



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:56 AM UTC

PDB ID : 6W1D / pdb_00006w1d
Title : Structure of human mitochondrial complex Nfs1-ISCU2 (WT)-ISD11 with E.coli ACP1 at 1.8 Å resolution (NIAU)2
Authors : Boniecki, M.T.; Cygler, M.
Deposited on : 2020-03-04
Resolution : 1.79 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

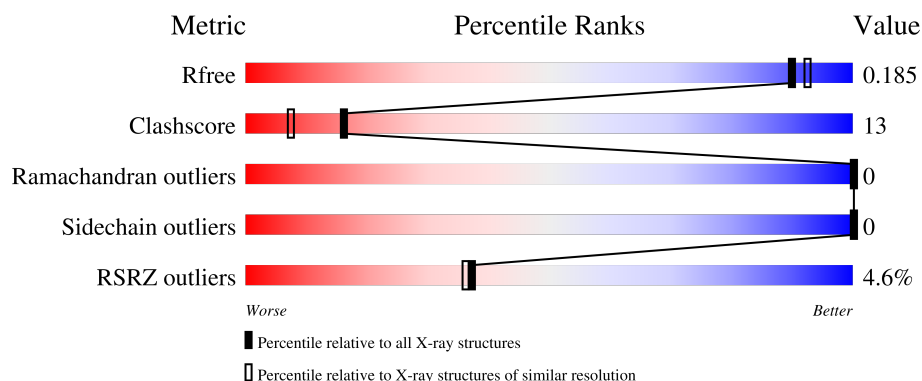
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	3% 78% 19% .
2	B	91	3% 79% 13% 8%
3	C	77	13% 90% 6% ..
4	D	143	5% 80% 8% 12%

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	P15	A	526	-	-	X	-
11	DTT	A	533	-	-	X	-
12	PGE	A	534	-	-	X	-
12	PGE	A	543	-	-	X	-
7	EDO	A	507	-	-	X	-
7	EDO	A	514	-	-	X	-
7	EDO	A	554	-	-	X	-
8	PEG	A	531	-	-	X	-
8	PEG	B	104	-	-	X	-
8	PEG	B	106	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 6266 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	395	Total	C	N	O	S	0	26	0
			3170	2007	541	600	22			

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	8	0
			723	458	141	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
			535	335	84	115	1			

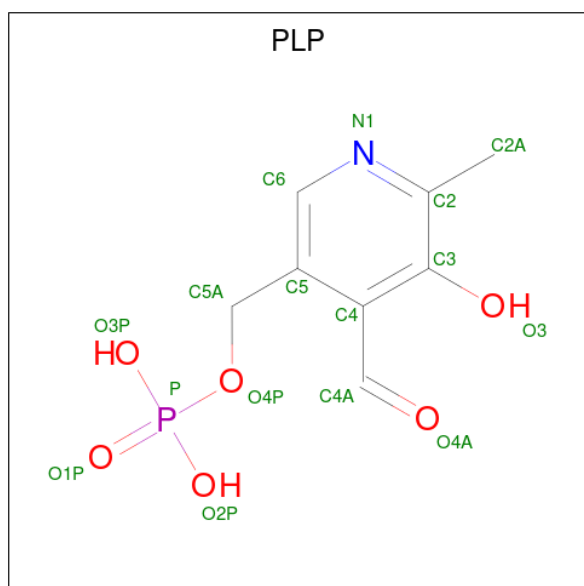
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	126	Total	C	N	O	S	0	6	0
			965	612	159	186	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 (CCD ID: 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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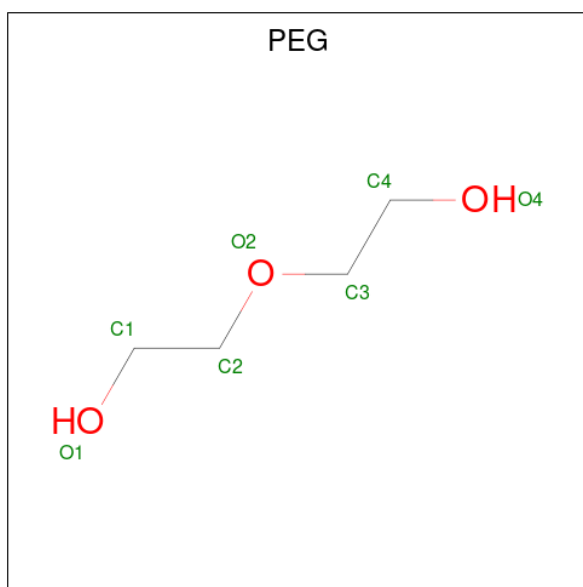
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total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

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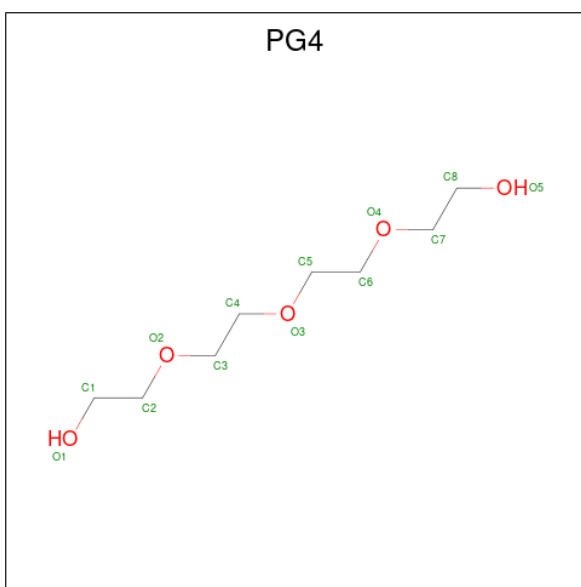
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



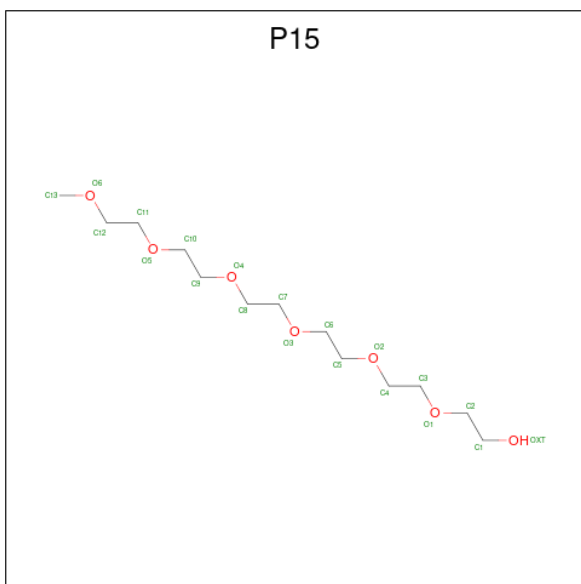
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	C	1	Total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

