



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:54 am BST

PDB ID : 6UXE
Title : Structure of the human mitochondrial desulfurase complex Nfs1-ISCU2(M140I)-ISD11 with E.coli ACP1 at 1.57 Å resolution showing flexibility of N terminal end of ISCU2
Authors : Boniecki, M.T.; Cygler, M.
Deposited on : 2019-11-07
Resolution : 1.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

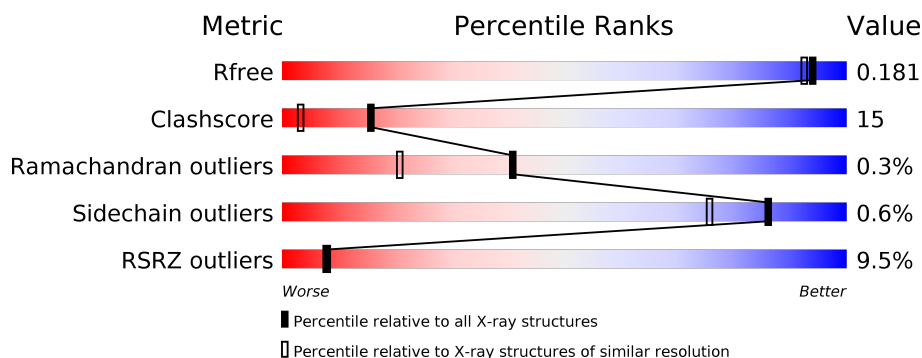
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>••</div> </div> </div>
2	B	91	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
3	C	77	<div> <div>48%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>••</div> </div> </div>
4	D	143	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>12%</div> </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	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	511	-	-	X	-
7	EDO	A	514	-	-	X	-
7	EDO	A	535	-	-	-	X
7	EDO	A	554	-	-	X	-
7	EDO	B	107	-	-	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 6265 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	22	0
			3141	1993	539	587	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	85	Total	C	N	O	S	0	8	0
			728	461	142	124	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			

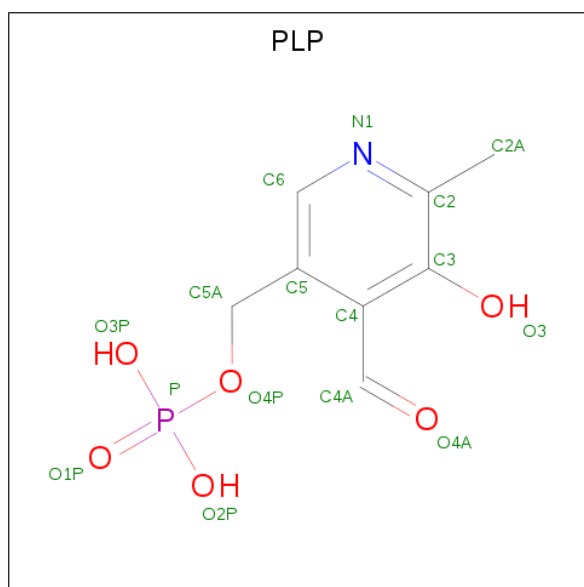
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	126	Total	C	N	O	S	0	7	0
			977	621	164	186	6			

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	140	ILE	MET	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: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by author).



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 (three-letter code: 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 (three-letter code: 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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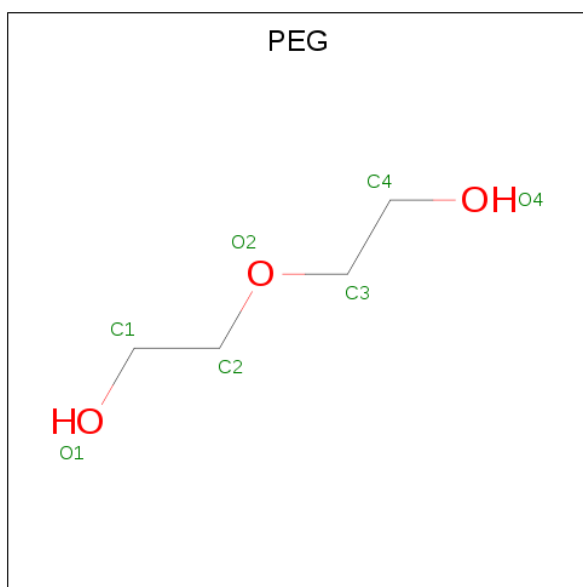
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	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

