wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 02:00 AM EDT

PDB ID	:	6WI2
Title	:	Structure of human mitochondrial complex Nfs1-ISCU2-ISD11 with E.coli ACP1 at 1.95 A resolution (NIAU)2. N-terminal mutation of ISCU2 (L35) traps Nfs1 Cys loop in the active site of ISCU2 without metal present.
Authors	:	Boniecki, M.T.; Cygler, M.
Deposited on	:	2020-04-08
Resolution	:	1.95 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

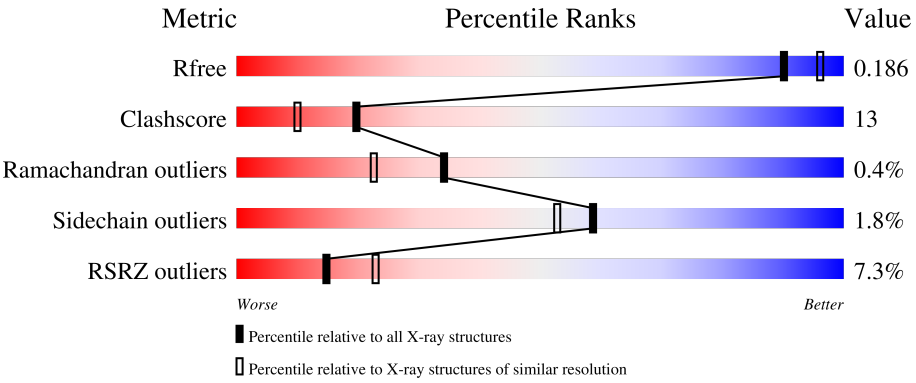
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

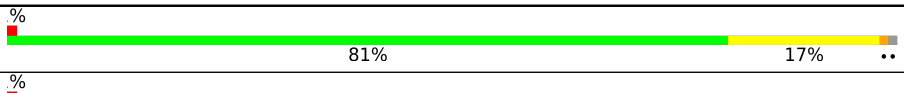
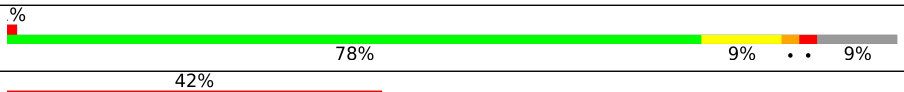
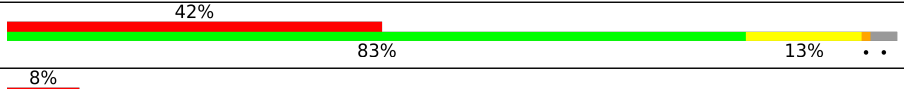
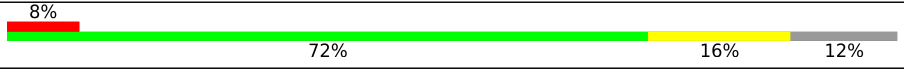
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	
2	B	91	
3	C	77	
4	D	143	

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
10	ETE	A	526	-	-	X	-
11	PGE	A	535	-	-	X	-
6	EDO	A	509	-	-	X	-
6	EDO	A	516	-	-	X	-
6	EDO	A	528	-	-	-	X
8	PEG	B	1607	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 6127 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	9	0
			3143	1978	548	596	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	83	Total	C	N	O	S	0	7	0
			727	457	147	122	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	1	0
			552	343	85	123	1			

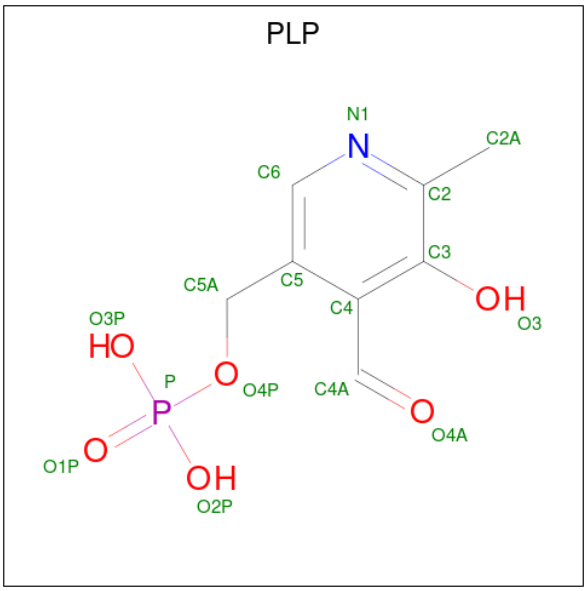
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	126	Total	C	N	O	S	1	3	0
			926	582	155	181	8			

There are 10 discrepancies between the modelled and reference sequences:

