



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 08:50 pm BST

PDB ID : 3BLV  
Title : Yeast Isocitrate Dehydrogenase with Citrate Bound in the Regulatory Subunits  
Authors : Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.  
Deposited on : 2007-12-11  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

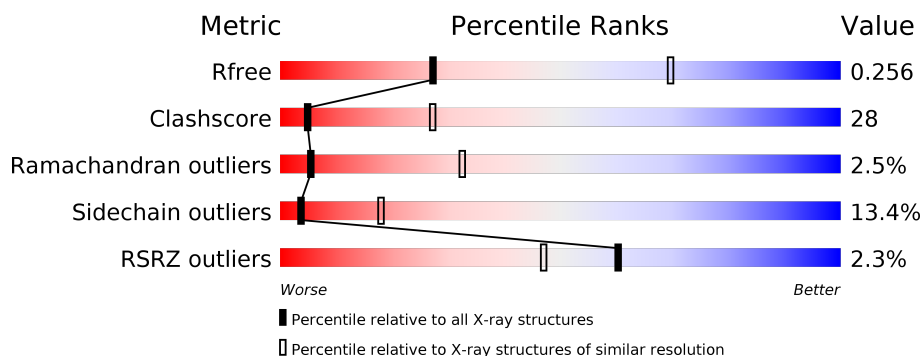
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	354	<div> <div></div> <div>60%</div> <div>31%</div> <div>6%</div> <div>• •</div> </div>
1	E	354	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>7%</div> <div>•</div> </div> </div>
1	G	354	<div> <div></div> <div>58%</div> <div>30%</div> <div>5%</div> <div>• 6%</div> </div>
2	B	354	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>9%</div> <div>• •</div> </div> </div>
2	D	354	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>39%</div> <div>10%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	354	
2	H	354	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	G	1004	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20849 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 Isocitrate dehydrogenase [NAD] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	Se	0	0	0
			2538	1605	442	484	7			
1	C	344	Total	C	N	O	Se	0	0	0
			2634	1664	461	502	7			
1	E	344	Total	C	N	O	Se	0	0	0
			2634	1664	461	502	7			
1	G	331	Total	C	N	O	Se	0	0	0
			2538	1605	442	484	7			

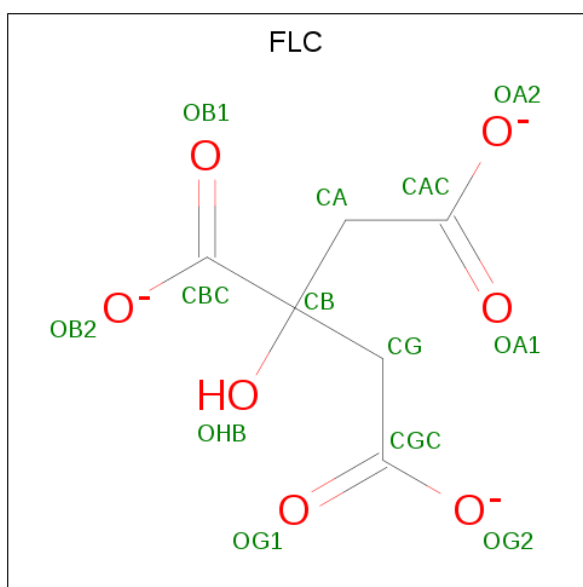
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	HIS	-	EXPRESSION TAG	UNP P28834
A	351	HIS	-	EXPRESSION TAG	UNP P28834
A	352	HIS	-	EXPRESSION TAG	UNP P28834
A	353	HIS	-	EXPRESSION TAG	UNP P28834
A	354	HIS	-	EXPRESSION TAG	UNP P28834
C	350	HIS	-	EXPRESSION TAG	UNP P28834
C	351	HIS	-	EXPRESSION TAG	UNP P28834
C	352	HIS	-	EXPRESSION TAG	UNP P28834
C	353	HIS	-	EXPRESSION TAG	UNP P28834
C	354	HIS	-	EXPRESSION TAG	UNP P28834
E	350	HIS	-	EXPRESSION TAG	UNP P28834
E	351	HIS	-	EXPRESSION TAG	UNP P28834
E	352	HIS	-	EXPRESSION TAG	UNP P28834
E	353	HIS	-	EXPRESSION TAG	UNP P28834
E	354	HIS	-	EXPRESSION TAG	UNP P28834
G	350	HIS	-	EXPRESSION TAG	UNP P28834
G	351	HIS	-	EXPRESSION TAG	UNP P28834
G	352	HIS	-	EXPRESSION TAG	UNP P28834
G	353	HIS	-	EXPRESSION TAG	UNP P28834
G	354	HIS	-	EXPRESSION TAG	UNP P28834

