



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 05:24 PM BST

PDB ID : 6WIH  
Title : N-terminal mutation of ISCU2 (L35H36) traps Nfs1 Cys loop in the active site of ISCU2 without metal present. Structure of human mitochondrial complex Nfs1-ISCU2(L35H36)-ISD11 with E.coli ACP1 at 1.9 Å resolution (NIAU)2.  
Authors : Boniecki, M.T.; Cygler, M.  
Deposited on : 2020-04-09  
Resolution : 1.90 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.

---

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 : 2.13.1  
buster-report : 1.1.7 (2018)  
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) : 2.13.1

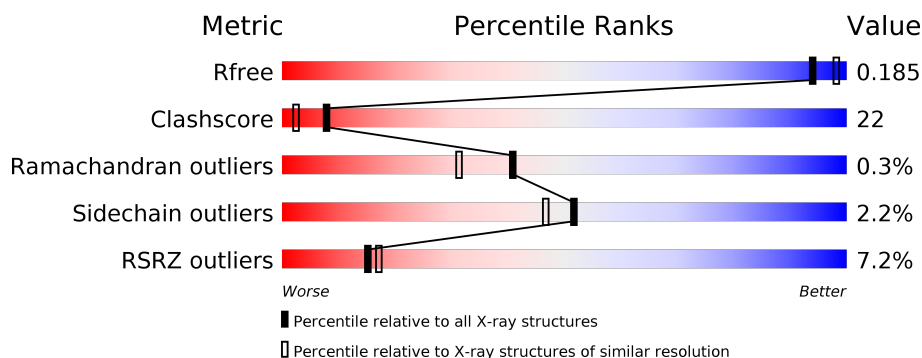
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	406	<div> <div>78%</div> <div>18%</div> <div>...</div> </div>
2	B	91	<div> <div>3%</div> <div>74%</div> <div>16%</div> <div>8%</div> </div>
3	C	77	<div> <div>39%</div> <div>83%</div> <div>10%</div> <div>...</div> </div>
4	D	143	<div> <div>7%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	P15	A	523	-	-	X	-
11	PGE	A	528	-	-	X	-
11	PGE	A	536	-	-	X	-
12	EDT	B	411	-	-	X	-
14	1PE	D	202	-	-	X	-
6	PEG	B	405	-	-	X	-
6	PEG	B	407	-	-	X	-
7	GOL	B	402	-	-	X	-
8	EDO	A	507	-	-	X	-
8	EDO	A	509	-	-	X	-
8	EDO	A	513	-	-	X	-
8	EDO	A	520	-	-	X	-
8	EDO	A	521	-	-	X	-
8	EDO	A	525	-	-	-	X
8	EDO	A	526	-	-	X	-
8	EDO	A	534	-	-	-	X
8	EDO	A	535	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 6194 atoms, of which 6 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	9	0
			3134	1977	542	594	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	initiating methionine	UNP Q9Y697
A	53	GLY	-	expression tag	UNP Q9Y697
A	54	SER	-	expression tag	UNP Q9Y697
A	55	SER	-	expression tag	UNP Q9Y697

- Molecule 2 is a protein called LYR motif-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	10	0
			741	469	148	123	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	SER	variant	UNP Q9HD34

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			550	343	85	121	1			

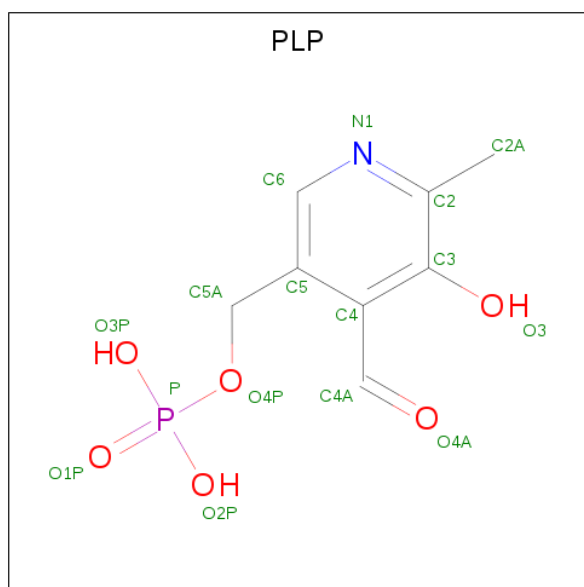
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	125	Total	C	N	O	S	0	1	0
			926	583	156	180	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	MET	-	initiating methionine	UNP Q9H1K1
D	34	ALA	-	expression tag	UNP Q9H1K1
D	36	HIS	SER	engineered mutation	UNP Q9H1K1
D	168	LEU	-	expression tag	UNP Q9H1K1
D	169	GLU	-	expression tag	UNP Q9H1K1
D	170	HIS	-	expression tag	UNP Q9H1K1
D	171	HIS	-	expression tag	UNP Q9H1K1
D	172	HIS	-	expression tag	UNP Q9H1K1
D	173	HIS	-	expression tag	UNP Q9H1K1
D	174	HIS	-	expression tag	UNP Q9H1K1
D	175	HIS	-	expression tag	UNP Q9H1K1

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			21	8	6	1	5	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



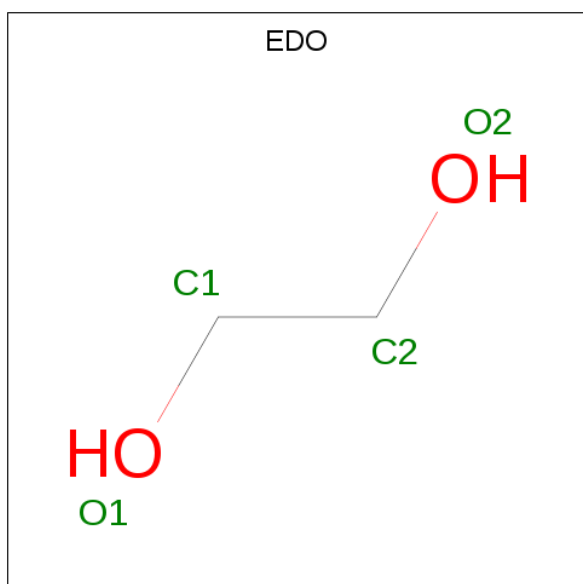
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