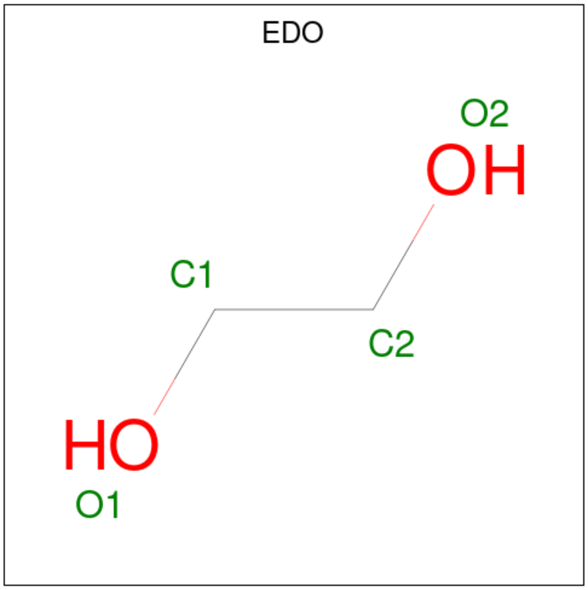
Chain	Residue	Modelled	Actual	Comment	Reference
D	33	MET	-	initiating methionine	UNP Q9H1K1
D	34	ALA	-	expression tag	UNP Q9H1K1
D	168	LEU	-	expression tag	UNP Q9H1K1
D	169	GLU	-	expression tag	UNP Q9H1K1
D	170	HIS	-	expression tag	UNP Q9H1K1
D	171	HIS	-	expression tag	UNP Q9H1K1
D	172	HIS	-	expression 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	N	O	P	0	0
			15	8	1	5	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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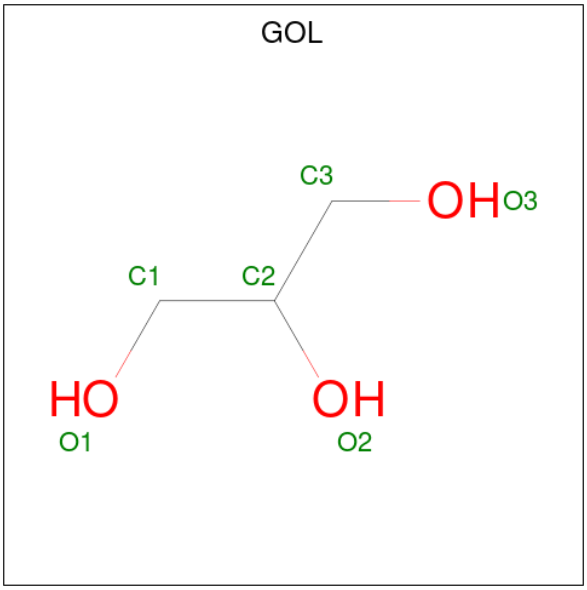
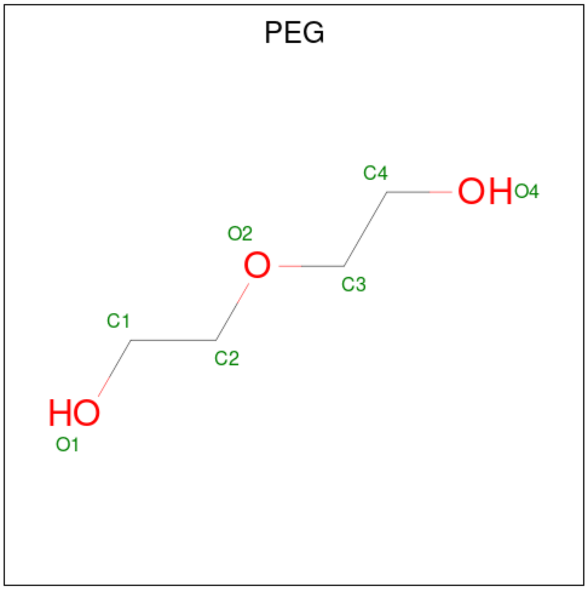
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



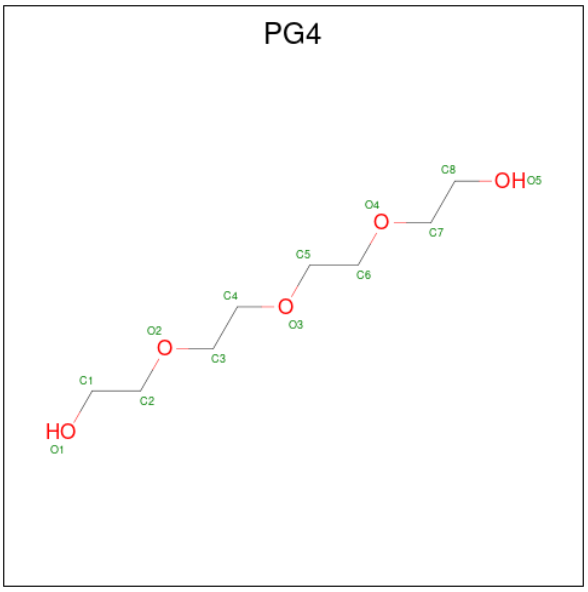
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



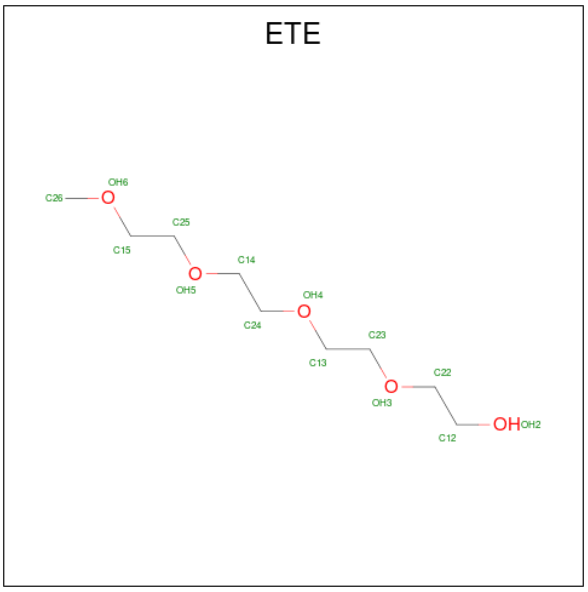
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



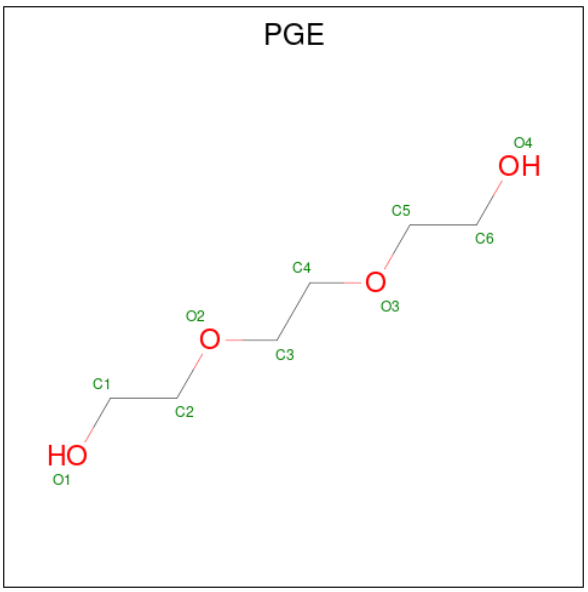
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 13 8 5	0	0
9	A	1	Total C O 13 8 5	0	0

- Molecule 10 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



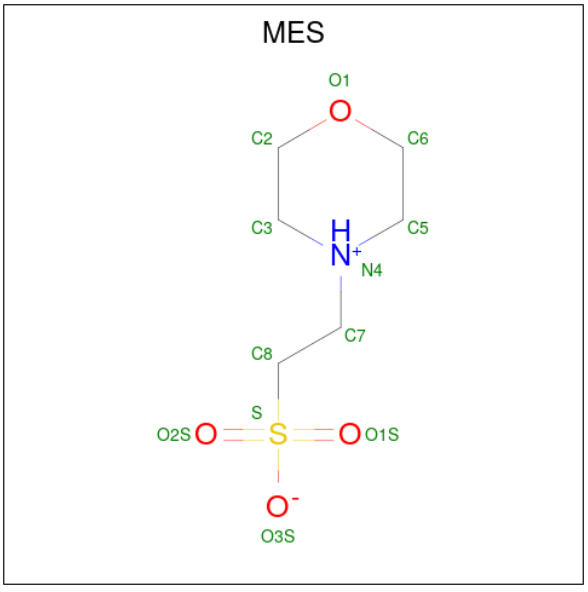
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 14 9 5	0	0