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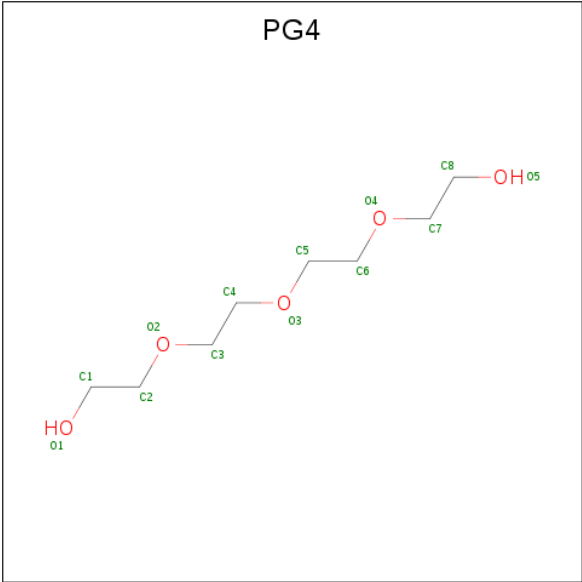
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



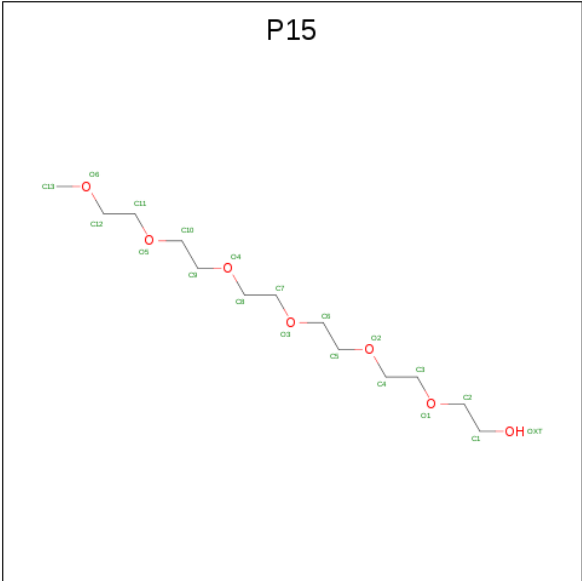
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	C	1	Total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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



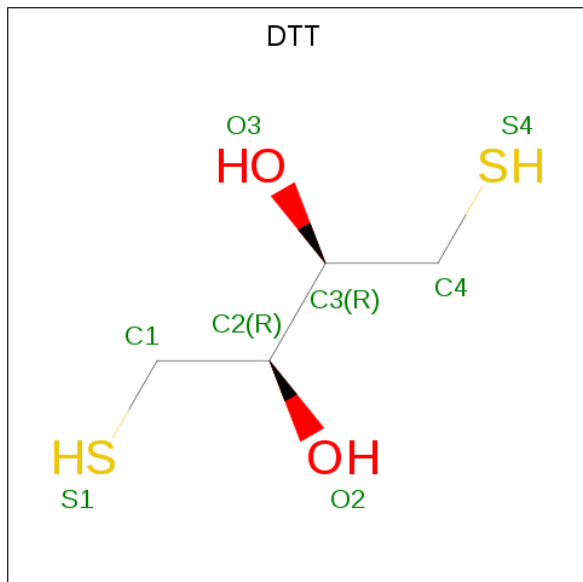
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (three-letter code: P15) (formula: C₁₃H₂₈O₇).



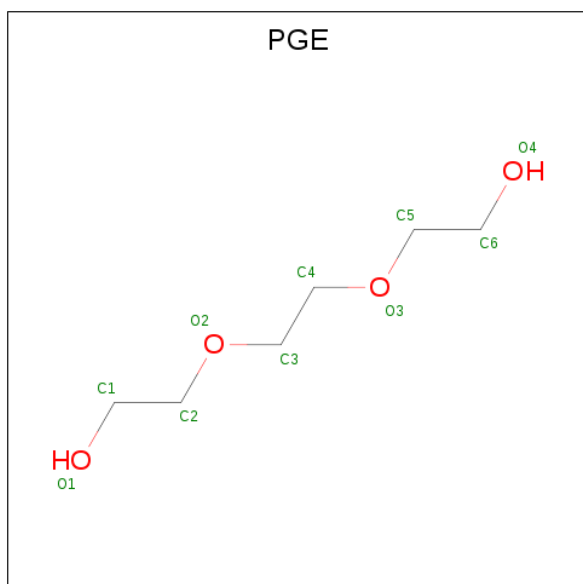
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			20	13	7		