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	345	Total	C	N	O	S	Se	0	0	0
			2600	1641	445	508	3	3			
2	D	347	Total	C	N	O	S	Se	0	0	0
			2617	1652	449	510	3	3			
2	F	347	Total	C	N	O	S	Se	0	0	0
			2617	1652	449	510	3	3			
2	H	348	Total	C	N	O	S	Se	0	0	0
			2619	1654	448	511	3	3			

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).

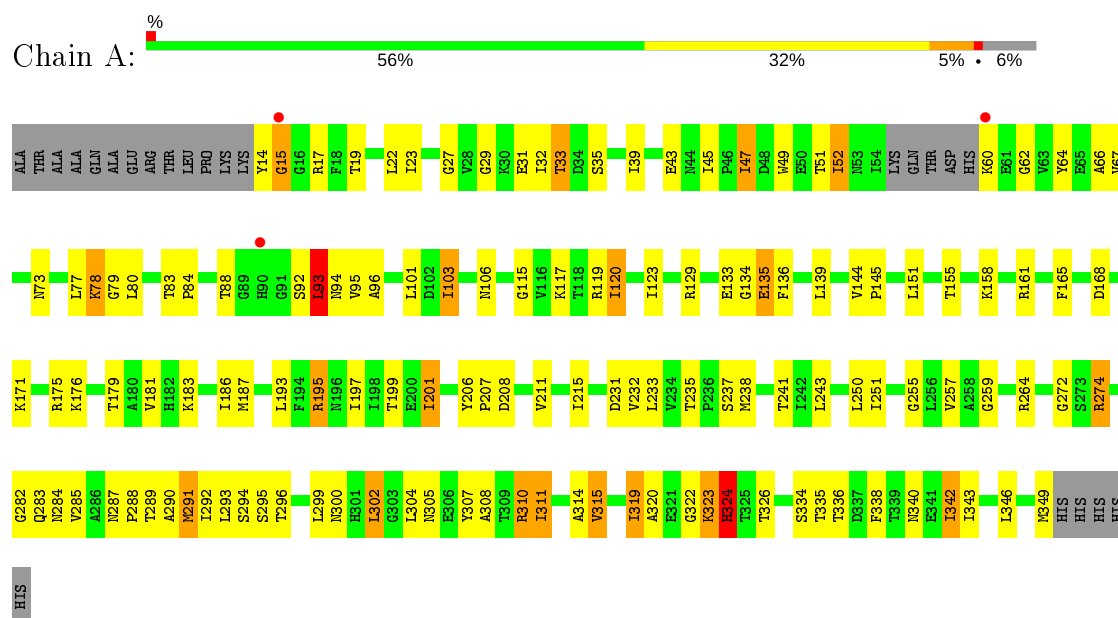


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		

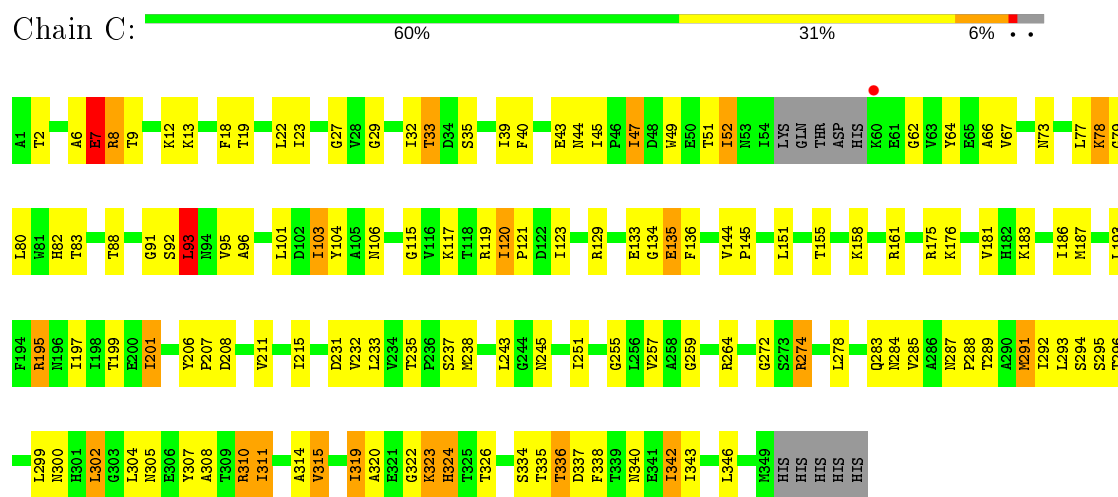
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

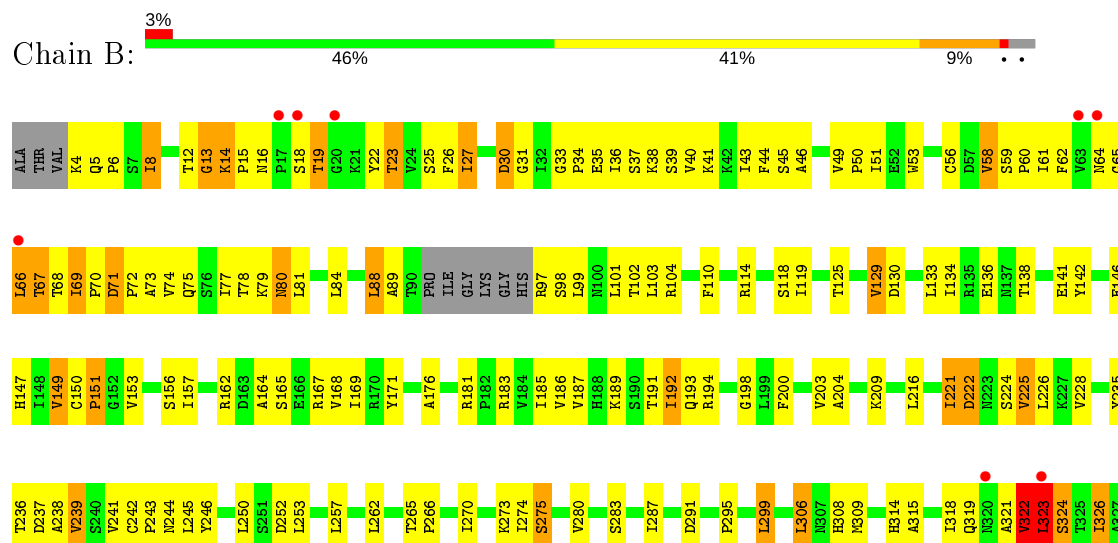
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