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



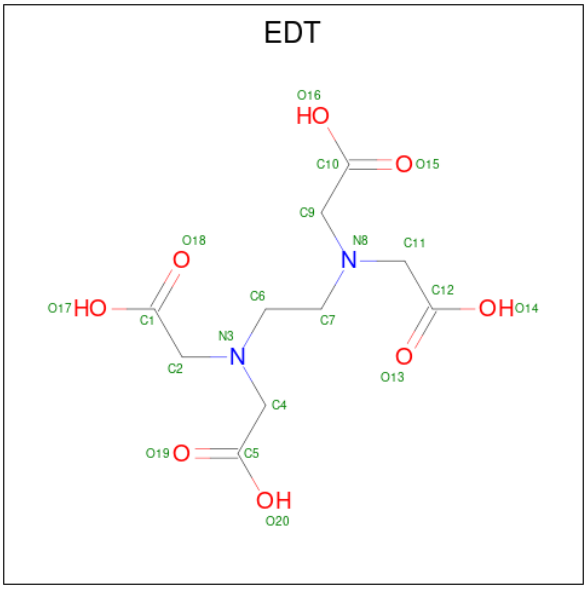
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	10	6	4	0	0

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



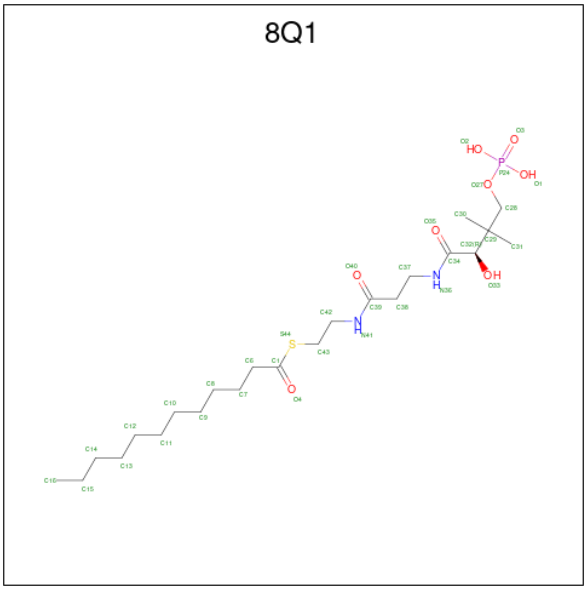
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
12	B	1	12	6	1	4	1	0	0

- Molecule 13 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



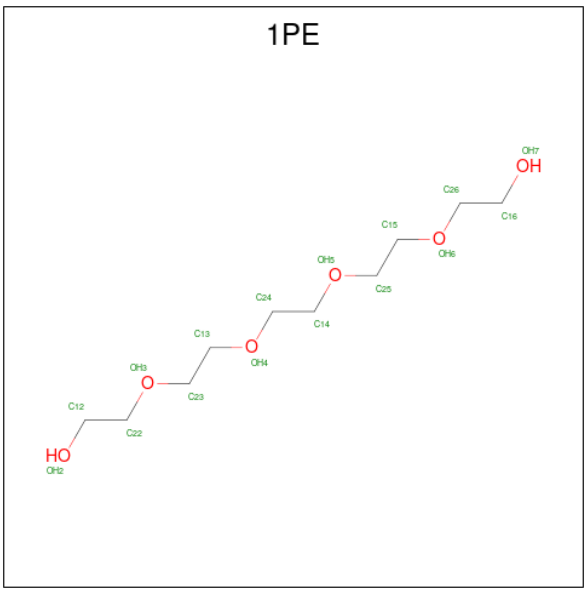
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 17 9 2 6	0	0

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



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

- Molecule 15 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

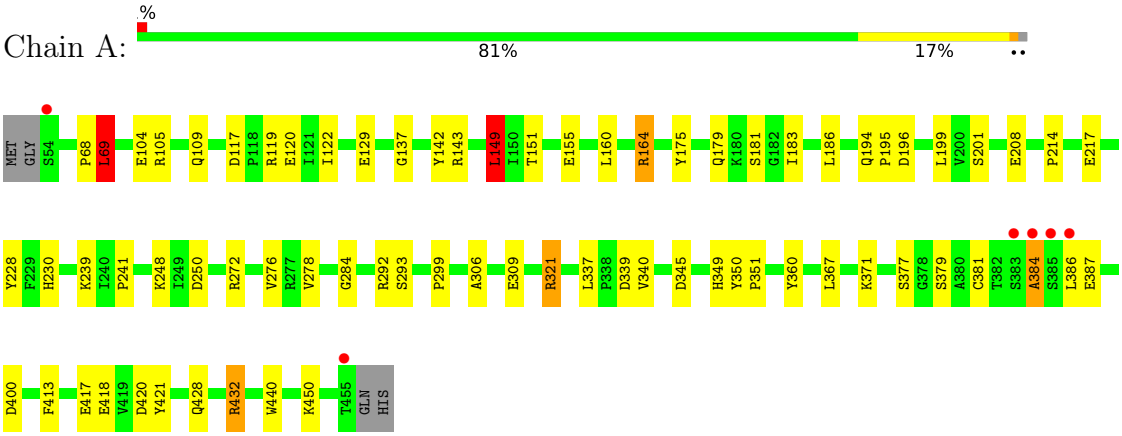
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	281	Total O 281 281	0	0
16	B	63	Total O 63 63	0	0
16	C	17	Total O 17 17	0	0
16	D	42	Total O 42 42	0	0

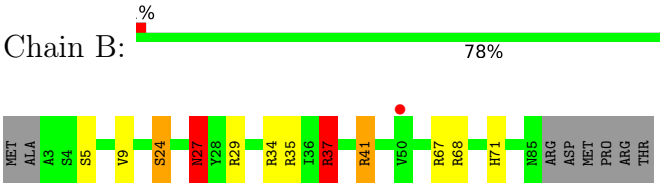
3 Residue-property plots (i)

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.