- Molecule 11 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: 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 (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



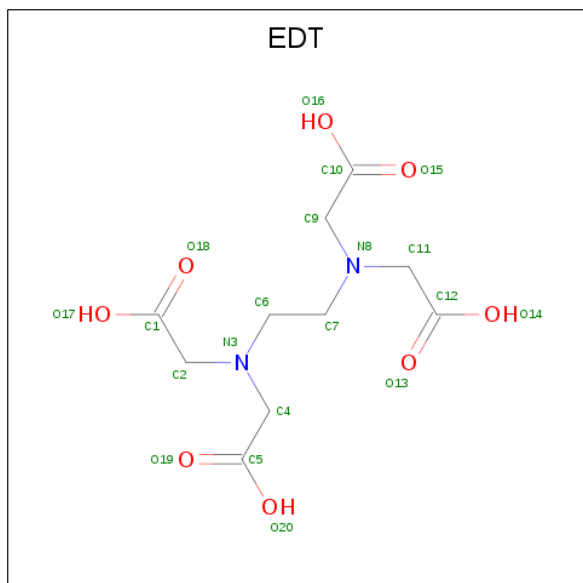
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		

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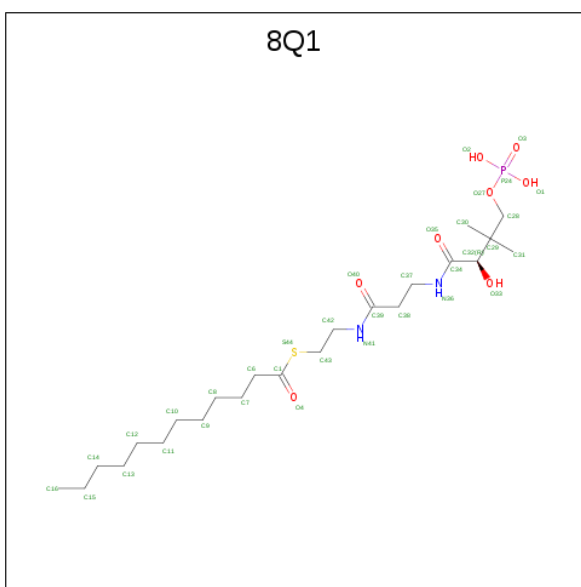
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		
12	A	1	Total	C	O	0	0
			10	6	4		

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



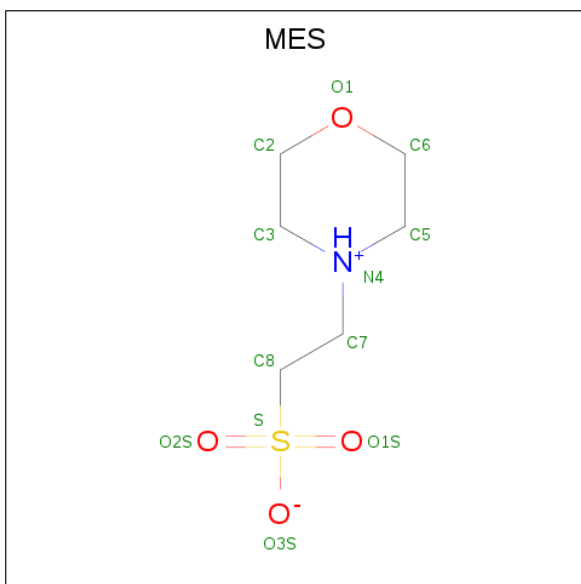
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by author).