[illegible]

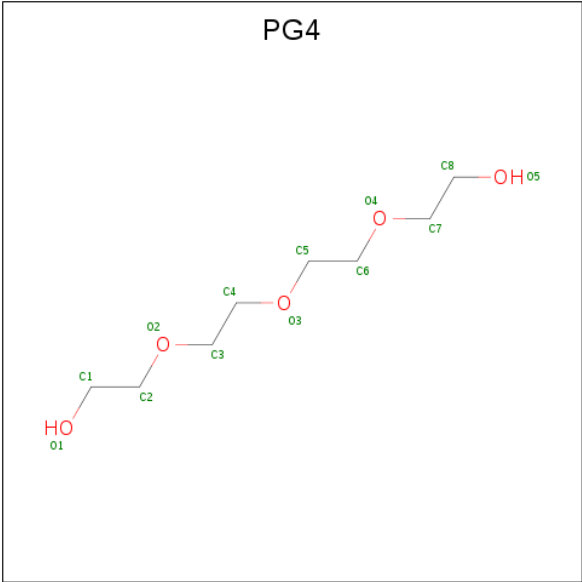
*Continued on next page...*



*Continued from previous page...*

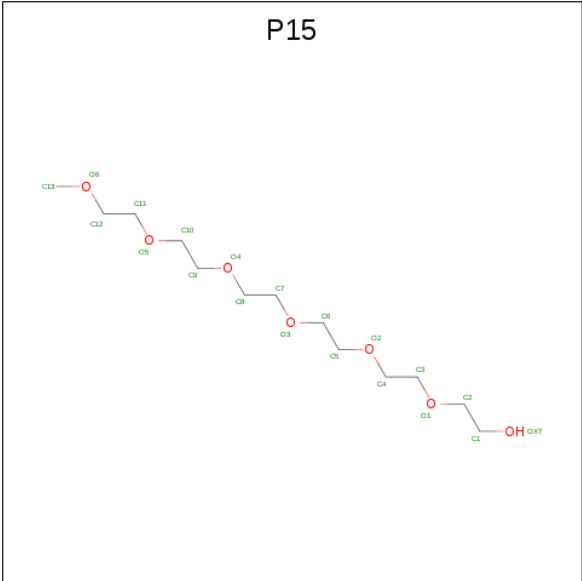
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



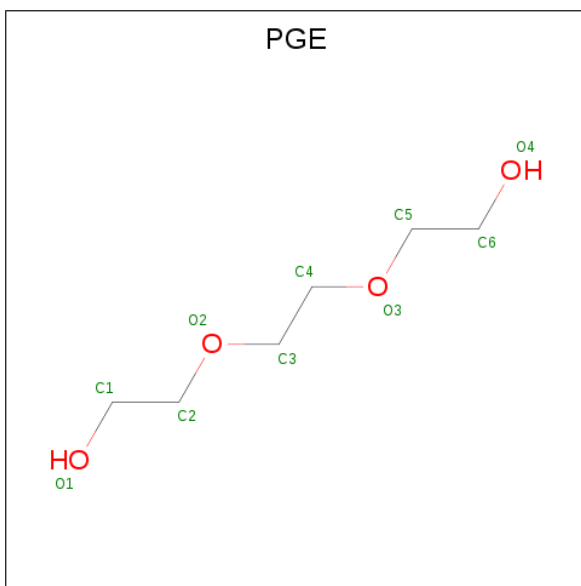
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (three-letter code: P15) (formula: C<sub>13</sub>H<sub>28</sub>O<sub>7</sub>).



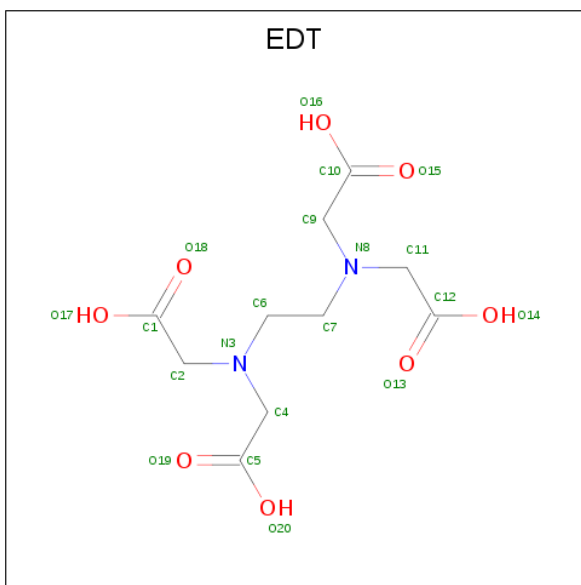
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			20	13	7		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



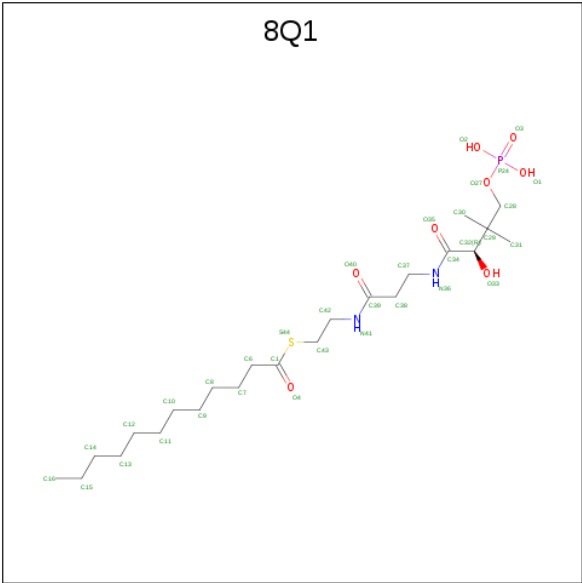
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			10	6	4		
11	A	1	Total	C	O	0	0
			10	6	4		
11	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula:  $C_{10}H_{16}N_2O_8$ ).