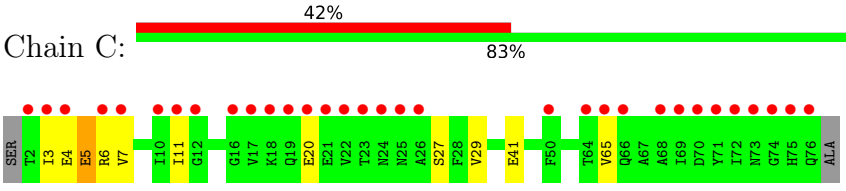
• Molecule 1: Cysteine desulfurase, mitochondrial



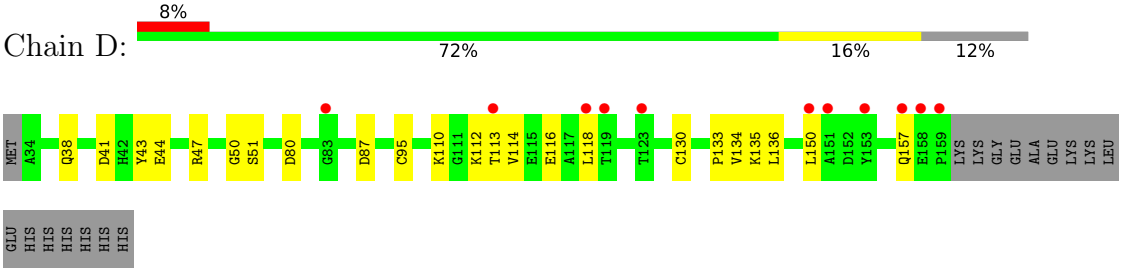
• Molecule 2: LYR motif-containing protein 4



• Molecule 3: Acyl carrier protein



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.43Å 86.43Å 246.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 1.95 49.01 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.01-1.95) 100.0 (49.01-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.150 , 0.185 0.161 , 0.186	Depositor DCC
R_{free} test set	3451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6127	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 3.32% 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, 0.333 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: 1PE, EDT, 8Q1, GOL, PGE, ETE, PG4, PEG, PLP, EDO, MES

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	1.01	12/3224 (0.4%)	0.90	4/4366 (0.1%)
2	B	1.04	6/757 (0.8%)	0.90	2/1014 (0.2%)
3	C	0.49	0/559	0.67	0/762
4	D	0.71	0/947	0.77	0/1284
All	All	0.93	18/5487 (0.3%)	0.86	6/7426 (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	4
2	B	0	5
All	All	0	9

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	GLU	CD-OE2	-7.01	1.18	1.25
2	B	37[A]	ARG	CA-C	6.42	1.69	1.52
2	B	37[B]	ARG	CA-C	6.42	1.69	1.52
1	A	104	GLU	CD-OE2	-5.95	1.19	1.25
1	A	309	GLU	CD-OE1	-5.88	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69[A]	LEU	CB-CG-CD1	-8.74	96.14	111.00
1	A	69[B]	LEU	CB-CG-CD1	-8.74	96.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69[A]	LEU	CB-CA-C	-7.86	95.27	110.20
1	A	69[B]	LEU	CB-CA-C	-7.86	95.27	110.20
2	B	37[A]	ARG	CA-C-N	-5.28	105.59	117.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432[A]	ARG	Mainchain
1	A	432[B]	ARG	Mainchain
1	A	69[A]	LEU	Mainchain
1	A	69[B]	LEU	Mainchain
2	B	24[B]	SER	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	3143	0	3136	80	0
2	B	727	0	764	19	0
3	C	552	0	489	8	0
4	D	926	0	926	30	0
5	A	15	0	7	0	0
6	A	96	0	140	26	0
6	B	24	0	36	4	0
6	C	8	0	12	1	0
6	D	16	0	24	3	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	63	0	90	8	0
8	B	7	0	10	5	0
9	A	26	0	36	2	0
10	A	14	0	20	9	0
11	A	10	0	14	13	0
12	B	12	0	13	1	0
13	B	17	0	10	5	0
14	C	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	D	16	0	22	3	0
16	A	281	0	0	13	0
16	B	63	0	0	5	0
16	C	17	0	0	0	0
16	D	42	0	0	3	0
All	All	6127	0	5773	146	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 13.

The worst 5 of 146 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:29:ARG:HH21	13:B:1609:EDT:H061	1.22	0.99
1:A:105[B]:ARG:HG2	6:A:513:EDO:H11	1.55	0.88
1:A:371:LYS:HD3	6:A:509:EDO:H22	1.53	0.88
4:D:95:CYS:SG	4:D:135:LYS:NZ	2.50	0.85
4:D:51:SER:H	6:D:203:EDO:H11	1.42	0.83

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	409/406 (101%)	399 (98%)	8 (2%)	2 (0%)	29 17
2	B	88/91 (97%)	87 (99%)	1 (1%)	0	100 100
3	C	74/77 (96%)	68 (92%)	5 (7%)	1 (1%)	11 3
4	D	127/143 (89%)	125 (98%)	2 (2%)	0	100 100
All	All	698/717 (97%)	679 (97%)	16 (2%)	3 (0%)	34 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ALA
1	A	450	LYS
3	C	5	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	340/346 (98%)	333 (98%)	7 (2%)	53	46
2	B	76/80 (95%)	74 (97%)	2 (3%)	46	36
3	C	54/66 (82%)	52 (96%)	2 (4%)	34	22
4	D	98/118 (83%)	96 (98%)	2 (2%)	55	48
All	All	568/610 (93%)	555 (98%)	13 (2%)	59	42

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

Mol	Chain	Res	Type
2	B	41[A]	ARG
2	B	41[B]	ARG
4	D	157	GLN
3	C	27	SER
4	D	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN

5.3.3 RNA (i)

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)

