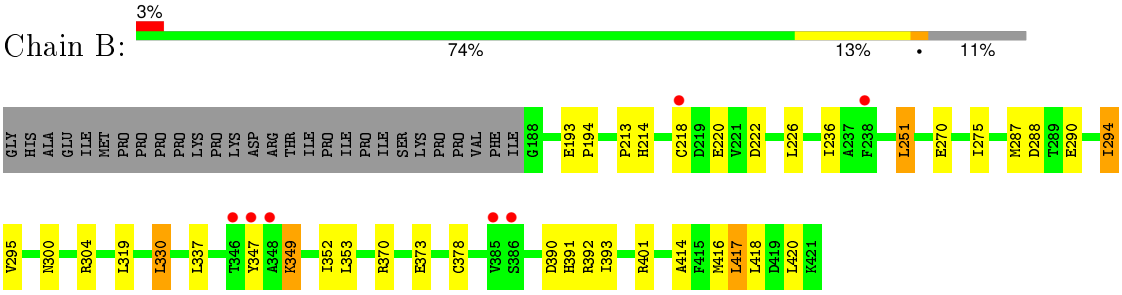
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain A:



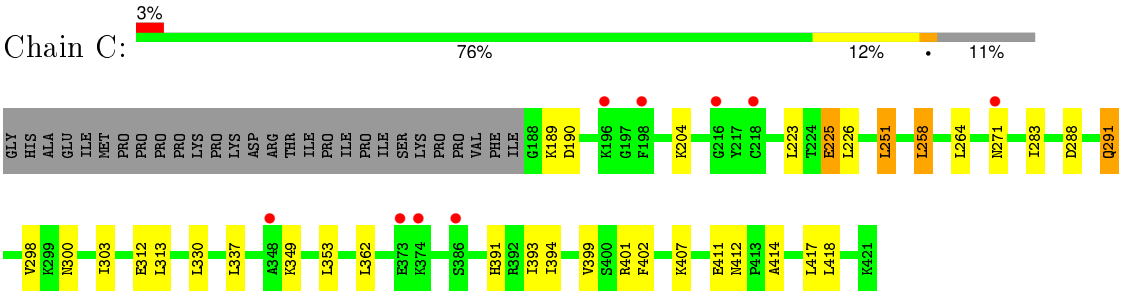
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain B:



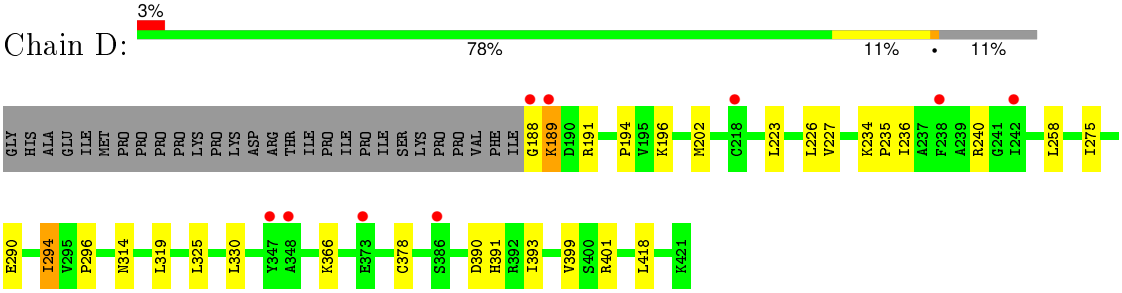
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain C:



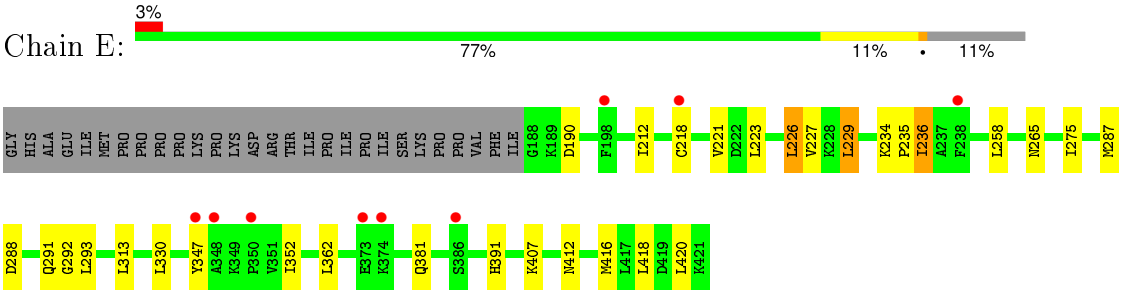
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain D:



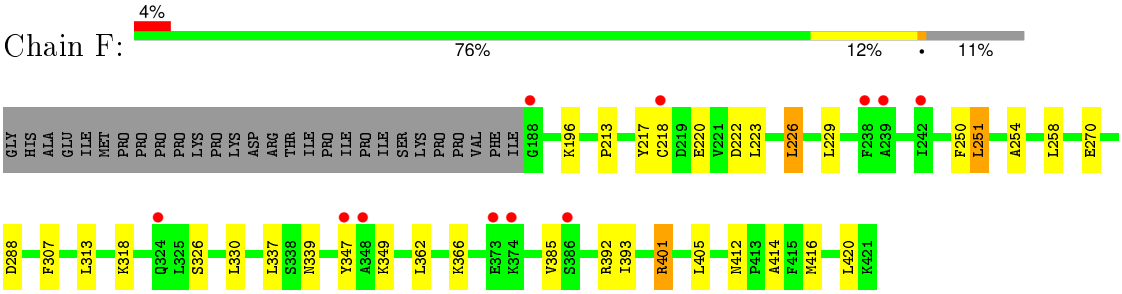
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain E:



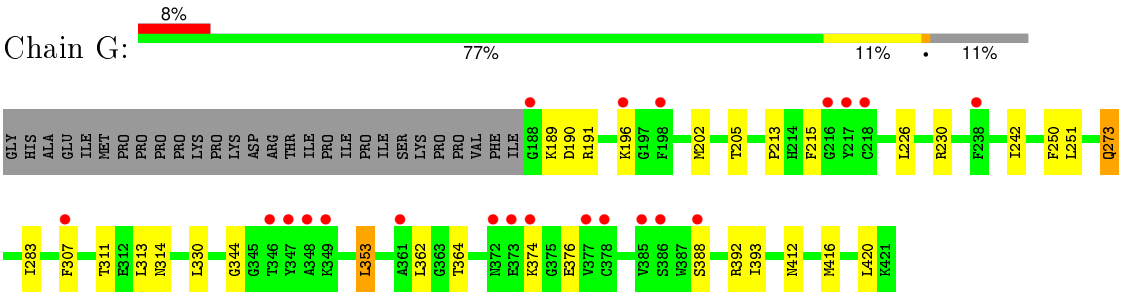
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain F:



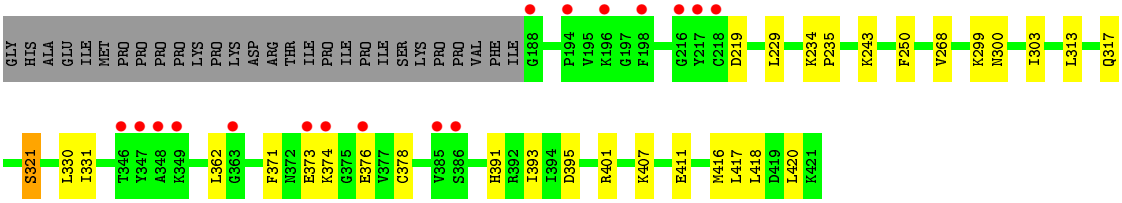
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain G:



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

Chain H:


GLY HIS ALA GLU ILE MET PRO PRO PRO PRO LYS PRO LYS ASP ARG THR ILE PRO ILE PRO ILE SER LYS PRO PRO VAL PHE ILE G188 P194 V195 K196 G197 F198 G216 Y217 C218 D219 L229 K234 P235 K243 F250 V268 K299 N300 I303 L313 Q317
S321 L330 I331 T346 Y347 A348 K349 L362 G363 F371 N372 E373 K374 G375 E376 V377 C378 V385 S386 H391 R392 I393 I394 D395 R401 K407 E411 M416 L417 L418 D419 L420 K421

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	195.23Å 195.23Å 172.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.59 45.26 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.59) 99.8 (45.26-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.94 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.229 0.172 , 0.226	Depositor DCC
R_{free} test set	3805 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.9	EDS
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 75817 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15112	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: COA, CL