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



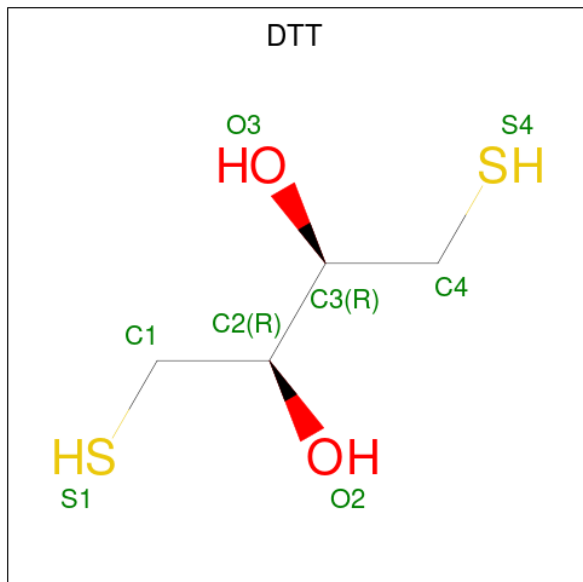
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (CCD ID: P15) (formula: $C_{13}H_{28}O_7$).



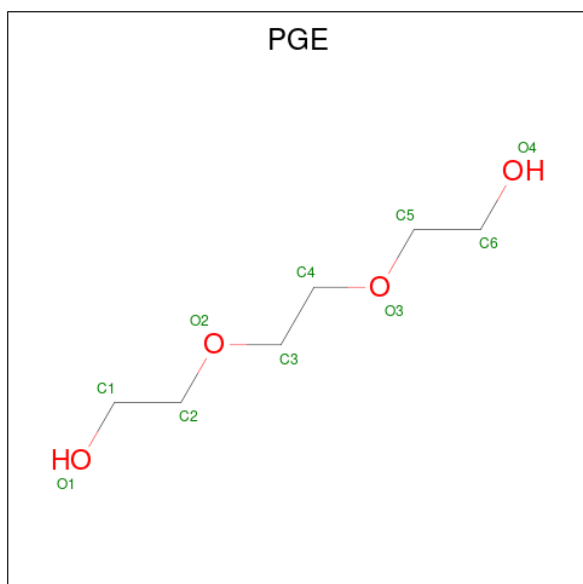
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			20	13	7		

- Molecule 11 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



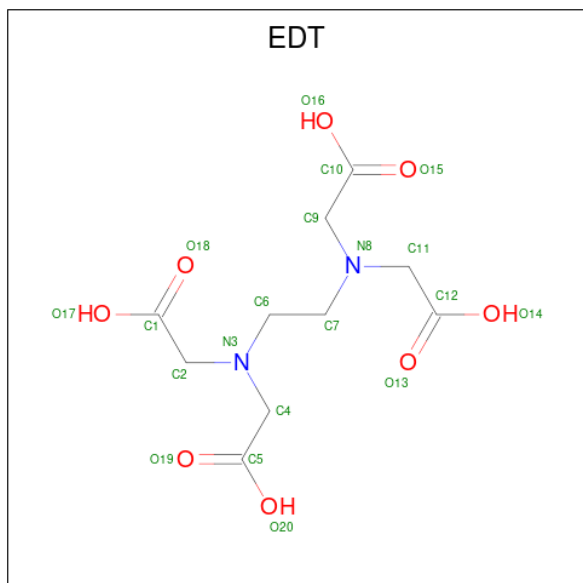
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		

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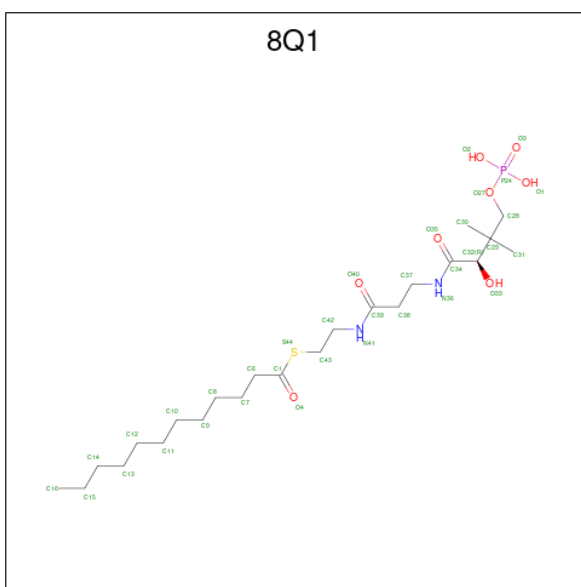
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		
12	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: C₁₀H₁₆N₂O₈).



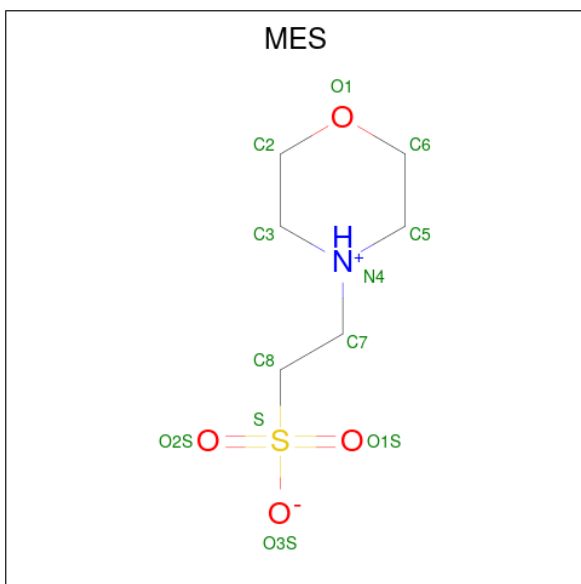
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