58 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	$\#\|Z\| > 2$
6	EDO	B	1606	-	3,3,3	0.46	0	2,2,2	0.45	0
8	PEG	A	527	-	6,6,6	0.48	0	5,5,5	0.30	0
6	EDO	A	512	-	3,3,3	0.52	0	2,2,2	0.19	0
6	EDO	A	518	-	3,3,3	0.69	0	2,2,2	0.62	0
9	PG4	A	521	-	12,12,12	0.58	0	11,11,11	0.49	0
9	PG4	A	520	-	12,12,12	0.56	0	11,11,11	0.58	0
6	EDO	B	1603	-	3,3,3	0.48	0	2,2,2	0.52	0
8	PEG	A	539	-	6,6,6	0.52	0	5,5,5	0.60	0
6	EDO	A	524	-	3,3,3	0.47	0	2,2,2	0.55	0
6	EDO	D	201	-	3,3,3	0.48	0	2,2,2	0.34	0
14	8Q1	C	301	-	27,33,34	2.19	6 (22%)	32,40,43	1.68	7 (21%)
13	EDT	B	1609	-	16,16,19	1.13	0	20,20,24	1.42	4 (20%)
12	MES	B	1604	-	12,12,12	2.02	3 (25%)	14,16,16	2.19	4 (28%)
6	EDO	A	534	-	3,3,3	0.52	0	2,2,2	0.33	0
6	EDO	B	1608	-	3,3,3	0.52	0	2,2,2	0.27	0
7	GOL	D	205	-	5,5,5	0.68	0	5,5,5	0.32	0
6	EDO	A	515	-	3,3,3	0.49	0	2,2,2	0.37	0
6	EDO	A	503	-	3,3,3	0.52	0	2,2,2	0.09	0
6	EDO	A	509	-	3,3,3	1.41	0	2,2,2	1.43	0
6	EDO	A	531	-	3,3,3	0.50	0	2,2,2	0.80	0
8	PEG	A	505	-	6,6,6	0.55	0	5,5,5	0.45	0
8	PEG	A	537	-	6,6,6	0.50	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	517	-	3,3,3	0.58	0	2,2,2	0.13	0
6	EDO	A	502	-	3,3,3	0.54	0	2,2,2	0.18	0
6	EDO	A	507	-	3,3,3	0.60	0	2,2,2	0.73	0
6	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	A	532	-	3,3,3	0.45	0	2,2,2	0.11	0
8	PEG	A	506	-	6,6,6	0.47	0	5,5,5	0.40	0
11	PGE	A	535	-	9,9,9	0.30	0	8,8,8	0.89	0
6	EDO	B	1602	-	3,3,3	0.54	0	2,2,2	0.50	0
6	EDO	A	513	-	3,3,3	0.48	0	2,2,2	0.66	0
8	PEG	A	540	-	6,6,6	0.49	0	5,5,5	0.30	0
6	EDO	A	533	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	D	206	-	3,3,3	0.50	0	2,2,2	0.23	0
5	PLP	A	501	-	15,15,16	1.63	3 (20%)	20,22,23	1.12	1 (5%)
8	PEG	A	519	-	6,6,6	0.56	0	5,5,5	0.80	0
8	PEG	A	529	-	6,6,6	0.49	0	5,5,5	0.37	0
6	EDO	A	530	-	3,3,3	0.54	0	2,2,2	0.13	0
6	EDO	A	511	-	3,3,3	0.72	0	2,2,2	0.93	0
6	EDO	C	303	-	3,3,3	0.50	0	2,2,2	0.09	0
6	EDO	A	528	-	3,3,3	0.60	0	2,2,2	0.26	0
6	EDO	A	523	-	3,3,3	0.50	0	2,2,2	0.35	0
8	PEG	B	1607	-	6,6,6	0.57	0	5,5,5	0.86	0
6	EDO	B	1601	-	3,3,3	0.66	0	2,2,2	0.85	0
6	EDO	A	514	-	3,3,3	0.29	0	2,2,2	0.66	0
6	EDO	A	536	-	3,3,3	0.53	0	2,2,2	0.20	0
6	EDO	A	538	-	3,3,3	0.52	0	2,2,2	0.26	0
6	EDO	B	1605	-	3,3,3	0.49	0	2,2,2	0.16	0
10	ETE	A	526	-	13,13,13	0.64	0	12,12,12	0.81	0
6	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.16	0
6	EDO	D	203	-	3,3,3	0.43	0	2,2,2	0.29	0
8	PEG	A	522	-	6,6,6	0.41	0	5,5,5	0.68	0
7	GOL	A	504	-	5,5,5	0.46	0	5,5,5	0.42	0
15	1PE	D	204	-	15,15,15	0.55	0	14,14,14	0.38	0
6	EDO	A	516	-	3,3,3	1.29	0	2,2,2	1.70	1 (50%)
7	GOL	A	508	-	5,5,5	0.89	0	5,5,5	1.33	1 (20%)
6	EDO	A	525	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	A	510	-	3,3,3	0.56	0	2,2,2	0.56	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
6	EDO	B	1606	-	-	0/1/1/1	-
8	PEG	A	527	-	-	2/4/4/4	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	A	518	-	-	1/1/1/1	-
9	PG4	A	521	-	-	4/10/10/10	-
9	PG4	A	520	-	-	7/10/10/10	-
6	EDO	B	1603	-	-	1/1/1/1	-
8	PEG	A	539	-	-	2/4/4/4	-
6	EDO	A	524	-	-	1/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
14	8Q1	C	301	-	-	0/38/40/41	-
13	EDT	B	1609	-	-	13/17/17/21	-
12	MES	B	1604	-	-	3/6/14/14	0/1/1/1
6	EDO	A	534	-	-	0/1/1/1	-
6	EDO	B	1608	-	-	0/1/1/1	-
7	GOL	D	205	-	-	2/4/4/4	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	A	503	-	-	1/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	A	531	-	-	1/1/1/1	-
8	PEG	A	505	-	-	2/4/4/4	-
8	PEG	A	537	-	-	4/4/4/4	-
6	EDO	A	517	-	-	0/1/1/1	-
6	EDO	A	502	-	-	0/1/1/1	-
6	EDO	A	507	-	-	0/1/1/1	-
6	EDO	C	302	-	-	1/1/1/1	-
6	EDO	A	532	-	-	0/1/1/1	-
8	PEG	A	506	-	-	1/4/4/4	-
11	PGE	A	535	-	-	3/7/7/7	-
6	EDO	B	1602	-	-	0/1/1/1	-
6	EDO	A	513	-	-	0/1/1/1	-
8	PEG	A	540	-	-	1/4/4/4	-
6	EDO	A	533	-	-	1/1/1/1	-
6	EDO	D	206	-	-	0/1/1/1	-
5	PLP	A	501	-	-	0/6/6/8	0/1/1/1
8	PEG	A	519	-	-	1/4/4/4	-
8	PEG	A	529	-	-	2/4/4/4	-
6	EDO	A	530	-	-	1/1/1/1	-
6	EDO	A	511	-	-	1/1/1/1	-
6	EDO	C	303	-	-	1/1/1/1	-
6	EDO	A	528	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	523	-	-	1/1/1/1	-
8	PEG	B	1607	-	-	3/4/4/4	-
6	EDO	B	1601	-	-	0/1/1/1	-
6	EDO	A	514	-	-	1/1/1/1	-
6	EDO	A	536	-	-	0/1/1/1	-
6	EDO	A	538	-	-	1/1/1/1	-
6	EDO	B	1605	-	-	1/1/1/1	-
10	ETE	A	526	-	-	4/11/11/11	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	D	203	-	-	0/1/1/1	-
8	PEG	A	522	-	-	2/4/4/4	-
7	GOL	A	504	-	-	4/4/4/4	-
15	1PE	D	204	-	-	9/13/13/13	-
6	EDO	A	516	-	-	1/1/1/1	-
7	GOL	A	508	-	-	1/4/4/4	-
6	EDO	A	525	-	-	0/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	C39-N41	5.50	1.45	1.33
14	C	301	8Q1	C34-N36	5.27	1.45	1.33
12	B	1604	MES	C8-S	4.62	1.84	1.77
14	C	301	8Q1	C6-C1	4.59	1.55	1.50
5	A	501	PLP	C3-C2	-3.75	1.37	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	1604	MES	O3S-S-O2S	-4.46	100.37	111.27
12	B	1604	MES	O1S-S-C8	4.21	111.98	106.92
14	C	301	8Q1	C37-N36-C34	-4.06	115.34	122.59
12	B	1604	MES	O2S-S-C8	3.66	111.32	106.92
14	C	301	8Q1	C38-C37-N36	-3.56	104.70	111.90