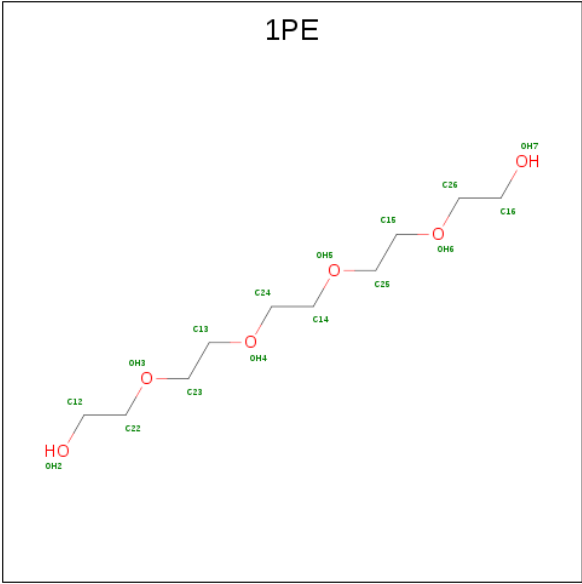
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	S	
			34	23	2	7	1	1	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 (three-letter code: 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		

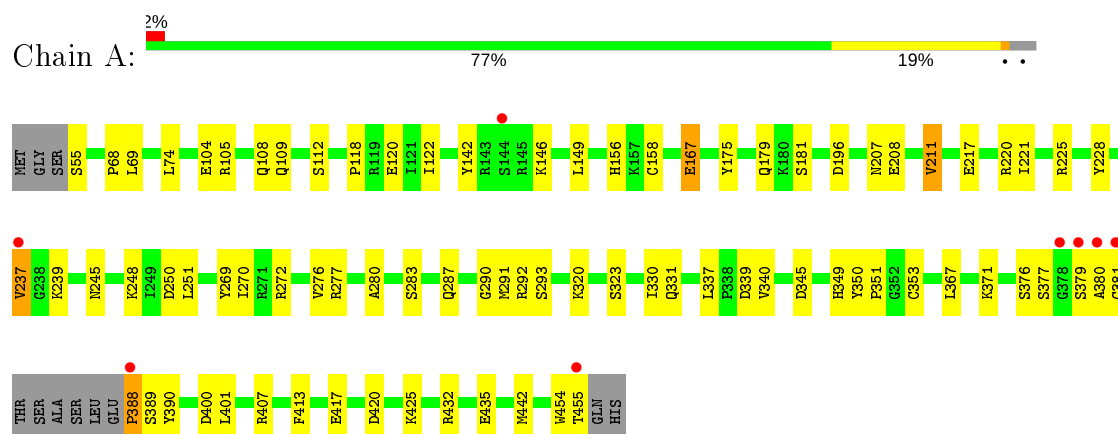
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	260	Total	O	0	0
			260	260		
17	B	71	Total	O	0	0
			71	71		
17	C	18	Total	O	0	0
			18	18		
17	D	41	Total	O	0	0
			41	41		

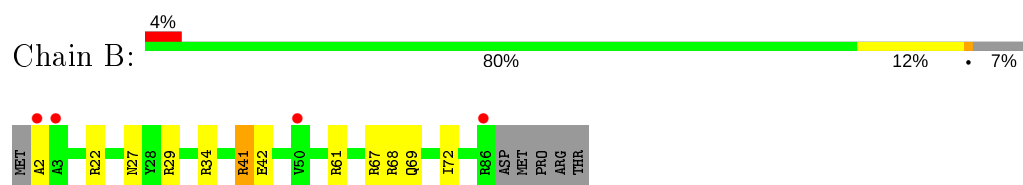
3 Residue-property plots [i](#)

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

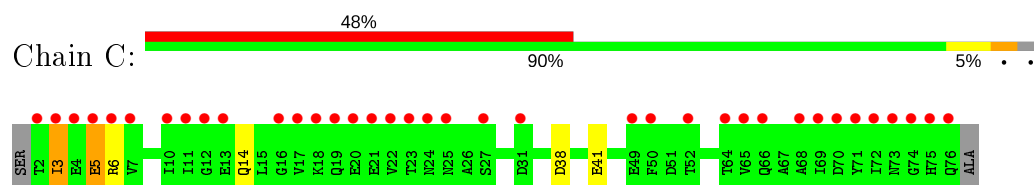
- Molecule 1: Cysteine desulfurase, mitochondrial