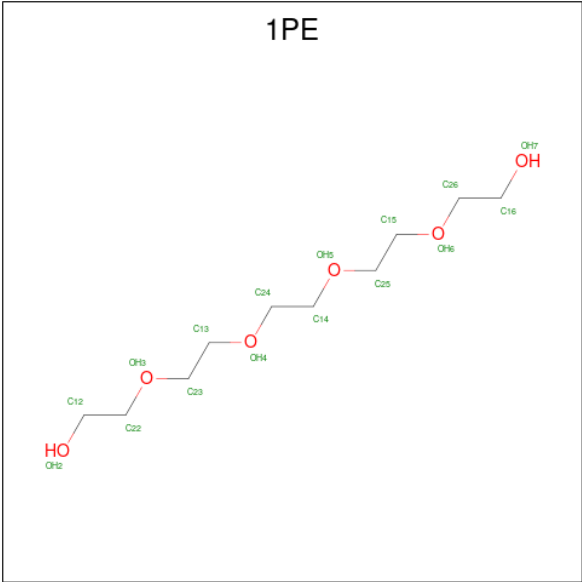
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	S	
			34	23	2	7	1	1	
								0	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 16 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

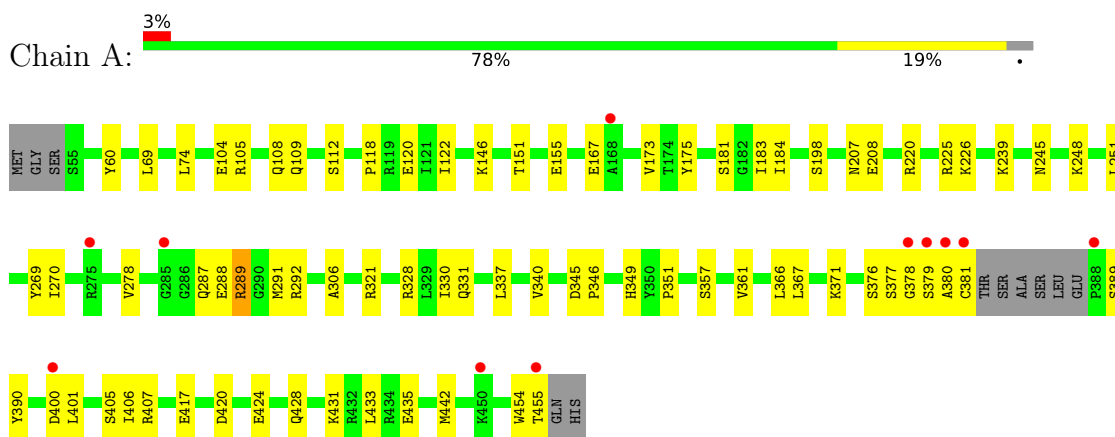
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	259	Total	O	0	0
			259	259		
17	B	69	Total	O	0	0
			69	69		
17	C	18	Total	O	0	0
			18	18		
17	D	41	Total	O	0	0
			41	41		

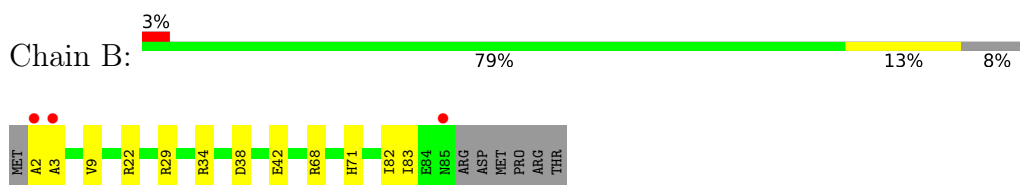
3 Residue-property plots [i](#)

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.

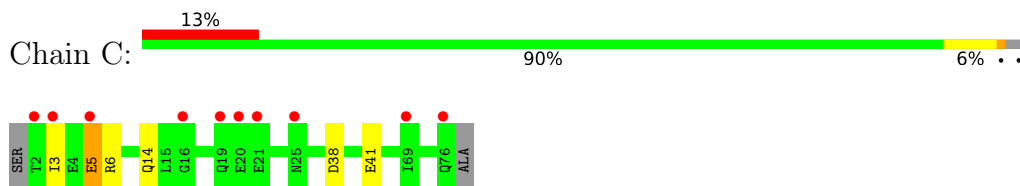
- Molecule 1: Cysteine desulfurase, mitochondrial



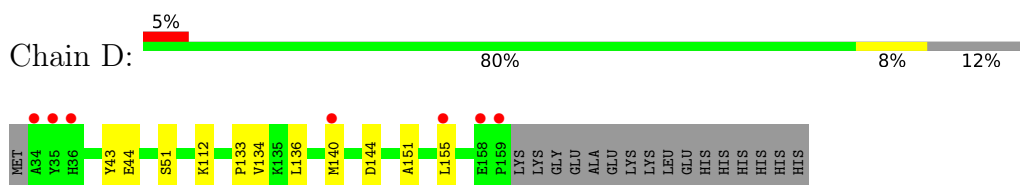
- Molecule 2: LYR motif-containing protein 4



- 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, α , β , γ	86.35Å 86.35Å 245.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 1.79 48.93 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-1.79) 99.9 (48.93-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.159 , 0.189 (Not available) , 0.185	Depositor DCC
R_{free} test set	2000 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6266	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PLP, P15, PG4, GOL, 1PE, 8Q1, EDT, EDO, DTT, PEG, MES, PGE

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	0.92	0/3289	0.87	1/4452 (0.0%)
2	B	0.85	0/756	0.81	0/1014
3	C	0.51	0/539	0.61	0/735
4	D	0.66	0/986	0.70	0/1336
All	All	0.84	0/5570	0.81	1/7537 (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	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	289	ARG	CG-CD-NE	-5.01	100.97	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	GLY	Peptide
3	C	5	GLU	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	3170	0	3192	94	0
2	B	723	0	764	20	0
3	C	535	0	472	7	0
4	D	965	0	956	12	0
5	A	15	0	7	0	0
6	A	30	0	39	6	0
6	D	6	0	8	0	0
7	A	132	0	193	42	0
7	B	32	0	47	5	0
7	C	12	0	18	3	0
7	D	16	0	24	3	0
8	A	56	0	80	10	0
8	B	14	0	20	9	0
8	C	7	0	10	1	0
9	A	26	0	36	4	0
10	A	20	0	28	9	0
11	A	8	0	10	4	0
12	A	30	0	42	17	0
13	B	20	0	12	6	0
14	C	34	0	0	0	0
15	C	12	0	13	1	0
16	D	16	0	22	2	0
17	A	259	0	0	16	0
17	B	69	0	0	6	0
17	C	18	0	0	0	0
17	D	41	0	0	1	0
All	All	6266	0	5993	156	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 156 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:A:245:ASN:HD21	11:A:533:DTT:H2	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:HH11	8:B:106:PEG:H22	1.23	1.01
1:A:381:CYS:HA	1:A:407:ARG:HH12	1.30	0.93
1:A:112:SER:HA	9:A:519:PG4:H11	1.51	0.93
1:A:175:TYR:HD1	8:A:531:PEG:H11	1.34	0.92