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1604	MES	C8-C7-N4-C3
13	B	1609	EDT	C7-C6-N3-C4
13	B	1609	EDT	C6-C7-N8-C9
13	B	1609	EDT	C12-C11-N8-C7
8	B	1607	PEG	C1-C2-O2-C3

There are no ring outliers.

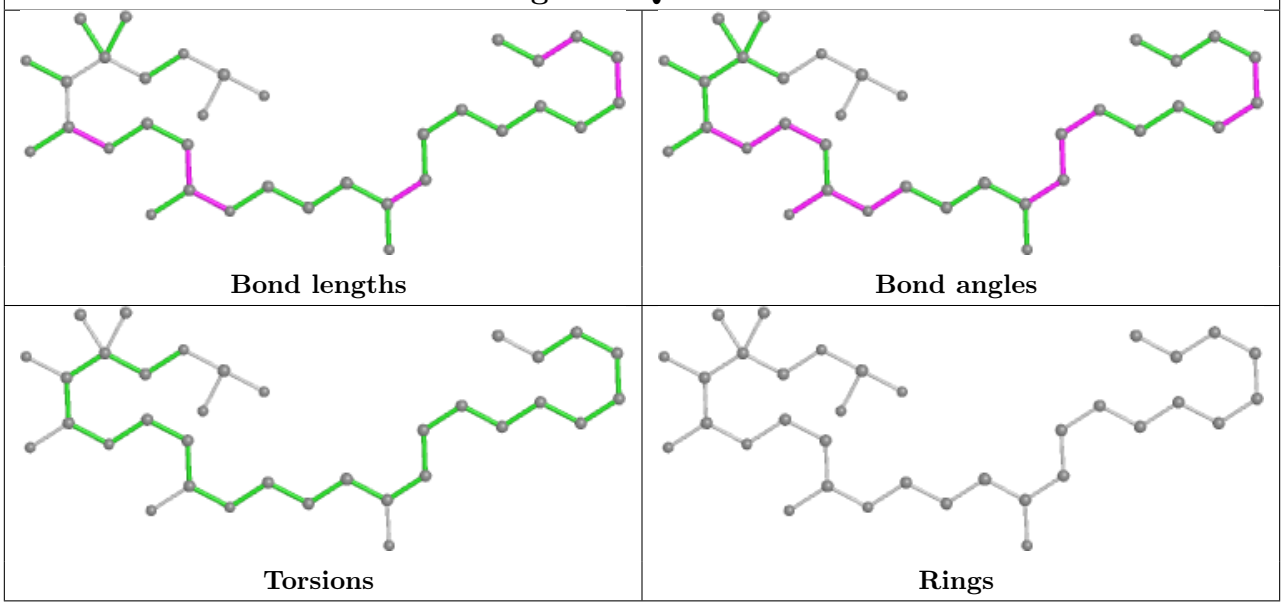
31 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1606	EDO	1	0
6	A	512	EDO	1	0
6	A	518	EDO	1	0
9	A	520	PG4	2	0
8	A	539	PEG	2	0
6	A	524	EDO	2	0
13	B	1609	EDT	5	0
12	B	1604	MES	1	0
6	A	534	EDO	2	0
6	A	503	EDO	1	0
6	A	509	EDO	6	0
6	A	502	EDO	1	0
6	A	507	EDO	1	0
6	C	302	EDO	1	0
8	A	506	PEG	2	0
11	A	535	PGE	13	0
6	A	513	EDO	1	0
8	A	540	PEG	1	0
8	A	519	PEG	1	0
8	A	529	PEG	1	0
6	A	530	EDO	2	0
6	A	528	EDO	1	0
6	A	523	EDO	1	0
8	B	1607	PEG	5	0
6	B	1601	EDO	3	0
6	A	538	EDO	2	0
10	A	526	ETE	9	0
6	D	203	EDO	3	0
8	A	522	PEG	1	0
15	D	204	1PE	3	0
6	A	516	EDO	4	0