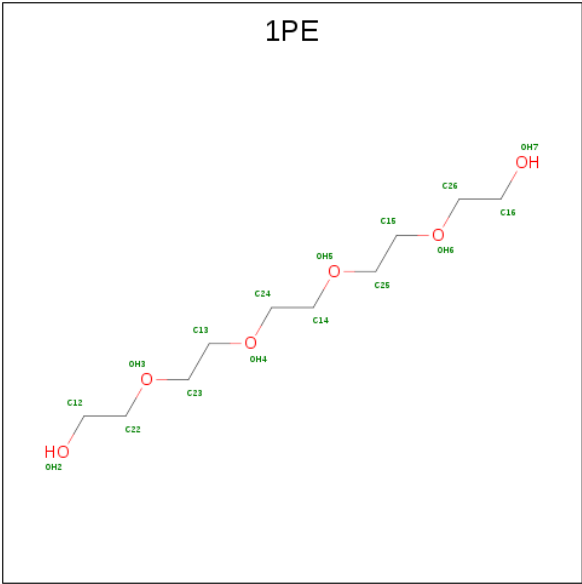
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 13 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	S	0	0
			34	23	2	7	1	1		

- Molecule 14 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			16	10	6		

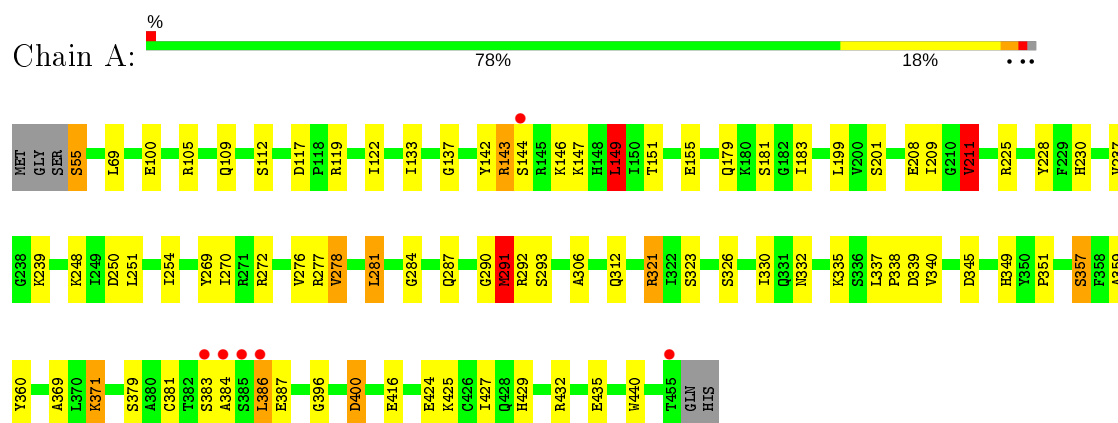
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	303	Total	O	0	0
			303	303		
15	B	60	Total	O	0	0
			60	60		
15	C	19	Total	O	0	0
			19	19		
15	D	49	Total	O	0	0
			49	49		

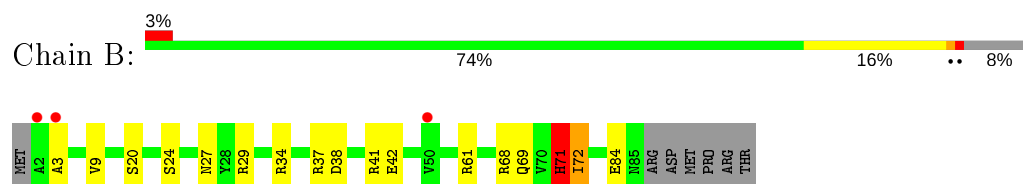
### 3 Residue-property plots [i](#)

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

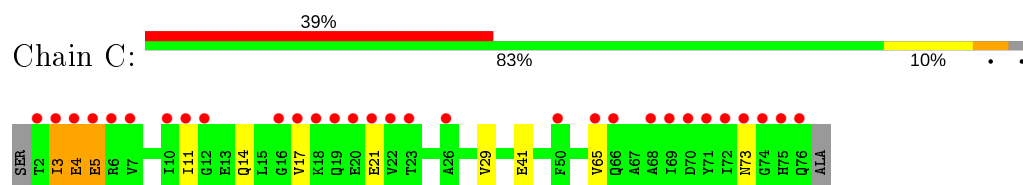
- Molecule 1: Cysteine desulfurase, mitochondrial



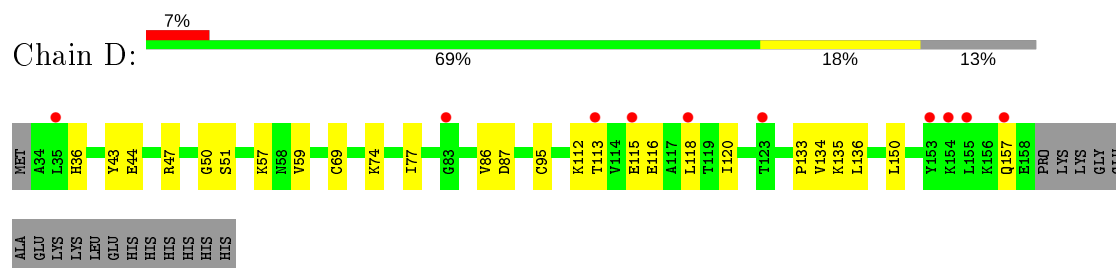
- Molecule 2: LYR motif-containing protein 4



- Molecule 3: Acyl carrier protein



- Molecule 4: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.35Å 86.35Å 245.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 1.90 48.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.97-1.90) 100.0 (48.97-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.151 , 0.186 0.159 , 0.185	Depositor DCC
$R_{free}$ test set	3717 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, PLP, EDO, 1PE, PG4, P15, EDT, 8Q1, PEG

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	8/3218 (0.2%)	0.88	6/4356 (0.1%)
2	B	1.05	3/780 (0.4%)	0.98	2/1045 (0.2%)
3	C	0.58	0/554	0.66	1/754 (0.1%)
4	D	0.65	0/941	0.73	0/1273
All	All	0.89	11/5493 (0.2%)	0.85	9/7428 (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	8
2	B	0	6
All	All	0	14