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	417/406 (103%)	407 (98%)	10 (2%)	0	100	100
2	B	90/91 (99%)	89 (99%)	1 (1%)	0	100	100
3	C	73/77 (95%)	69 (94%)	4 (6%)	0	100	100
4	D	129/143 (90%)	128 (99%)	1 (1%)	0	100	100
All	All	709/717 (99%)	693 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	349/346 (101%)	349 (100%)	0	100	100
2	B	76/80 (95%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	49/66 (74%)	49 (100%)	0	100	100
4	D	100/118 (85%)	100 (100%)	0	100	100
All	All	574/610 (94%)	574 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	194	GLN
1	A	312	GLN
1	A	343	ASN
1	A	444	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

77 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
7	EDO	D	201	-	3,3,3	0.52	0	2,2,2	0.71	0
7	EDO	A	530	-	3,3,3	0.41	0	2,2,2	0.50	0
7	EDO	A	522	-	3,3,3	0.79	0	2,2,2	0.84	0
7	EDO	A	516	-	3,3,3	0.48	0	2,2,2	0.33	0
7	EDO	B	101	-	3,3,3	0.82	0	2,2,2	0.29	0
7	EDO	C	304	-	3,3,3	0.35	0	2,2,2	0.10	0
7	EDO	A	540	-	3,3,3	0.43	0	2,2,2	0.44	0
8	PEG	A	548	-	6,6,6	0.51	0	5,5,5	0.51	0
10	P15	A	526	-	19,19,19	0.66	0	18,18,18	0.74	0
8	PEG	A	531	-	6,6,6	0.52	0	5,5,5	0.52	0
7	EDO	B	107	-	3,3,3	0.47	0	2,2,2	0.31	0
7	EDO	A	535	-	3,3,3	0.38	0	2,2,2	0.55	0
7	EDO	A	554	-	3,3,3	0.45	0	2,2,2	0.04	0
7	EDO	A	514	-	3,3,3	1.33	0	2,2,2	0.66	0
6	GOL	D	204	-	5,5,5	0.72	0	5,5,5	0.37	0
12	PGE	A	534	-	9,9,9	0.48	0	8,8,8	0.63	0
8	PEG	B	104	-	6,6,6	0.59	0	5,5,5	0.32	0
6	GOL	A	504	-	5,5,5	0.53	0	5,5,5	0.40	0
7	EDO	A	537	-	3,3,3	0.41	0	2,2,2	0.19	0
8	PEG	A	532	-	6,6,6	0.49	0	5,5,5	0.58	0
12	PGE	A	544	-	9,9,9	0.35	0	8,8,8	0.42	0
7	EDO	A	513	-	3,3,3	0.49	0	2,2,2	0.59	0
7	EDO	A	509	-	3,3,3	0.72	0	2,2,2	1.30	0
7	EDO	B	111	-	3,3,3	0.46	0	2,2,2	0.24	0
7	EDO	A	517	-	3,3,3	0.25	0	2,2,2	0.35	0
8	PEG	A	527	-	6,6,6	0.54	0	5,5,5	0.53	0
6	GOL	A	502	-	5,5,5	0.66	0	5,5,5	1.95	2 (40%)
9	PG4	A	519	-	12,12,12	0.53	0	11,11,11	0.53	0
7	EDO	A	506	-	3,3,3	0.39	0	2,2,2	0.23	0
16	1PE	D	202	-	15,15,15	0.54	0	14,14,14	0.29	0
7	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.28	0
7	EDO	D	205	-	3,3,3	0.48	0	2,2,2	0.58	0
6	GOL	A	503	-	5,5,5	0.42	0	5,5,5	0.63	0
7	EDO	A	524	-	3,3,3	0.41	0	2,2,2	0.46	0
7	EDO	A	536	-	3,3,3	0.49	0	2,2,2	1.05	0
7	EDO	A	542	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	A	510	-	3,3,3	0.41	0	2,2,2	0.46	0
7	EDO	C	306	-	3,3,3	0.42	0	2,2,2	0.25	0
5	PLP	A	501	1	15,15,16	1.44	2 (13%)	21,22,23	1.07	2 (9%)
7	EDO	A	545	-	3,3,3	0.41	0	2,2,2	0.32	0
7	EDO	B	105	-	3,3,3	0.41	0	2,2,2	0.38	0
7	EDO	A	546	-	3,3,3	0.78	0	2,2,2	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	553	-	3,3,3	0.36	0	2,2,2	0.39	0
7	EDO	A	539	-	3,3,3	0.42	0	2,2,2	0.22	0
13	EDT	B	108	-	19,19,19	1.32	1 (5%)	24,24,24	1.38	3 (12%)
7	EDO	B	109	-	3,3,3	0.39	0	2,2,2	0.29	0
8	PEG	B	106	-	6,6,6	0.92	0	5,5,5	0.71	0
7	EDO	A	512	-	3,3,3	0.39	0	2,2,2	0.75	0
7	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.70	0
7	EDO	A	523	-	3,3,3	0.44	0	2,2,2	0.29	0
8	PEG	C	305	-	6,6,6	0.52	0	5,5,5	0.36	0
7	EDO	A	552	-	3,3,3	0.51	0	2,2,2	0.70	0
7	EDO	D	203	-	3,3,3	0.47	0	2,2,2	0.21	0
7	EDO	A	528	-	3,3,3	0.72	0	2,2,2	0.60	0
7	EDO	B	102	-	3,3,3	0.48	0	2,2,2	0.85	0
7	EDO	A	507	-	3,3,3	1.75	1 (33%)	2,2,2	1.43	0
11	DTT	A	533	-	7,7,7	0.64	0	4,8,8	1.27	0
7	EDO	A	525	-	3,3,3	0.43	0	2,2,2	0.24	0
12	PGE	A	543	-	9,9,9	0.26	0	8,8,8	0.58	0
14	8Q1	C	301	3	28,33,34	2.02	8 (28%)	32,40,43	1.83	7 (21%)
7	EDO	A	547	-	3,3,3	0.43	0	2,2,2	0.69	0
8	PEG	A	518	-	6,6,6	0.62	0	5,5,5	0.80	0
8	PEG	A	550	-	6,6,6	0.48	0	5,5,5	0.17	0