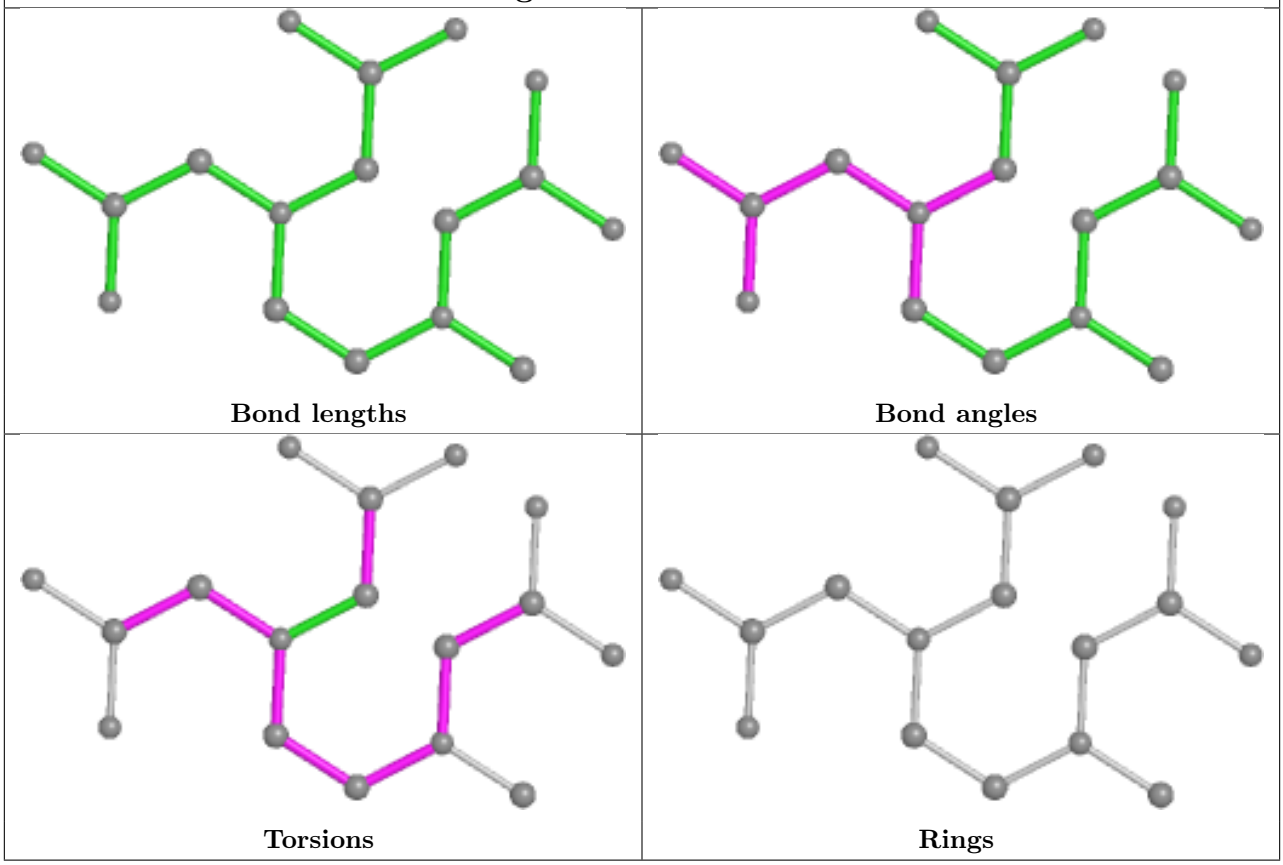
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

Ligand 8Q1 C 301



Ligand EDT B 1609



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^{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	402/406 (99%)	-0.21	6 (1%)	73	81	19, 29, 60, 99	7 (1%)
2	B	83/91 (91%)	-0.34	1 (1%)	79	84	22, 31, 57, 85	0
3	C	75/77 (97%)	1.77	32 (42%)	0	0	39, 68, 111, 138	0
4	D	126/143 (88%)	0.12	11 (8%)	10	16	27, 46, 73, 83	1 (0%)
All	All	686/717 (95%)	0.05	50 (7%)	15	23	19, 34, 77, 138	8 (1%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	159	PRO	7.4
3	C	17	VAL	6.4
4	D	158	GLU	6.1
1	A	384	ALA	6.1
3	C	76	GLN	6.0

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
6	EDO	A	530	4/4	0.47	0.29	56,58,58,58	4
9	PG4	A	521	13/13	0.47	0.36	88,95,102,102	0
13	EDT	B	1609	17/20	0.55	0.27	54,70,75,77	17
7	GOL	A	504	6/6	0.56	0.38	74,88,89,90	0
6	EDO	A	532	4/4	0.58	0.31	79,80,80,80	0
6	EDO	A	517	4/4	0.59	0.20	66,67,68,68	0
6	EDO	A	533	4/4	0.61	0.20	85,85,85,85	0
8	PEG	A	527	7/7	0.61	0.31	72,75,83,84	0
6	EDO	A	528	4/4	0.62	0.41	41,43,44,45	4
6	EDO	D	206	4/4	0.64	0.21	80,80,80,81	0
8	PEG	A	506	7/7	0.66	0.26	93,97,99,99	0
8	PEG	B	1607	7/7	0.67	0.22	39,52,61,63	0
9	PG4	A	520	13/13	0.68	0.32	55,64,67,67	13
6	EDO	A	536	4/4	0.70	0.16	68,76,78,80	0
10	ETE	A	526	14/14	0.70	0.26	36,83,90,90	0
6	EDO	C	303	4/4	0.70	0.38	79,81,82,82	0
6	EDO	A	525	4/4	0.71	0.25	84,84,85,85	0
6	EDO	D	203	4/4	0.72	0.23	59,60,68,70	0
6	EDO	B	1603	4/4	0.72	0.24	76,80,84,87	0
6	EDO	A	502	4/4	0.73	0.19	60,72,74,77	0
12	MES	B	1604	12/12	0.73	0.28	121,122,127,128	0
6	EDO	D	202	4/4	0.73	0.24	73,75,77,78	0
6	EDO	A	531	4/4	0.75	0.33	51,51,53,53	4
8	PEG	A	537	7/7	0.75	0.25	53,69,77,78	0
8	PEG	A	539	7/7	0.76	0.25	65,72,76,77	0
7	GOL	A	508	6/6	0.77	0.18	20,31,37,40	6
8	PEG	A	505	7/7	0.77	0.22	58,66,76,76	0
6	EDO	A	523	4/4	0.77	0.29	45,45,46,48	4
8	PEG	A	529	7/7	0.78	0.16	78,81,83,83	0
6	EDO	B	1608	4/4	0.78	0.17	71,74,76,77	0
6	EDO	A	534	4/4	0.78	0.38	59,63,66,68	0
15	1PE	D	204	16/16	0.78	0.24	65,80,82,82	0
6	EDO	A	524	4/4	0.79	0.27	63,63,63,63	4
8	PEG	A	540	7/7	0.80	0.17	88,89,89,89	0
6	EDO	B	1602	4/4	0.80	0.17	67,68,71,72	0
6	EDO	A	512	4/4	0.81	0.17	63,68,68,69	0
6	EDO	A	503	4/4	0.81	0.36	43,51,52,55	0
7	GOL	D	205	6/6	0.81	0.17	49,52,56,56	6
6	EDO	B	1605	4/4	0.81	0.15	54,63,67,71	0
6	EDO	A	538	4/4	0.81	0.20	59,63,68,70	0
8	PEG	A	519	7/7	0.81	0.15	53,57,60,62	0
6	EDO	A	510	4/4	0.83	0.11	60,63,65,68	0
6	EDO	B	1606	4/4	0.83	0.16	73,73,74,74	0