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24[A]	SER	CA-C	5.93	1.68	1.52
2	B	24[B]	SER	CA-C	5.93	1.68	1.52
1	A	208	GLU	CD-OE1	-5.87	1.19	1.25
2	B	84	GLU	CD-OE2	-5.76	1.19	1.25
1	A	357[A]	SER	CA-C	5.67	1.67	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	GLU	CB-CA-C	5.83	122.05	110.40
1	A	321[A]	ARG	NE-CZ-NH1	-5.71	117.44	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321[B]	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	A	291[A]	MET	N-CA-C	5.47	125.76	111.00
1	A	291[B]	MET	N-CA-C	5.47	125.76	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149[A]	LEU	Mainchain
1	A	149[B]	LEU	Mainchain
1	A	211[A]	VAL	Mainchain
1	A	69[A]	LEU	Mainchain
1	A	69[B]	LEU	Mainchain

## 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	3134	0	3147	135	0
2	B	741	0	790	31	0
3	C	550	0	496	10	0
4	D	926	0	934	36	0
5	A	15	6	7	0	0
6	A	49	0	70	7	0
6	B	14	0	20	20	0
7	A	18	0	24	5	0
7	B	6	0	8	5	0
7	D	6	0	8	0	0
8	A	100	0	146	64	0
8	B	28	0	42	5	0
8	C	12	0	18	3	0
8	D	12	0	18	4	0
9	A	26	0	36	8	0
10	A	20	0	28	15	0
11	A	30	0	42	31	0
12	B	20	0	12	9	0
13	C	34	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	16	0	22	9	0
15	A	303	0	0	31	0
15	B	60	0	0	6	0
15	C	19	0	0	0	0
15	D	49	0	0	7	0
All	All	6188	6	5868	251	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 22.

The worst 5 of 251 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:B:34[A]:ARG:HH21	7:B:402:GOL:H12	1.06	1.16
4:D:112:LYS:HG2	14:D:202:1PE:H222	1.37	1.06
1:A:381:CYS:SG	4:D:135:LYS:NZ	2.32	1.01
2:B:68:ARG:HH11	6:B:407:PEG:H22	1.28	0.97
9:A:517:PG4:H12	15:A:691:HOH:O	1.63	0.97

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	408/406 (100%)	399 (98%)	9 (2%)	0	100	100
2	B	92/91 (101%)	89 (97%)	2 (2%)	1 (1%)	14	5
3	C	73/77 (95%)	69 (94%)	3 (4%)	1 (1%)	11	3
4	D	124/143 (87%)	123 (99%)	1 (1%)	0	100	100
All	All	697/717 (97%)	680 (98%)	15 (2%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ALA
3	C	3	ILE

### 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	342/346 (99%)	332 (97%)	10 (3%)	42	35
2	B	78/80 (98%)	78 (100%)	0	100	100
3	C	54/66 (82%)	53 (98%)	1 (2%)	57	53
4	D	98/118 (83%)	96 (98%)	2 (2%)	55	51
All	All	572/610 (94%)	559 (98%)	13 (2%)	52	45

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291[B]	MET
1	A	371	LYS
3	C	4	GLU
1	A	291[A]	MET
1	A	400	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	312	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