8	PEG	A	521	-	6,6,6	0.49	0	5,5,5	0.67	0
6	GOL	A	505	-	5,5,5	0.98	0	5,5,5	0.87	0
7	EDO	B	103	-	3,3,3	0.40	0	2,2,2	0.29	0
7	EDO	B	110	-	3,3,3	0.48	0	2,2,2	0.08	0
15	MES	C	302	-	12,12,12	2.11	4 (33%)	15,16,16	2.04	4 (26%)
6	GOL	A	551	-	5,5,5	0.49	0	5,5,5	0.72	0
7	EDO	A	538	-	3,3,3	0.50	0	2,2,2	0.39	0
7	EDO	A	541	-	3,3,3	0.46	0	2,2,2	0.30	0
7	EDO	A	515	-	3,3,3	0.53	0	2,2,2	0.18	0
7	EDO	A	508	-	3,3,3	0.45	0	2,2,2	0.15	0
9	PG4	A	520	-	12,12,12	0.60	0	11,11,11	0.57	0
7	EDO	D	206	-	3,3,3	0.41	0	2,2,2	0.56	0
8	PEG	A	549	-	6,6,6	0.52	0	5,5,5	0.28	0
7	EDO	A	529	-	3,3,3	0.45	0	2,2,2	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
7	EDO	D	201	-	-	1/1/1/1	-
7	EDO	A	530	-	-	0/1/1/1	-
7	EDO	A	522	-	-	0/1/1/1	-
7	EDO	A	516	-	-	1/1/1/1	-
7	EDO	B	101	-	-	1/1/1/1	-
7	EDO	C	304	-	-	1/1/1/1	-
7	EDO	A	540	-	-	1/1/1/1	-
8	PEG	A	548	-	-	2/4/4/4	-
10	P15	A	526	-	-	10/17/17/17	-
8	PEG	A	531	-	-	2/4/4/4	-
7	EDO	B	107	-	-	0/1/1/1	-
7	EDO	A	535	-	-	1/1/1/1	-
7	EDO	A	554	-	-	0/1/1/1	-
7	EDO	A	514	-	-	1/1/1/1	-
6	GOL	D	204	-	-	0/4/4/4	-
12	PGE	A	534	-	-	6/7/7/7	-
8	PEG	B	104	-	-	3/4/4/4	-
6	GOL	A	504	-	-	4/4/4/4	-
7	EDO	A	537	-	-	1/1/1/1	-
8	PEG	A	532	-	-	2/4/4/4	-
12	PGE	A	544	-	-	3/7/7/7	-
7	EDO	A	513	-	-	1/1/1/1	-
7	EDO	A	509	-	-	0/1/1/1	-
7	EDO	B	111	-	-	0/1/1/1	-
7	EDO	A	517	-	-	1/1/1/1	-
8	PEG	A	527	-	-	1/4/4/4	-
6	GOL	A	502	-	-	0/4/4/4	-
9	PG4	A	519	-	-	4/10/10/10	-
7	EDO	A	506	-	-	1/1/1/1	-
16	1PE	D	202	-	-	11/13/13/13	-
7	EDO	C	303	-	-	1/1/1/1	-
7	EDO	D	205	-	-	0/1/1/1	-
6	GOL	A	503	-	-	4/4/4/4	-
7	EDO	A	524	-	-	1/1/1/1	-
7	EDO	A	536	-	-	1/1/1/1	-
7	EDO	A	542	-	-	1/1/1/1	-
7	EDO	A	510	-	-	1/1/1/1	-
7	EDO	C	306	-	-	1/1/1/1	-
5	PLP	A	501	1	-	0/6/6/8	0/1/1/1
7	EDO	A	545	-	-	1/1/1/1	-
7	EDO	B	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	546	-	-	0/1/1/1	-
7	EDO	A	553	-	-	1/1/1/1	-
7	EDO	A	539	-	-	1/1/1/1	-
13	EDT	B	108	-	-	12/21/21/21	-
7	EDO	B	109	-	-	1/1/1/1	-
8	PEG	B	106	-	-	2/4/4/4	-
7	EDO	A	512	-	-	1/1/1/1	-
7	EDO	A	511	-	-	0/1/1/1	-
7	EDO	A	523	-	-	1/1/1/1	-
8	PEG	C	305	-	-	1/4/4/4	-
7	EDO	A	552	-	-	0/1/1/1	-
7	EDO	D	203	-	-	1/1/1/1	-
7	EDO	A	528	-	-	1/1/1/1	-
7	EDO	B	102	-	-	1/1/1/1	-
7	EDO	A	507	-	-	1/1/1/1	-
11	DTT	A	533	-	-	3/8/8/8	-
7	EDO	A	525	-	-	1/1/1/1	-
12	PGE	A	543	-	-	4/7/7/7	-
14	8Q1	C	301	3	-	1/38/40/41	-
7	EDO	A	547	-	-	1/1/1/1	-
8	PEG	A	518	-	-	1/4/4/4	-
8	PEG	A	550	-	-	1/4/4/4	-
8	PEG	A	521	-	-	1/4/4/4	-
6	GOL	A	505	-	-	3/4/4/4	-
7	EDO	B	103	-	-	1/1/1/1	-
7	EDO	B	110	-	-	1/1/1/1	-
15	MES	C	302	-	-	3/6/14/14	0/1/1/1
6	GOL	A	551	-	-	4/4/4/4	-
7	EDO	A	538	-	-	0/1/1/1	-
7	EDO	A	541	-	-	0/1/1/1	-
7	EDO	A	515	-	-	1/1/1/1	-
7	EDO	A	508	-	-	1/1/1/1	-
9	PG4	A	520	-	-	6/10/10/10	-
7	EDO	D	206	-	-	0/1/1/1	-
8	PEG	A	549	-	-	3/4/4/4	-
7	EDO	A	529	-	-	1/1/1/1	-

The worst 5 of 16 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	C39-N41	5.00	1.45	1.33
14	C	301	8Q1	C34-N36	4.70	1.44	1.33
15	C	302	MES	C8-S	4.60	1.84	1.77
5	A	501	PLP	C3-C2	-3.61	1.37	1.41
14	C	301	8Q1	C6-C1	3.26	1.54	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	302	MES	O1S-S-C8	4.91	114.15	106.73
14	C	301	8Q1	C42-N41-C39	-4.69	114.10	122.82
14	C	301	8Q1	C37-N36-C34	-4.37	114.69	122.55
6	A	502	GOL	C3-C2-C1	-3.73	98.11	111.80
13	B	108	EDT	C11-N8-C9	3.72	120.38	111.66

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	O1-C1-C2-C3
6	A	504	GOL	C1-C2-C3-O3
6	A	551	GOL	C1-C2-C3-O3
6	A	551	GOL	O2-C2-C3-O3
11	A	533	DTT	C1-C2-C3-C4

There are no ring outliers.