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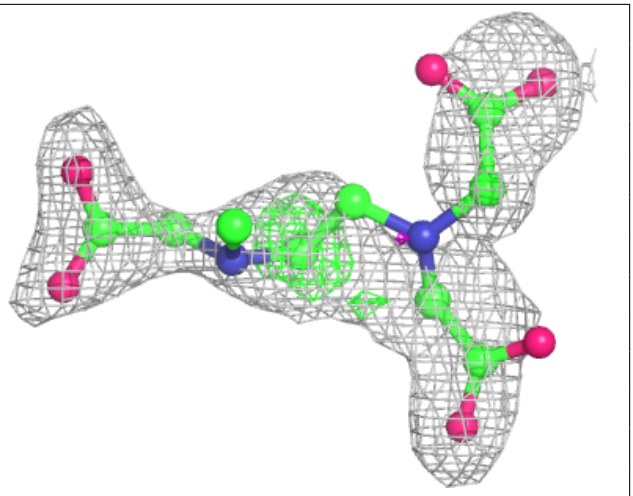
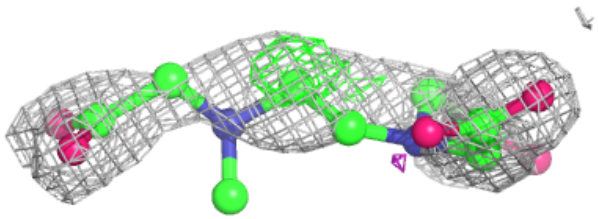
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	201	4/4	0.83	0.19	91,91,92,93	0
6	EDO	A	513	4/4	0.85	0.22	42,42,45,46	4
11	PGE	A	535	10/10	0.90	0.16	35,51,59,59	10
6	EDO	A	511	4/4	0.90	0.23	41,46,51,52	4
6	EDO	B	1601	4/4	0.90	0.20	44,47,50,59	0
8	PEG	A	522	7/7	0.90	0.10	55,57,63,67	0
6	EDO	C	302	4/4	0.91	0.27	47,50,55,57	4
6	EDO	A	507	4/4	0.91	0.25	45,46,54,62	0
6	EDO	A	514	4/4	0.92	0.15	42,42,45,49	4
6	EDO	A	518	4/4	0.93	0.17	25,31,33,33	4
14	8Q1	C	301	34/35	0.94	0.09	31,40,48,50	0
6	EDO	A	515	4/4	0.94	0.12	56,58,62,62	0
6	EDO	A	516	4/4	0.96	0.21	21,24,25,27	4
6	EDO	A	509	4/4	0.97	0.20	17,18,22,25	4
5	PLP	A	501	15/16	0.99	0.11	18,23,29,31	0

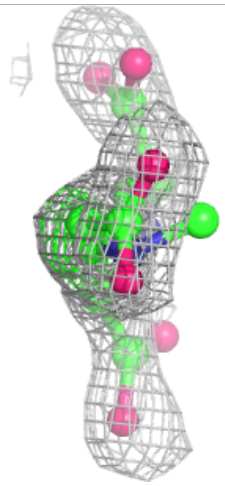
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDT B 1609:

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

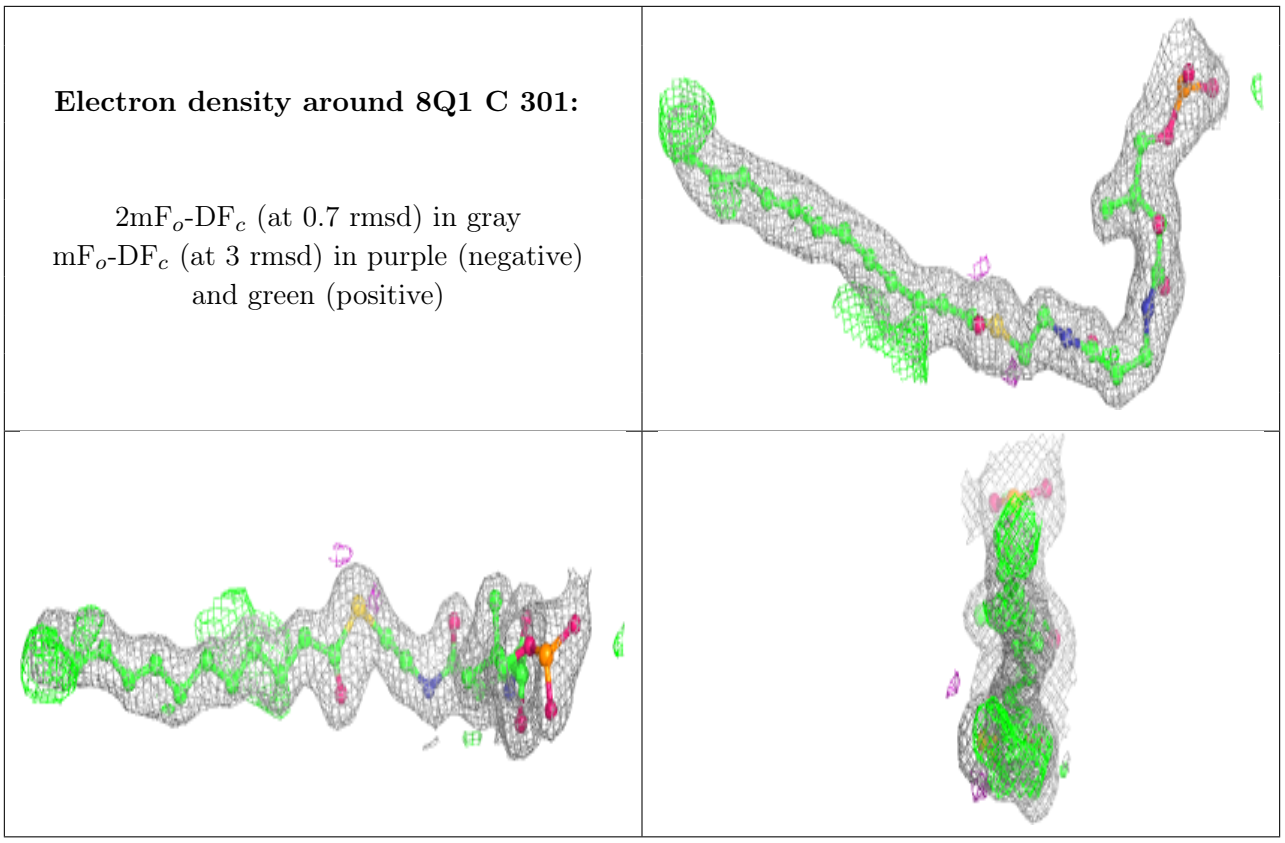






Electron density around 8Q1 C 301:

$2mF_o$-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 (i)

There are no such residues in this entry.