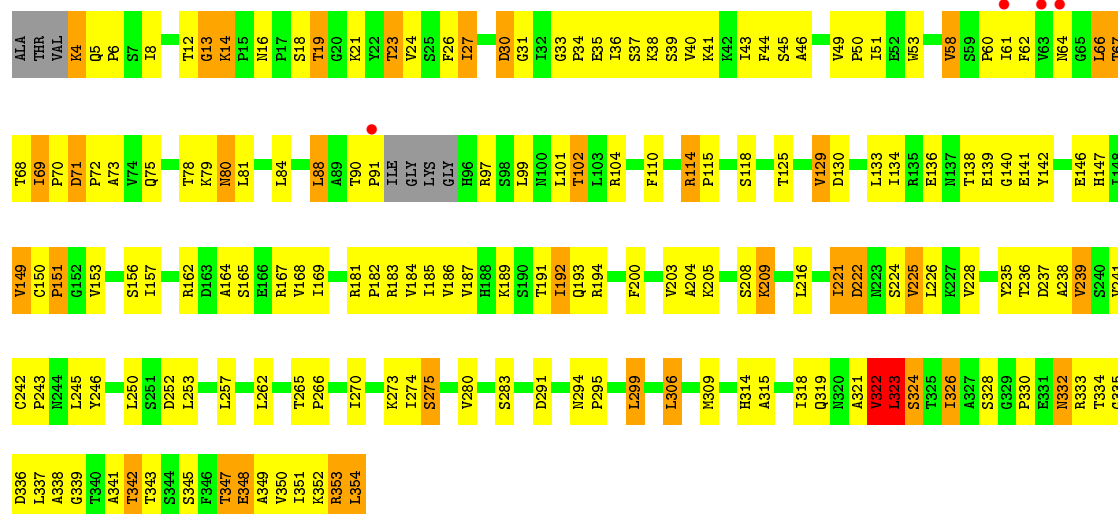


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

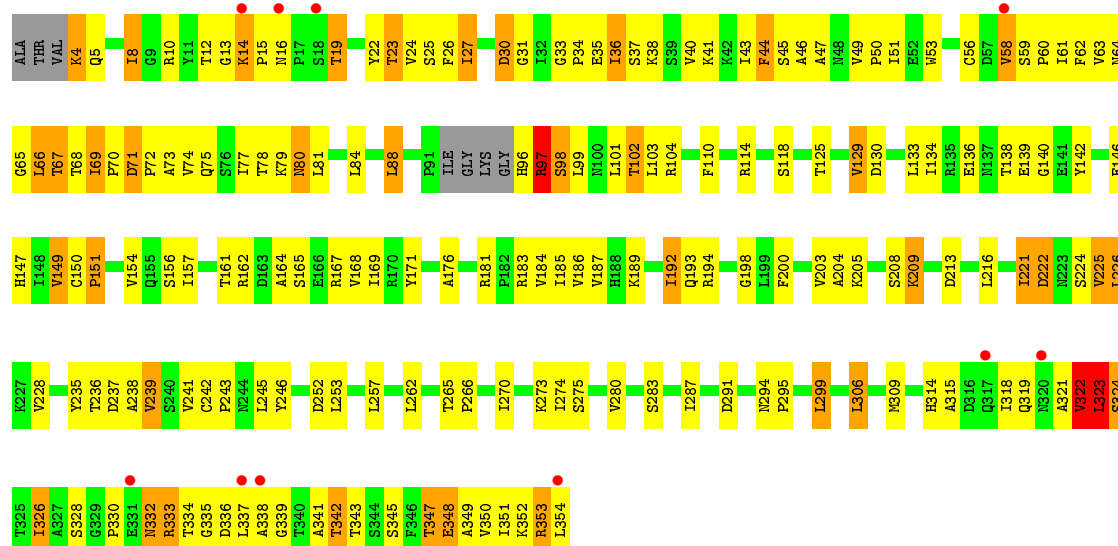




• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



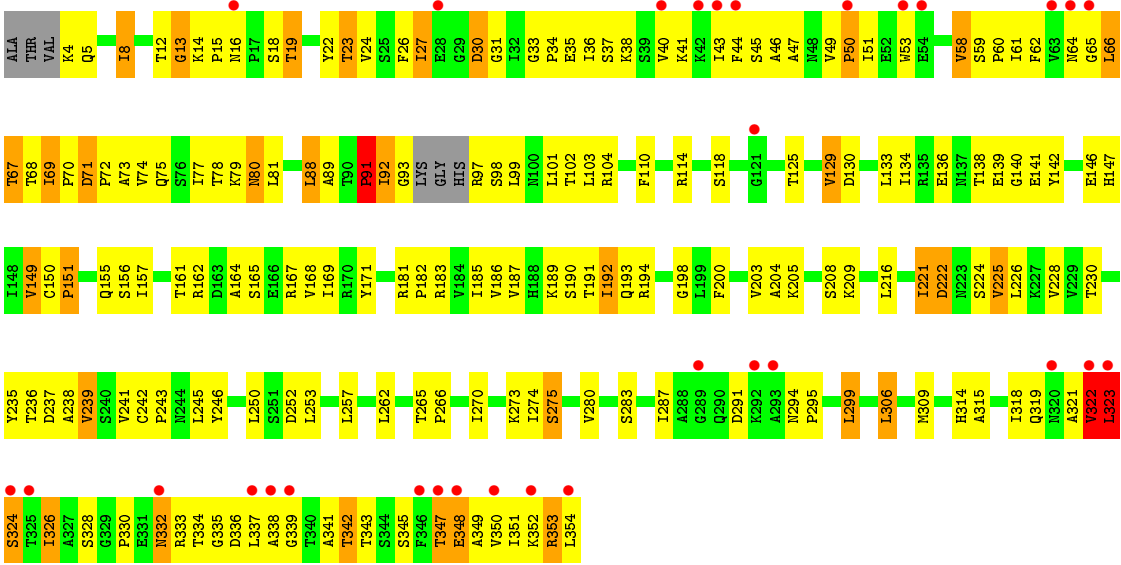
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	256.90Å 112.95Å 125.62Å 90.00° 106.67° 90.00°	Depositor
Resolution (Å)	49.35 – 3.20 49.34 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.35-3.20) 95.8 (49.34-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.221 , 0.265 0.210 , 0.256	Depositor DCC
$R_{free}$ test set	2772 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC

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	0.40	0/2574	0.76	4/3469 (0.1%)
1	C	0.41	0/2671	0.62	3/3600 (0.1%)
1	E	0.39	0/2671	0.63	3/3600 (0.1%)
1	G	0.41	0/2574	0.61	3/3469 (0.1%)
2	B	0.37	0/2641	0.57	0/3585
2	D	0.39	0/2660	0.56	0/3612
2	F	0.38	0/2660	0.57	0/3612
2	H	0.39	0/2661	0.59	1/3613 (0.0%)
All	All	0.39	0/21112	0.61	14/28560 (0.0%)

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	E	0	1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	-19.14	110.73	120.30
1	A	264	ARG	NE-CZ-NH2	18.22	129.41	120.30
1	A	264	ARG	CD-NE-CZ	8.81	135.94	123.60