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	0.94	0/1837	0.88	3/2481 (0.1%)
1	B	0.98	2/1837 (0.1%)	0.92	5/2481 (0.2%)
1	C	0.96	1/1837 (0.1%)	0.90	1/2481 (0.0%)
1	D	0.90	1/1837 (0.1%)	0.89	1/2481 (0.0%)
1	E	0.92	0/1837	0.93	2/2481 (0.1%)
1	F	0.94	2/1837 (0.1%)	0.85	2/2481 (0.1%)
1	G	0.89	0/1837	0.87	1/2481 (0.0%)
1	H	0.96	0/1837	0.90	4/2481 (0.2%)
All	All	0.94	6/14696 (0.0%)	0.89	19/19848 (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	C	0	1
1	E	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	270	GLU	CG-CD	6.13	1.61	1.51
1	F	270	GLU	CB-CG	5.73	1.63	1.52
1	C	225	GLU	CG-CD	5.67	1.60	1.51
1	B	378	CYS	CB-SG	-5.59	1.72	1.81
1	D	378	CYS	CB-SG	-5.16	1.73	1.81

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	293	LEU	N-CA-C	-9.46	85.47	111.00
1	G	190	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	202	MET	CG-SD-CE	6.29	110.26	100.20
1	H	378	CYS	CA-CB-SG	-5.61	103.89	114.00
1	H	401	ARG	NE-CZ-NH2	-5.41	117.59	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	291	GLN	Peptide
1	E	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	28	0
1	B	1803	0	1859	17	0
1	C	1803	0	1859	15	0
1	D	1803	0	1859	10	0
1	E	1803	0	1859	15	0
1	F	1803	0	1859	19	0
1	G	1803	0	1859	15	0
1	H	1803	0	1859	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	0	0
3	C	48	0	32	2	0
3	D	48	0	32	1	0
3	E	48	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	48	0	32	2	0
3	G	48	0	32	2	0
3	H	48	0	32	1	0
4	A	46	0	0	3	0
4	B	34	0	0	0	0
4	C	37	0	0	0	0
4	D	33	0	0	0	0
4	E	39	0	0	1	0
4	F	36	0	0	0	0
4	G	26	0	0	0	0
4	H	41	0	0	0	0
All	All	15112	0	15128	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 124 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD13	1:B:337:LEU:HD12	1.55	0.87
1:A:229:LEU:HD13	1:F:414:ALA:HB1	1.56	0.86
1:C:264:LEU:HD23	1:C:394:ILE:HD13	1.62	0.81
1:E:221:VAL:HG13	1:E:407:LYS:HG3	1.65	0.79
1:C:393:ILE:HG13	1:C:394:ILE:HG13	1.67	0.76

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%)	225 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	39 65
1	C	232/262 (88%)	226 (97%)	6 (3%)	0	100 100
1	D	232/262 (88%)	225 (97%)	6 (3%)	1 (0%)	39 65
1	E	232/262 (88%)	223 (96%)	9 (4%)	0	100 100
1	F	232/262 (88%)	224 (97%)	8 (3%)	0	100 100
1	G	232/262 (88%)	224 (97%)	8 (3%)	0	100 100
1	H	232/262 (88%)	224 (97%)	8 (3%)	0	100 100
All	All	1856/2096 (88%)	1794 (97%)	60 (3%)	2 (0%)	56 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	189	LYS
1	B	290	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	196/222 (88%)	182 (93%)	14 (7%)	18 36
1	B	196/222 (88%)	185 (94%)	11 (6%)	26 50
1	C	196/222 (88%)	181 (92%)	15 (8%)	16 31
1	D	196/222 (88%)	182 (93%)	14 (7%)	18 36
1	E	196/222 (88%)	184 (94%)	12 (6%)	23 46
1	F	196/222 (88%)	183 (93%)	13 (7%)	21 40
1	G	196/222 (88%)	185 (94%)	11 (6%)	26 50
1	H	196/222 (88%)	184 (94%)	12 (6%)	23 46
All	All	1568/1776 (88%)	1466 (94%)	102 (6%)	21 42