47 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	201	EDO	3	0
7	A	530	EDO	1	0
7	A	522	EDO	1	0
7	A	516	EDO	1	0
7	B	101	EDO	2	0
7	C	304	EDO	3	0
8	A	548	PEG	1	0
10	A	526	P15	9	0
8	A	531	PEG	4	0
7	A	535	EDO	3	0

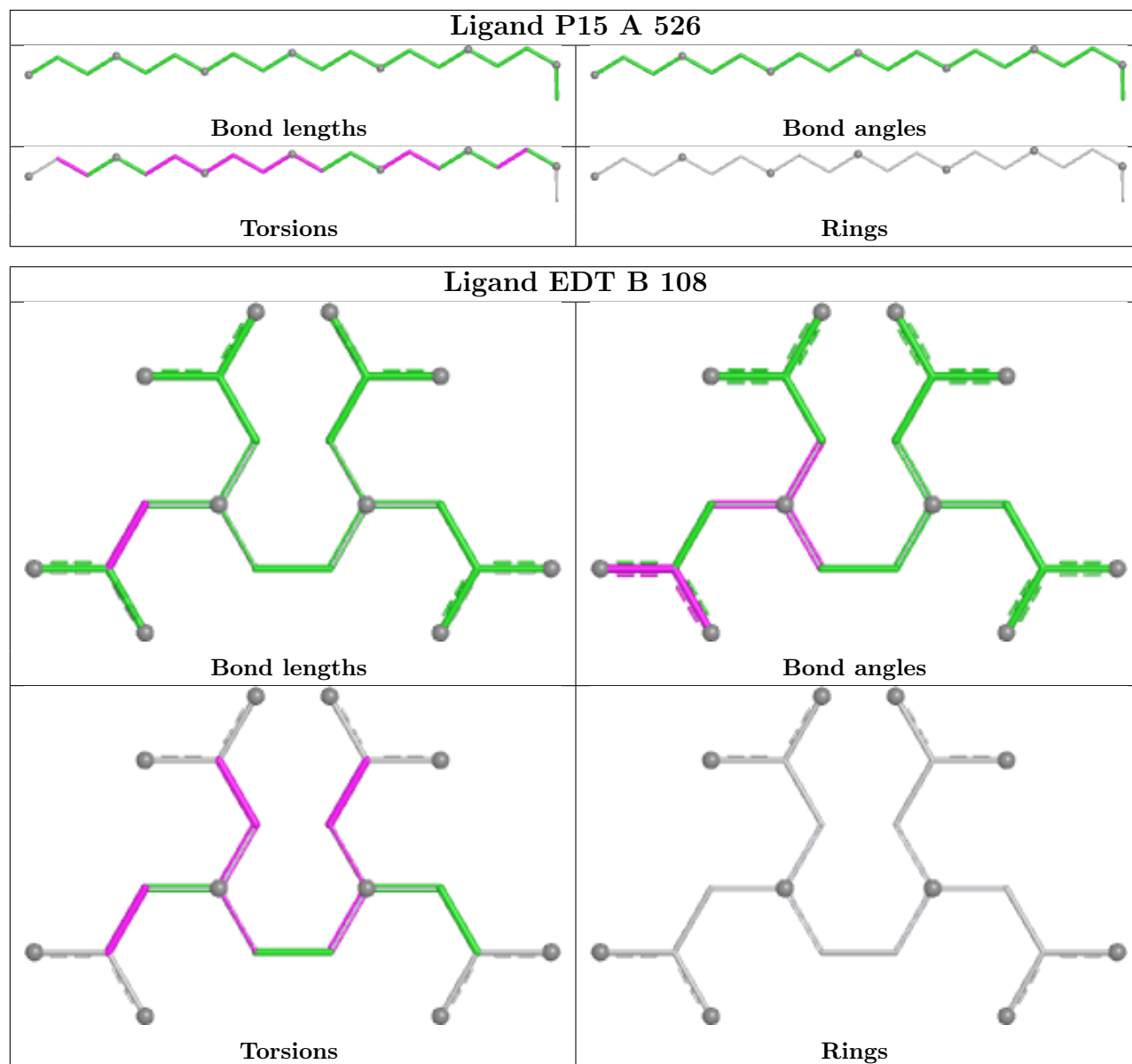
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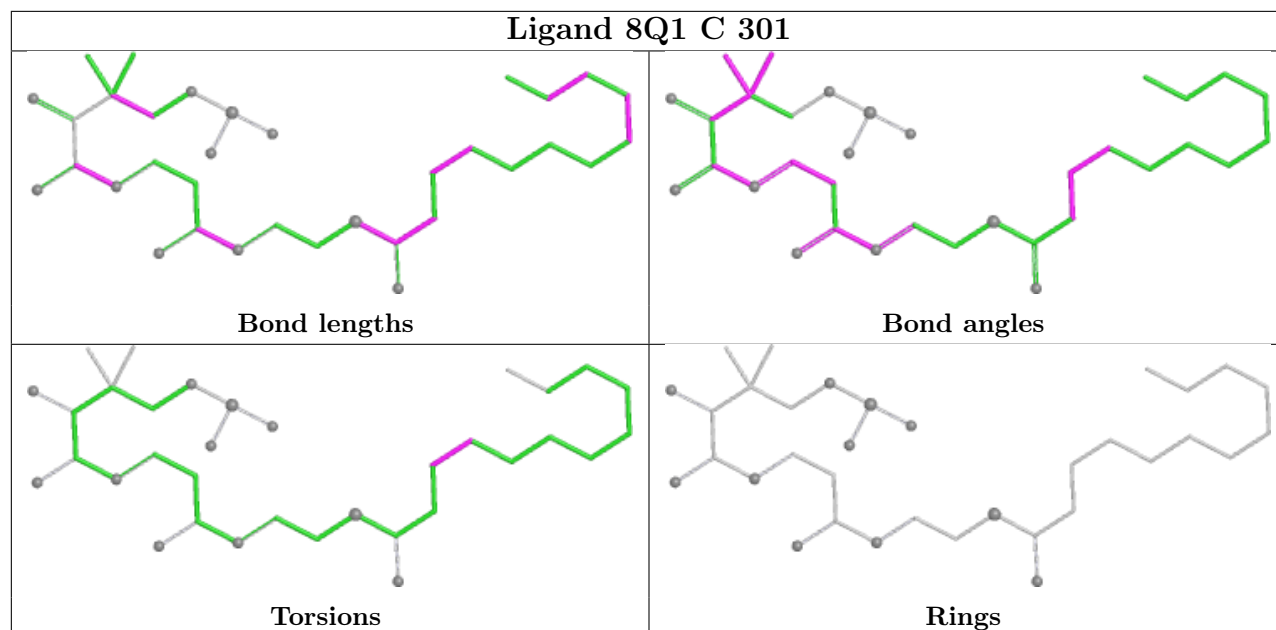
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	554	EDO	4	0
7	A	514	EDO	7	0
12	A	534	PGE	9	0
8	B	104	PEG	5	0
6	A	504	GOL	2	0
7	A	537	EDO	1	0
8	A	532	PEG	2	0
7	A	513	EDO	1	0
7	A	517	EDO	3	0
9	A	519	PG4	3	0
7	A	506	EDO	1	0
16	D	202	1PE	2	0
6	A	503	GOL	1	0
7	A	510	EDO	1	0
7	A	553	EDO	2	0
13	B	108	EDT	6	0
7	B	109	EDO	1	0
8	B	106	PEG	4	0
7	A	511	EDO	2	0
7	A	523	EDO	1	0
8	C	305	PEG	1	0
7	A	552	EDO	3	0
7	A	507	EDO	7	0
11	A	533	DTT	4	0
12	A	543	PGE	8	0
7	A	547	EDO	1	0
8	A	518	PEG	1	0
8	A	550	PEG	1	0
6	A	505	GOL	2	0
7	B	103	EDO	1	0
7	B	110	EDO	1	0
15	C	302	MES	1	0
6	A	551	GOL	1	0
7	A	538	EDO	1	0
7	A	515	EDO	2	0
9	A	520	PG4	1	0
8	A	549	PEG	1	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 [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 [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, 95th 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	395/406 (97%)	-0.35	11 (2%) 55 55	6, 18, 43, 90	33 (8%)
2	B	84/91 (92%)	-0.12	3 (3%) 46 46	8, 21, 45, 63	8 (9%)
3	C	75/77 (97%)	1.06	10 (13%) 7 6	27, 50, 79, 98	0
4	D	126/143 (88%)	0.26	7 (5%) 30 29	9, 33, 59, 110	6 (4%)
All	All	680/717 (94%)	-0.05	31 (4%) 37 36	6, 23, 60, 110	47 (6%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	ALA	9.7
4	D	35[A]	TYR	9.1
4	D	34[A]	ALA	8.2
1	A	381	CYS	6.3
1	A	378	GLY	6.3