1	C	264	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	264	ARG	NE-CZ-NH1	7.06	123.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2538	0	2571	119	0
1	C	2634	0	2679	120	0
1	E	2634	0	2679	135	0
1	G	2538	0	2571	121	0
2	B	2600	0	2648	168	0
2	D	2617	0	2662	174	0
2	F	2617	0	2662	188	0
2	H	2619	0	2669	186	0
3	A	13	0	5	3	0
3	C	13	0	5	3	0
3	E	13	0	5	3	0
3	G	13	0	5	4	0
All	All	20849	0	21161	1156	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 28.

The worst 5 of 1156 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:C:135:GLU:HG3	1:C:238:MSE:HB2	1.36	1.07
1:E:7:GLU:HB3	1:E:10:LEU:HD11	1.37	1.04
1:G:135:GLU:HG3	1:G:238:MSE:HB2	1.36	1.03
1:A:135:GLU:HG3	1:A:238:MSE:HB2	1.38	1.01
1:E:135:GLU:HG3	1:E:238:MSE:HB2	1.38	1.01

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	327/354 (92%)	296 (90%)	26 (8%)	5 (2%)	10	44
1	C	340/354 (96%)	307 (90%)	28 (8%)	5 (2%)	10	44
1	E	340/354 (96%)	304 (89%)	31 (9%)	5 (2%)	10	44
1	G	327/354 (92%)	296 (90%)	27 (8%)	4 (1%)	13	49
2	B	341/354 (96%)	288 (84%)	40 (12%)	13 (4%)	3	22
2	D	343/354 (97%)	291 (85%)	43 (12%)	9 (3%)	5	31
2	F	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	22
2	H	344/354 (97%)	290 (84%)	40 (12%)	14 (4%)	3	21
All	All	2705/2832 (96%)	2361 (87%)	276 (10%)	68 (2%)	5	32