62 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	$\# Z  > 2$
8	EDO	A	530	-	3,3,3	0.47	0	2,2,2	0.14	0
14	1PE	D	202	-	15,15,15	0.52	0	14,14,14	0.31	0
6	PEG	A	502	-	6,6,6	0.60	0	5,5,5	0.78	0
8	EDO	A	512	-	3,3,3	0.47	0	2,2,2	0.28	0
8	EDO	A	526	-	3,3,3	0.48	0	2,2,2	0.37	0
8	EDO	B	403	-	3,3,3	0.75	0	2,2,2	1.08	0
6	PEG	B	407	-	6,6,6	0.72	0	5,5,5	0.77	0
8	EDO	A	531	-	3,3,3	0.53	0	2,2,2	0.25	0
8	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.16	0
8	EDO	A	542	-	3,3,3	0.56	0	2,2,2	0.22	0
8	EDO	D	205	-	3,3,3	0.48	0	2,2,2	0.03	0
10	P15	A	523	-	19,19,19	0.61	0	18,18,18	0.46	0
8	EDO	A	506	-	3,3,3	0.53	0	2,2,2	0.15	0
8	EDO	A	529	-	3,3,3	0.52	0	2,2,2	1.01	0
9	PG4	A	517	-	12,12,12	0.55	0	11,11,11	0.27	0
8	EDO	A	515	-	3,3,3	0.71	0	2,2,2	0.93	0
8	EDO	B	404	-	3,3,3	0.53	0	2,2,2	0.59	0
8	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.64	0
6	PEG	A	540	-	6,6,6	0.52	0	5,5,5	0.36	0
7	GOL	A	504	-	5,5,5	0.54	0	5,5,5	0.25	0
8	EDO	A	525	-	3,3,3	0.49	0	2,2,2	0.27	0
6	PEG	A	524	-	6,6,6	0.52	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	A	521	-	3,3,3	0.44	0	2,2,2	0.59	0
8	EDO	A	539	-	3,3,3	0.51	0	2,2,2	0.45	0
8	EDO	A	533	-	3,3,3	0.48	0	2,2,2	0.31	0
8	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.22	0
11	PGE	A	536	-	9,9,9	0.32	0	8,8,8	0.49	0
8	EDO	C	304	-	3,3,3	0.47	0	2,2,2	0.30	0
8	EDO	A	509	-	3,3,3	0.56	0	2,2,2	0.43	0
8	EDO	A	532	-	3,3,3	0.47	0	2,2,2	0.09	0
6	PEG	A	516	-	6,6,6	0.50	0	5,5,5	0.71	0
8	EDO	A	535	-	3,3,3	0.47	0	2,2,2	0.32	0
8	EDO	B	410	-	3,3,3	0.50	0	2,2,2	0.57	0
8	EDO	B	408	-	3,3,3	0.47	0	2,2,2	0.73	0
8	EDO	D	201	-	3,3,3	0.49	0	2,2,2	0.45	0
8	EDO	A	508	-	3,3,3	0.51	0	2,2,2	0.27	0
8	EDO	A	522	-	3,3,3	0.47	0	2,2,2	0.19	0
7	GOL	A	503	-	5,5,5	0.61	0	5,5,5	1.08	0
8	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.21	0
8	EDO	A	510	-	3,3,3	0.48	0	2,2,2	0.13	0
12	EDT	B	411	-	7,19,19	0.47	0	12,24,24	2.00	5 (41%)
11	PGE	A	528	-	9,9,9	0.49	0	8,8,8	0.72	0
8	EDO	A	507	-	3,3,3	1.51	0	2,2,2	1.63	1 (50%)
6	PEG	A	541	-	6,6,6	0.47	0	5,5,5	0.48	0
8	EDO	A	511	-	3,3,3	0.32	0	2,2,2	0.36	0
8	EDO	A	514	-	3,3,3	0.56	0	2,2,2	0.12	0
13	8Q1	C	301	3	27,33,34	2.18	7 (25%)	32,40,43	1.72	7 (21%)
8	EDO	A	534	-	3,3,3	0.51	0	2,2,2	0.13	0
8	EDO	C	302	-	3,3,3	0.51	0	2,2,2	0.29	0
8	EDO	D	203	-	3,3,3	0.51	0	2,2,2	0.29	0
7	GOL	A	505	-	5,5,5	0.14	0	5,5,5	0.44	0
9	PG4	A	518	-	12,12,12	0.56	0	11,11,11	0.37	0
6	PEG	A	527	-	6,6,6	0.49	0	5,5,5	0.23	0
8	EDO	A	513	-	3,3,3	1.05	0	2,2,2	0.89	0
7	GOL	B	402	-	5,5,5	0.51	0	5,5,5	0.83	0
6	PEG	A	519	-	6,6,6	0.48	0	5,5,5	0.64	0
5	PLP	A	501	-	15,15,16	1.44	1 (6%)	20,22,23	0.90	1 (5%)
8	EDO	A	520	-	3,3,3	0.63	0	2,2,2	1.10	0
8	EDO	A	538	-	3,3,3	0.50	0	2,2,2	0.38	0
11	PGE	A	537	-	9,9,9	0.37	0	8,8,8	0.26	0
6	PEG	B	405	-	6,6,6	0.56	0	5,5,5	0.56	0
7	GOL	D	204	-	5,5,5	0.60	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	530	-	-	1/1/1/1	-
14	1PE	D	202	-	-	9/13/13/13	-
6	PEG	A	502	-	-	2/4/4/4	-
8	EDO	A	512	-	-	1/1/1/1	-
8	EDO	A	526	-	-	0/1/1/1	-
8	EDO	B	403	-	-	1/1/1/1	-
6	PEG	B	407	-	-	3/4/4/4	-
8	EDO	A	531	-	-	1/1/1/1	-
8	EDO	C	303	-	-	1/1/1/1	-
8	EDO	A	542	-	-	1/1/1/1	-
8	EDO	D	205	-	-	1/1/1/1	-
10	P15	A	523	-	-	9/17/17/17	-
8	EDO	A	506	-	-	0/1/1/1	-
8	EDO	A	529	-	-	1/1/1/1	-
9	PG4	A	517	-	-	6/10/10/10	-
8	EDO	A	515	-	-	1/1/1/1	-
8	EDO	B	404	-	-	0/1/1/1	-
8	EDO	B	401	-	-	1/1/1/1	-
6	PEG	A	540	-	-	4/4/4/4	-
7	GOL	A	504	-	-	4/4/4/4	-
8	EDO	A	525	-	-	1/1/1/1	-
6	PEG	A	524	-	-	1/4/4/4	-
8	EDO	A	521	-	-	0/1/1/1	-
8	EDO	A	539	-	-	0/1/1/1	-
8	EDO	A	533	-	-	0/1/1/1	-
8	EDO	B	409	-	-	0/1/1/1	-
11	PGE	A	536	-	-	3/7/7/7	-
8	EDO	C	304	-	-	0/1/1/1	-
8	EDO	A	509	-	-	1/1/1/1	-
8	EDO	A	532	-	-	0/1/1/1	-
6	PEG	A	516	-	-	1/4/4/4	-
8	EDO	A	535	-	-	0/1/1/1	-
8	EDO	B	410	-	-	0/1/1/1	-
8	EDO	B	408	-	-	1/1/1/1	-
8	EDO	D	201	-	-	0/1/1/1	-
8	EDO	A	508	-	-	0/1/1/1	-
8	EDO	A	522	-	-	1/1/1/1	-
7	GOL	A	503	-	-	2/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	406	-	-	0/1/1/1	-
8	EDO	A	510	-	-	0/1/1/1	-
12	EDT	B	411	-	-	8/13/21/21	-
11	PGE	A	528	-	-	5/7/7/7	-
8	EDO	A	507	-	-	0/1/1/1	-
6	PEG	A	541	-	-	2/4/4/4	-
8	EDO	A	511	-	-	1/1/1/1	-
8	EDO	A	514	-	-	0/1/1/1	-
13	8Q1	C	301	3	-	1/38/40/41	-
8	EDO	A	534	-	-	1/1/1/1	-
8	EDO	C	302	-	-	1/1/1/1	-
8	EDO	D	203	-	-	0/1/1/1	-
7	GOL	A	505	-	-	2/4/4/4	-
9	PG4	A	518	-	-	5/10/10/10	-
6	PEG	A	527	-	-	3/4/4/4	-
8	EDO	A	513	-	-	1/1/1/1	-
7	GOL	B	402	-	-	4/4/4/4	-
6	PEG	A	519	-	-	2/4/4/4	-
5	PLP	A	501	-	-	0/6/6/8	0/1/1/1
8	EDO	A	520	-	-	0/1/1/1	-
8	EDO	A	538	-	-	1/1/1/1	-
11	PGE	A	537	-	-	4/7/7/7	-
6	PEG	B	405	-	-	1/4/4/4	-
7	GOL	D	204	-	-	0/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	301	8Q1	C39-N41	5.65	1.46	1.33
13	C	301	8Q1	C34-N36	5.36	1.45	1.33
13	C	301	8Q1	C6-C1	3.56	1.54	1.50
5	A	501	PLP	C3-C2	-3.47	1.37	1.40
13	C	301	8Q1	C38-C39	2.51	1.56	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	301	8Q1	C37-N36-C34	-4.54	114.49	122.59
12	B	411	EDT	C11-N8-C9	4.50	118.59	110.72
13	C	301	8Q1	C42-N41-C39	-3.97	115.47	122.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	301	8Q1	C38-C37-N36	-3.01	105.81	111.90
13	C	301	8Q1	O40-C39-N41	-2.72	117.89	123.01

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	GOL	O1-C1-C2-O2
7	A	504	GOL	O1-C1-C2-C3
7	A	504	GOL	C1-C2-C3-O3
7	A	504	GOL	O2-C2-C3-O3
7	A	505	GOL	C1-C2-C3-O3

There are no ring outliers.