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	294	ILE
1	E	258	LEU
1	H	321	SER
1	D	314	ASN
1	D	393	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN
1	D	381	GLN
1	H	274	ASN
1	D	324	GLN
1	E	274	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	COA	A	500	-	40,50,50	1.58	3 (7%)	50,75,75	1.96	6 (12%)
3	COA	B	500	-	40,50,50	1.59	3 (7%)	50,75,75	2.39	11 (22%)
3	COA	C	500	-	40,50,50	1.65	3 (7%)	50,75,75	2.00	5 (10%)
3	COA	D	500	-	40,50,50	1.64	3 (7%)	50,75,75	2.13	8 (16%)
3	COA	E	500	-	40,50,50	1.48	2 (5%)	50,75,75	2.58	11 (22%)
3	COA	F	500	-	40,50,50	1.73	3 (7%)	50,75,75	2.09	2 (4%)
3	COA	G	500	-	40,50,50	1.68	3 (7%)	50,75,75	2.73	7 (14%)
3	COA	H	500	-	40,50,50	1.67	3 (7%)	50,75,75	2.41	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	500	-	-	0/44/64/64	0/3/3/3
3	COA	B	500	-	-	0/44/64/64	0/3/3/3
3	COA	C	500	-	-	0/44/64/64	0/3/3/3
3	COA	D	500	-	-	0/44/64/64	0/3/3/3
3	COA	E	500	-	-	0/44/64/64	0/3/3/3
3	COA	F	500	-	-	0/44/64/64	0/3/3/3
3	COA	G	500	-	-	0/44/64/64	0/3/3/3
3	COA	H	500	-	-	0/44/64/64	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	COA	C2A-N1A	2.32	1.38	1.33
3	D	500	COA	C2A-N1A	2.32	1.38	1.33
3	A	500	COA	C2A-N1A	2.39	1.38	1.33
3	G	500	COA	C2A-N1A	2.41	1.38	1.33
3	H	500	COA	C2A-N3A	3.02	1.37	1.32

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	500	COA	N3A-C2A-N1A	-16.08	116.58	128.89
3	E	500	COA	N3A-C2A-N1A	-14.90	117.48	128.89
3	B	500	COA	N3A-C2A-N1A	-13.14	118.83	128.89
3	H	500	COA	N3A-C2A-N1A	-12.44	119.37	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	500	COA	N3A-C2A-N1A	-12.30	119.47	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	COA	2	0
3	C	500	COA	2	0
3	D	500	COA	1	0
3	E	500	COA	2	0
3	F	500	COA	2	0
3	G	500	COA	2	0
3	H	500	COA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	234/262 (89%)	-0.06	9 (3%)	44	36	28, 37, 58, 70	0
1	B	234/262 (89%)	-0.01	7 (2%)	54	47	28, 36, 56, 61	0
1	C	234/262 (89%)	-0.05	9 (3%)	44	36	29, 38, 57, 69	0
1	D	234/262 (89%)	0.05	9 (3%)	44	36	30, 39, 60, 66	0
1	E	234/262 (89%)	-0.01	9 (3%)	44	36	30, 39, 56, 69	0
1	F	234/262 (89%)	0.12	11 (4%)	35	28	30, 40, 58, 64	0
1	G	234/262 (89%)	0.28	21 (8%)	12	8	32, 41, 60, 69	0
1	H	234/262 (89%)	0.15	17 (7%)	18	12	28, 37, 59, 68	0
All	All	1872/2096 (89%)	0.06	92 (4%)	33	26	28, 39, 58, 70	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	GLY	4.5
1	H	374	LYS	4.2
1	F	238	PHE	4.2
1	H	218	CYS	4.1
1	H	348	ALA	4.1

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	E	806	1/1	0.94	0.34	2.03	76,76,76,76	0
2	CL	C	803	1/1	0.98	0.25	2.00	63,63,63,63	0
2	CL	G	811	1/1	0.98	0.40	1.91	75,75,75,75	0
2	CL	F	804	1/1	0.98	0.29	1.69	71,71,71,71	0
2	CL	H	809	1/1	0.94	0.33	1.32	65,65,65,65	0
2	CL	A	802	1/1	0.97	0.24	1.17	61,61,61,61	0
2	CL	C	807	1/1	0.98	0.13	1.00	39,39,39,39	0
2	CL	D	805	1/1	0.95	0.24	0.81	71,71,71,71	0
2	CL	B	801	1/1	0.93	0.18	-0.04	66,66,66,66	0
2	CL	D	808	1/1	0.96	0.11	-0.14	41,41,41,41	0
3	COA	F	500	48/48	0.94	0.13	-0.48	48,54,63,65	0
3	COA	D	500	48/48	0.94	0.12	-0.94	42,52,63,65	0
3	COA	H	500	48/48	0.97	0.11	-1.11	32,43,54,58	0
3	COA	B	500	48/48	0.97	0.10	-1.19	31,42,55,61	0
3	COA	E	500	48/48	0.97	0.10	-1.22	31,37,53,57	0
3	COA	C	500	48/48	0.96	0.10	-1.23	38,43,57,60	0
3	COA	G	500	48/48	0.96	0.10	-1.25	35,43,56,58	0
3	COA	A	500	48/48	0.96	0.10	-1.47	34,42,53,55	0
2	CL	G	810	1/1	0.98	0.17	-	42,42,42,42	1
2	CL	H	812	1/1	0.97	0.12	-	39,39,39,39	1

6.5 Other polymers

There are no such residues in this entry.