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LEU
2	B	13	GLY
2	B	98	SER
2	B	151	PRO
2	B	322	VAL

### 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	275/287 (96%)	246 (90%)	29 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	284/287 (99%)	254 (89%)	30 (11%)	6	27
1	E	284/287 (99%)	254 (89%)	30 (11%)	6	27
1	G	275/287 (96%)	248 (90%)	27 (10%)	8	31
2	B	291/294 (99%)	245 (84%)	46 (16%)	2	12
2	D	293/294 (100%)	246 (84%)	47 (16%)	2	11
2	F	293/294 (100%)	244 (83%)	49 (17%)	2	10
2	H	293/294 (100%)	245 (84%)	48 (16%)	2	11
All	All	2288/2324 (98%)	1982 (87%)	306 (13%)	4	18

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	262	LEU
1	E	291	MSE
2	H	162	ARG
2	D	306	LEU
1	E	47	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	245	ASN
1	C	301	HIS
2	F	64	ASN
1	C	106	ASN
2	F	193	GLN

### 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

4 ligands are modelled in this entry.

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	FLC	C	1002	-	3,12,12	0.94	0	3,17,17	2.77	2 (66%)
3	FLC	E	1003	-	3,12,12	0.92	0	3,17,17	2.76	2 (66%)
3	FLC	G	1004	-	3,12,12	0.92	0	3,17,17	2.77	2 (66%)
3	FLC	A	1001	-	3,12,12	0.95	0	3,17,17	2.09	2 (66%)

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	FLC	C	1002	-	-	6/6/16/16	-
3	FLC	E	1003	-	-	6/6/16/16	-
3	FLC	G	1004	-	-	3/6/16/16	-
3	FLC	A	1001	-	-	3/6/16/16	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1004	FLC	CB-CA-CAC	-3.40	109.53	114.98
3	C	1002	FLC	CB-CG-CGC	-3.40	109.55	114.98
3	E	1003	FLC	CB-CA-CAC	-3.39	109.56	114.98
3	C	1002	FLC	CB-CA-CAC	-3.38	109.57	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1004	FLC	CB-CG-CGC	-3.38	109.58	114.98

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1002	FLC	CAC-CA-CB-CBC
3	C	1002	FLC	CA-CB-CG-CGC
3	C	1002	FLC	CBC-CB-CG-CGC
3	E	1003	FLC	CAC-CA-CB-CBC
3	E	1003	FLC	CA-CB-CG-CGC

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	FLC	3	0
3	E	1003	FLC	3	0
3	G	1004	FLC	4	0
3	A	1001	FLC	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	324/354 (91%)	-0.15	3 (0%) 84 75	48, 66, 95, 124	0
1	C	337/354 (95%)	-0.24	1 (0%) 94 92	48, 64, 93, 125	0
1	E	337/354 (95%)	-0.20	3 (0%) 84 75	47, 66, 95, 138	0
1	G	324/354 (91%)	-0.20	1 (0%) 94 92	47, 64, 91, 123	0
2	B	342/354 (96%)	-0.04	9 (2%) 56 40	43, 76, 108, 123	0
2	D	344/354 (97%)	-0.04	4 (1%) 79 67	43, 74, 103, 128	0
2	F	344/354 (97%)	0.16	10 (2%) 51 36	44, 76, 107, 122	0
2	H	345/354 (97%)	0.29	31 (8%) 9 5	43, 77, 109, 124	0
All	All	2697/2832 (95%)	-0.05	62 (2%) 60 47	43, 70, 103, 138	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	VAL	4.4
2	H	346	PHE	3.9
2	H	324	SER	3.9
2	H	348	GLU	3.7
2	H	64	ASN	3.7

### 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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FLC	E	1003	13/13	0.91	0.23	62,86,94,96	0
3	FLC	A	1001	13/13	0.92	0.25	76,83,99,99	0
3	FLC	C	1002	13/13	0.94	0.21	71,82,94,94	0
3	FLC	G	1004	13/13	0.95	0.20	53,77,84,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.