46 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	530	EDO	1	0
14	D	202	1PE	9	0
8	A	512	EDO	1	0
8	A	526	EDO	5	0
8	B	403	EDO	1	0
6	B	407	PEG	12	0
8	A	531	EDO	2	0
8	C	303	EDO	2	0
8	A	542	EDO	1	0
8	D	205	EDO	1	0
10	A	523	P15	15	0
8	A	506	EDO	3	0
9	A	517	PG4	5	0
8	A	515	EDO	3	0
6	A	540	PEG	3	0
7	A	504	GOL	1	0
6	A	524	PEG	1	0
8	A	521	EDO	7	0
8	A	539	EDO	1	0
11	A	536	PGE	12	0
8	A	509	EDO	4	0
8	A	532	EDO	2	0
6	A	516	PEG	1	0
8	A	535	EDO	2	0

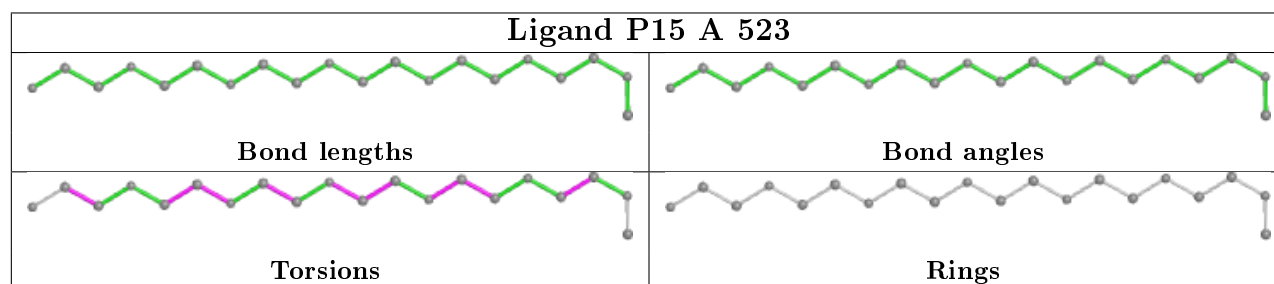
*Continued on next page...*

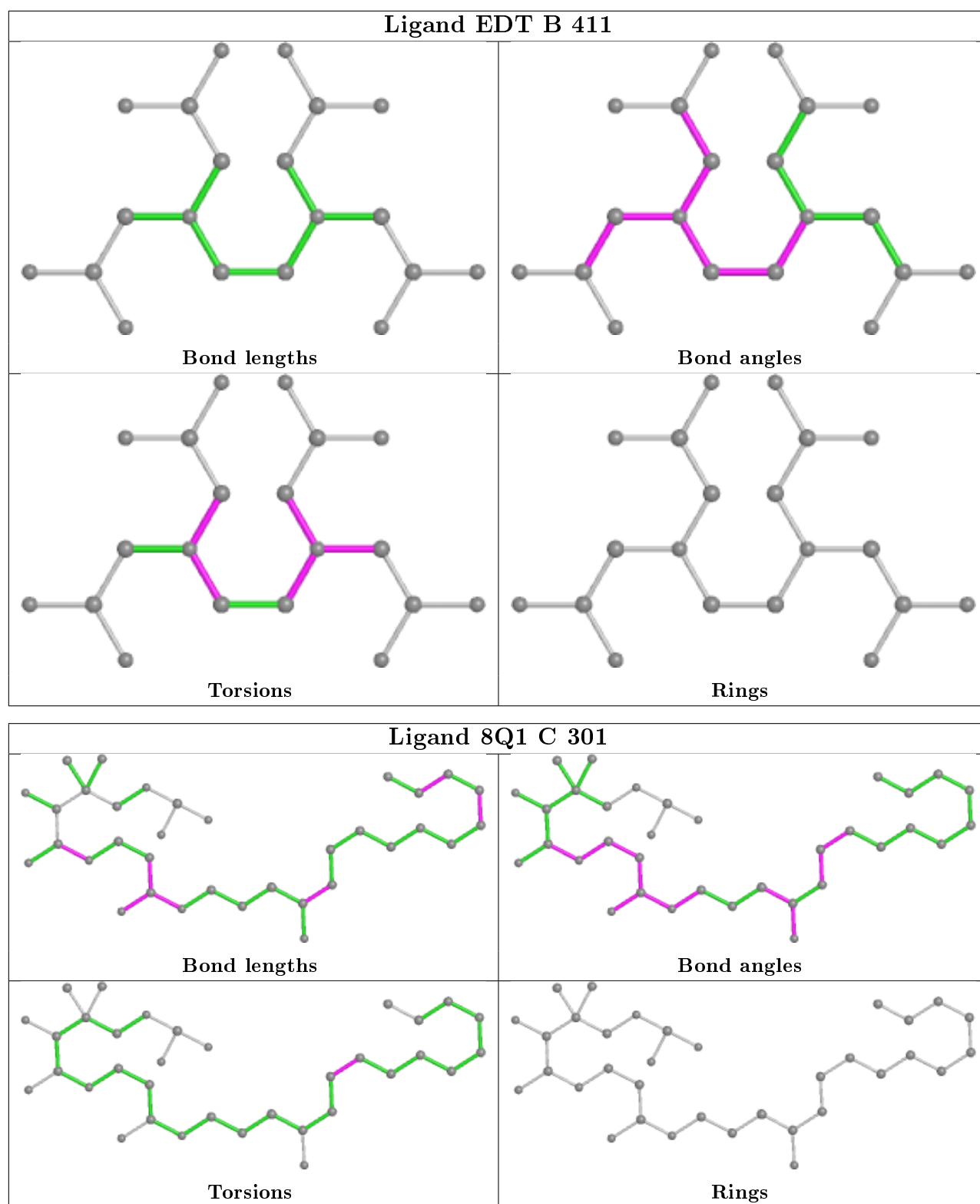


*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	408	EDO	3	0
8	D	201	EDO	3	0
8	A	508	EDO	1	0
8	A	522	EDO	3	0
7	A	503	GOL	3	0
8	B	406	EDO	1	0
12	B	411	EDT	9	0
11	A	528	PGE	15	0
8	A	507	EDO	9	0
6	A	541	PEG	2	0
8	A	511	EDO	1	0
8	A	514	EDO	3	0
8	A	534	EDO	1	0
8	C	302	EDO	1	0
7	A	505	GOL	1	0
9	A	518	PG4	3	0
8	A	513	EDO	8	0
7	B	402	GOL	5	0
8	A	520	EDO	5	0
8	A	538	EDO	1	0
11	A	537	PGE	4	0
6	B	405	PEG	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	401/406 (98%)	-0.15	6 (1%) 73 76	16, 25, 51, 107	10 (2%)
2	B	84/91 (92%)	-0.13	3 (3%) 42 45	19, 28, 53, 108	0
3	C	75/77 (97%)	1.78	30 (40%) 0 0	34, 62, 98, 117	0
4	D	125/143 (87%)	0.18	10 (8%) 12 13	23, 41, 69, 107	1 (0%)
All	All	685/717 (95%)	0.13	49 (7%) 15 17	16, 29, 74, 117	11 (1%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	17	VAL	6.6
3	C	22	VAL	6.5
2	B	3	ALA	5.7
1	A	386	LEU	5.4
3	C	20	GLU	5.4

### 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 monosaccharides 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
8	EDO	A	525	4/4	0.13	0.41	91,92,92,94	0
12	EDT	B	411	20/20	0.53	0.35	53,63,78,79	20
8	EDO	A	522	4/4	0.55	0.27	85,86,87,87	0