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 oligosaccharides 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, 95th 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	PEG	C	305	7/7	0.60	0.28	65,71,73,73	0
7	EDO	A	553	4/4	0.65	0.27	69,69,73,76	0
6	GOL	A	551	6/6	0.68	0.27	41,65,76,81	0
7	EDO	A	540	4/4	0.68	0.23	71,73,76,78	0
7	EDO	B	109	4/4	0.69	0.26	74,75,76,77	0
13	EDT	B	108	20/20	0.69	0.27	47,57,71,72	20
8	PEG	A	550	7/7	0.70	0.21	69,73,75,76	0
7	EDO	A	524	4/4	0.70	0.19	54,54,54,55	4
7	EDO	A	547	4/4	0.70	0.22	48,55,60,62	0
7	EDO	A	529	4/4	0.71	0.29	84,85,87,87	0
7	EDO	A	525	4/4	0.72	0.20	56,57,57,59	0
9	PG4	A	520	13/13	0.72	0.24	36,59,67,67	13
8	PEG	B	104	7/7	0.72	0.25	34,51,68,70	0
7	EDO	A	542	4/4	0.73	0.20	53,58,62,67	0
7	EDO	C	306	4/4	0.73	0.20	65,69,69,69	0
7	EDO	D	203	4/4	0.73	0.21	57,61,63,66	0
7	EDO	A	554	4/4	0.73	0.28	85,85,85,85	0
8	PEG	A	548	7/7	0.75	0.26	69,71,79,81	0
9	PG4	A	519	13/13	0.75	0.23	31,51,58,61	13
7	EDO	A	530	4/4	0.76	0.30	52,58,60,61	4
8	PEG	A	532	7/7	0.76	0.20	56,64,67,68	0
7	EDO	B	105	4/4	0.76	0.26	70,71,73,73	0
8	PEG	A	549	7/7	0.77	0.21	42,66,73,73	0
7	EDO	B	111	4/4	0.78	0.18	61,62,62,63	0
7	EDO	D	205	4/4	0.78	0.18	41,43,45,52	4
8	PEG	A	527	7/7	0.78	0.21	61,64,67,68	0
7	EDO	B	103	4/4	0.78	0.20	72,73,76,79	0
10	P15	A	526	20/20	0.79	0.23	18,69,74,74	0
12	PGE	A	544	10/10	0.79	0.21	78,80,82,82	0
7	EDO	A	528	4/4	0.79	0.22	31,33,36,37	4
7	EDO	A	541	4/4	0.80	0.17	44,52,55,56	0
7	EDO	D	206	4/4	0.80	0.16	62,62,63,63	0
8	PEG	A	518	7/7	0.80	0.17	35,44,49,53	0
7	EDO	A	515	4/4	0.80	0.21	54,55,56,57	0
7	EDO	A	545	4/4	0.80	0.19	51,59,65,69	0
6	GOL	A	503	6/6	0.81	0.17	32,55,60,61	0
7	EDO	B	110	4/4	0.81	0.16	57,60,61,63	0
7	EDO	B	102	4/4	0.81	0.16	44,49,50,53	0
7	EDO	A	537	4/4	0.81	0.19	60,64,67,70	0
7	EDO	A	539	4/4	0.81	0.18	61,62,63,65	0
7	EDO	A	538	4/4	0.82	0.20	59,62,65,67	0
7	EDO	A	535	4/4	0.82	0.19	32,37,38,38	4
7	EDO	A	536	4/4	0.82	0.18	29,32,33,33	4