8	EDO	A	533	4/4	0.55	0.21	79,79,79,79	0
9	PG4	A	518	13/13	0.55	0.38	81,87,91,91	0
6	PEG	A	541	7/7	0.61	0.32	73,82,88,90	0
8	EDO	D	203	4/4	0.62	0.24	74,77,78,80	0
6	PEG	A	524	7/7	0.65	0.29	62,66,67,70	0
8	EDO	A	534	4/4	0.69	0.47	70,73,75,75	0
8	EDO	B	404	4/4	0.69	0.17	58,63,63,66	0
8	EDO	A	514	4/4	0.69	0.22	61,63,66,66	0
8	EDO	A	535	4/4	0.70	0.60	59,62,67,72	4
11	PGE	A	537	10/10	0.70	0.20	81,86,88,88	0
9	PG4	A	517	13/13	0.71	0.31	51,59,63,63	13
8	EDO	D	205	4/4	0.71	0.22	75,77,77,77	0
8	EDO	A	532	4/4	0.73	0.20	73,73,73,73	0
8	EDO	A	526	4/4	0.73	0.31	67,68,70,71	0
8	EDO	A	521	4/4	0.74	0.24	58,59,60,63	4
6	PEG	A	502	7/7	0.74	0.26	41,53,66,67	0
7	GOL	A	504	6/6	0.74	0.35	59,74,76,79	0
6	PEG	B	405	7/7	0.74	0.28	48,60,74,76	0
8	EDO	A	539	4/4	0.75	0.21	54,60,63,63	0
8	EDO	B	409	4/4	0.75	0.22	74,74,75,77	0
8	EDO	C	304	4/4	0.77	0.24	66,71,73,74	0
8	EDO	A	530	4/4	0.77	0.33	75,76,76,78	0
10	P15	A	523	20/20	0.77	0.29	28,77,81,82	20
6	PEG	B	407	7/7	0.78	0.22	32,36,48,51	7
7	GOL	B	402	6/6	0.79	0.19	37,61,62,65	0
14	1PE	D	202	16/16	0.79	0.22	59,71,75,77	0
8	EDO	C	303	4/4	0.80	0.61	38,45,45,48	4
8	EDO	B	406	4/4	0.80	0.20	65,69,69,70	0
8	EDO	A	529	4/4	0.80	0.32	34,38,38,40	4
8	EDO	A	509	4/4	0.82	0.29	36,49,52,62	0
8	EDO	A	531	4/4	0.82	0.33	72,75,77,77	0
8	EDO	B	410	4/4	0.83	0.15	66,67,68,70	0
8	EDO	A	542	4/4	0.83	0.23	52,55,59,60	0
8	EDO	B	401	4/4	0.84	0.14	83,84,84,85	0
8	EDO	A	538	4/4	0.85	0.17	67,74,77,79	0
8	EDO	B	408	4/4	0.85	0.25	29,32,33,45	4
6	PEG	A	519	7/7	0.85	0.17	54,55,58,61	0
11	PGE	A	528	10/10	0.85	0.29	25,40,47,48	10
8	EDO	A	506	4/4	0.85	0.16	51,55,59,61	0
7	GOL	D	204	6/6	0.85	0.29	41,49,54,55	6

Continued on next page...

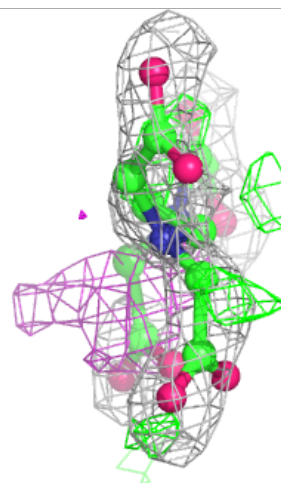
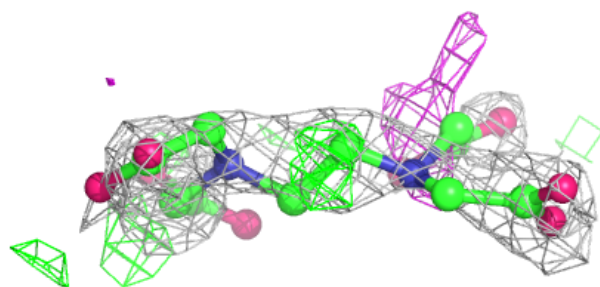
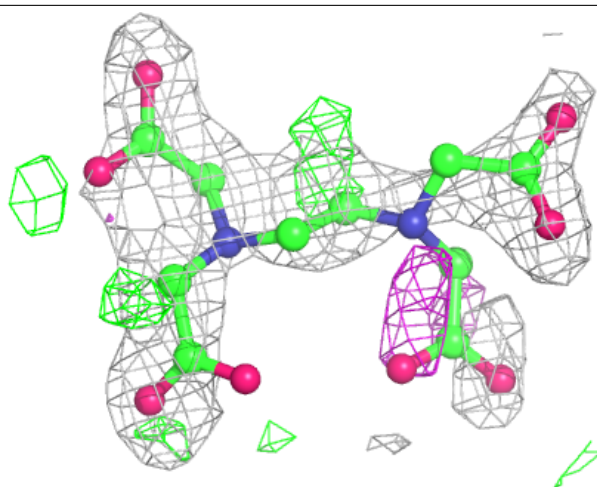
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	A	516	7/7	0.86	0.13	49,53,55,59	0
8	EDO	D	201	4/4	0.86	0.19	48,50,52,53	0
8	EDO	A	508	4/4	0.86	0.14	51,55,57,58	0
7	GOL	A	505	6/6	0.87	0.24	32,36,40,40	6
8	EDO	A	511	4/4	0.87	0.21	33,33,34,37	4
8	EDO	C	302	4/4	0.87	0.23	41,45,50,50	4
6	PEG	A	540	7/7	0.87	0.18	45,62,66,67	0
6	PEG	A	527	7/7	0.88	0.11	64,70,72,72	0
7	GOL	A	503	6/6	0.88	0.16	16,23,30,32	6
8	EDO	A	520	4/4	0.88	0.36	26,31,33,39	4
8	EDO	A	510	4/4	0.89	0.15	62,64,64,66	0
11	PGE	A	536	10/10	0.89	0.17	44,57,64,64	10
8	EDO	A	512	4/4	0.89	0.17	50,56,61,66	0
8	EDO	A	515	4/4	0.95	0.24	23,25,29,30	4
13	8Q1	C	301	34/35	0.95	0.10	27,34,43,47	0
8	EDO	B	403	4/4	0.95	0.15	29,34,38,46	4
8	EDO	A	513	4/4	0.96	0.22	17,20,24,29	4
8	EDO	A	507	4/4	0.97	0.22	10,11,16,20	4
5	PLP	A	501	15/16	0.99	0.10	17,20,25,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

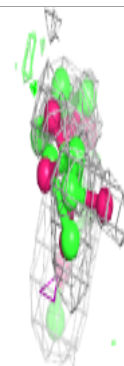
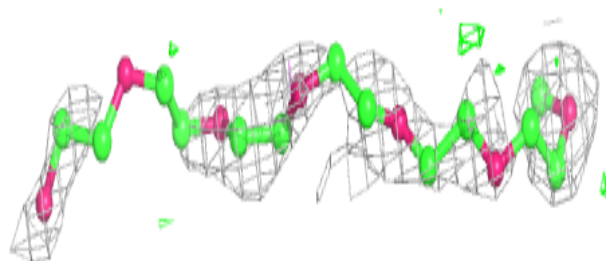
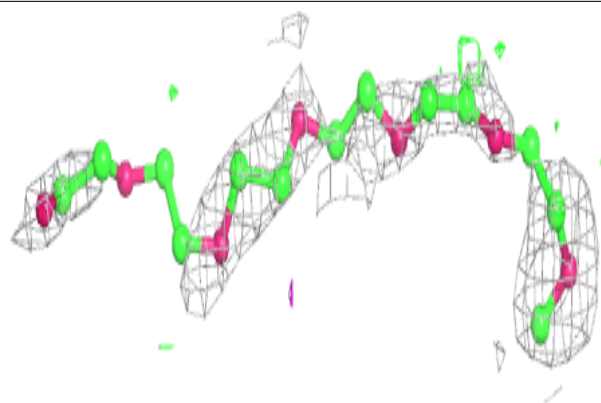
**Electron density around EDT B 411:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

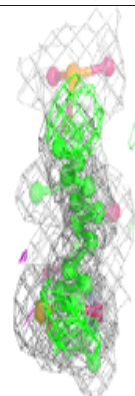
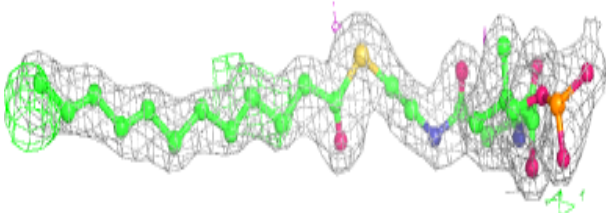
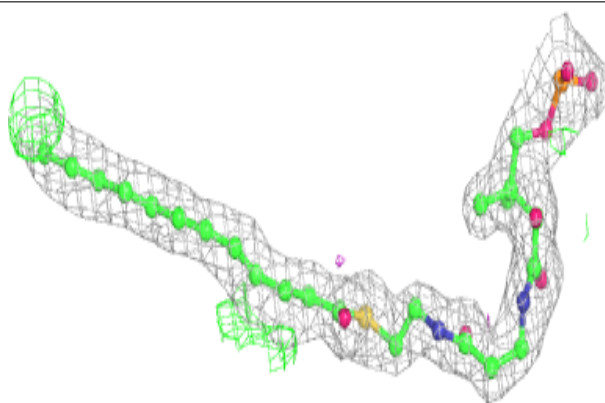


**Electron density around P15 A 523:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 8Q1 C 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.