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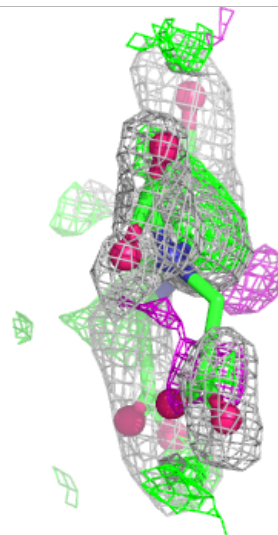
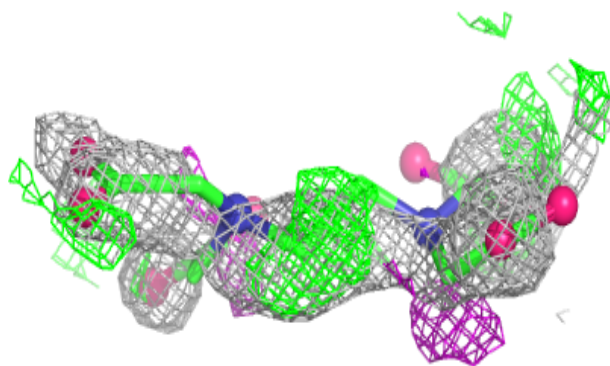
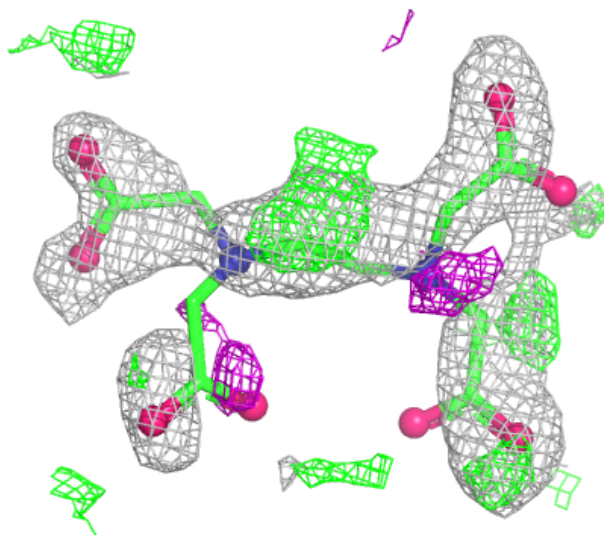
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	504	6/6	0.82	0.16	38,57,61,67	0
7	EDO	B	107	4/4	0.82	0.18	57,60,61,64	0
11	DTT	A	533	8/8	0.83	0.18	45,60,65,70	8
7	EDO	A	523	4/4	0.83	0.16	28,32,33,35	4
7	EDO	A	552	4/4	0.83	0.23	39,41,42,44	0
15	MES	C	302	12/12	0.83	0.16	60,62,64,66	0
7	EDO	A	510	4/4	0.84	0.15	48,51,53,56	0
7	EDO	A	512	4/4	0.84	0.18	35,36,38,39	4
8	PEG	A	531	7/7	0.85	0.19	23,42,66,70	7
8	PEG	A	521	7/7	0.85	0.14	39,48,56,61	0
7	EDO	A	509	4/4	0.85	0.16	23,27,30,31	4
8	PEG	B	106	7/7	0.85	0.16	18,29,37,42	7
7	EDO	A	508	4/4	0.86	0.13	48,50,51,53	0
7	EDO	A	546	4/4	0.86	0.17	26,32,33,38	4
12	PGE	A	543	10/10	0.86	0.18	23,41,51,52	10
12	PGE	A	534	10/10	0.87	0.16	29,39,45,45	10
16	1PE	D	202	16/16	0.87	0.15	59,64,69,70	0
7	EDO	A	517	4/4	0.88	0.16	16,22,28,34	4
7	EDO	A	506	4/4	0.88	0.16	39,39,43,43	4
6	GOL	A	502	6/6	0.88	0.16	9,20,25,28	6
6	GOL	D	204	6/6	0.88	0.13	30,35,39,43	6
7	EDO	C	304	4/4	0.88	0.17	28,32,33,36	4
7	EDO	B	101	4/4	0.90	0.16	19,24,26,27	4
7	EDO	D	201	4/4	0.90	0.12	26,26,35,40	4
7	EDO	C	303	4/4	0.91	0.15	37,37,39,39	4
6	GOL	A	505	6/6	0.91	0.14	23,32,36,37	6
7	EDO	A	511	4/4	0.92	0.11	34,34,36,37	4
7	EDO	A	513	4/4	0.92	0.15	35,42,42,44	4
7	EDO	A	516	4/4	0.93	0.11	11,12,15,20	4
7	EDO	A	522	4/4	0.93	0.16	19,24,35,36	4
14	8Q1	C	301	34/35	0.96	0.08	19,29,39,40	0
7	EDO	A	507	4/4	0.96	0.11	9,11,12,19	4
7	EDO	A	514	4/4	0.96	0.14	14,15,18,25	4
5	PLP	A	501	15/16	0.99	0.04	11,13,16,21	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.

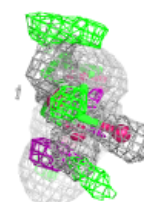
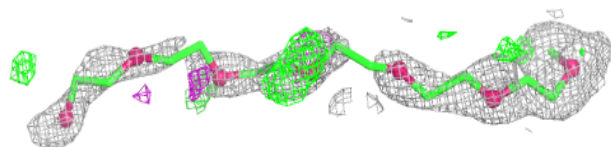
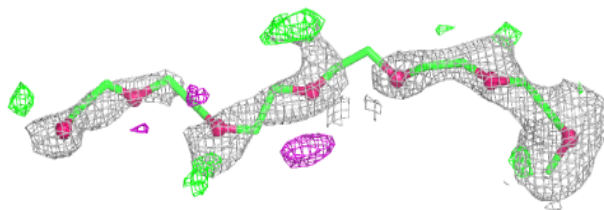
Electron density around EDT B 108:

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

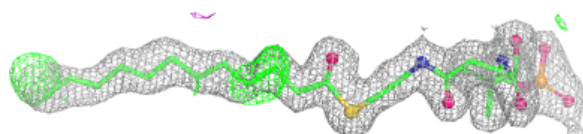
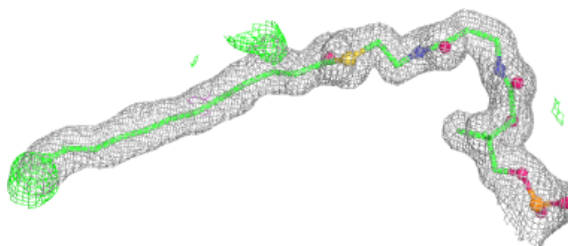


Electron density around P15 A 526:

$2mF_o-DF_c$ (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.