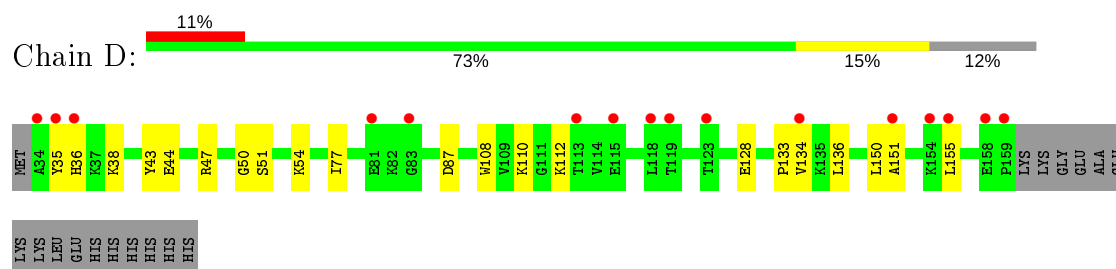
- Molecule 2: LYR motif-containing protein 4



- 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	86.41Å 86.41Å 245.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.57 48.98 – 1.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-1.57) 100.0 (48.98-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.156 , 0.180 0.160 , 0.181	Depositor DCC
R_{free} test set	6521 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.7	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	0.97	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: GOL, PGE, EDT, PLP, EDO, 1PE, PG4, P15, MES, 8Q1, PEG, DTT

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	1.04	6/3260 (0.2%)	0.94	5/4410 (0.1%)
2	B	0.90	0/761	0.83	0/1021
3	C	0.51	0/539	0.67	0/735
4	D	0.65	0/1002	0.75	0/1357
All	All	0.92	6/5562 (0.1%)	0.87	5/7523 (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
3	C	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237[A]	VAL	CA-C	7.64	1.72	1.52
1	A	237[B]	VAL	CA-C	7.64	1.72	1.52
1	A	217	GLU	CD-OE1	-6.30	1.18	1.25
1	A	353	CYS	C-O	-5.25	1.13	1.23
1	A	167	GLU	CD-OE2	-5.17	1.20	1.25
1	A	217	GLU	CD-OE2	-5.08	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220[A]	ARG	NE-CZ-NH1	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220[B]	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	211[A]	VAL	CB-CA-C	-6.09	99.84	111.40
1	A	211[B]	VAL	CB-CA-C	-6.09	99.84	111.40
1	A	388	PRO	CA-N-CD	-6.08	103.00	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211[A]	VAL	Mainchain
1	A	211[B]	VAL	Mainchain
1	A	237[A]	VAL	Mainchain
1	A	237[B]	VAL	Mainchain
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	3141	0	3188	108	0
2	B	728	0	766	19	0
3	C	535	0	472	7	0
4	D	977	0	984	19	0
5	A	15	0	7	0	0
6	A	30	0	40	7	0
6	D	6	0	8	0	0
7	A	132	0	193	45	0
7	B	36	0	53	8	0
7	C	12	0	18	3	0
7	D	20	0	30	4	0
8	A	56	0	80	10	0
8	B	14	0	20	12	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	5	0
12	A	30	0	42	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	20	0	12	4	0
14	C	34	0	0	0	0
15	C	12	0	13	1	0
16	D	16	0	22	3	0
17	A	260	0	0	14	0
17	B	71	0	0	6	0
17	C	18	0	0	1	0
17	D	41	0	0	1	0
All	All	6265	0	6032	175	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 15.

All (175) 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:68:ARG:HH11	8:B:106:PEG:H22	1.14	1.04
6:A:503:GOL:H12	2:B:34[A]:ARG:HH21	1.25	1.02
1:A:245:ASN:HD21	11:A:533:DTT:H2	1.28	0.97
1:A:208[A]:GLU:HG2	1:A:379:SER:O	1.67	0.94
1:A:112:SER:HA	9:A:519:PG4:H11	1.53	0.89
1:A:371:LYS:HD3	7:A:507:EDO:H22	1.52	0.88
1:A:349:HIS:H	7:A:552:EDO:H21	1.39	0.85
9:A:519:PG4:H12	17:A:753:HOH:O	1.77	0.83
1:A:293:SER:H	7:A:554:EDO:H12	1.42	0.83
2:B:29:ARG:HH21	13:B:110:EDT:H061	1.41	0.83
7:B:107:EDO:O2	17:B:201:HOH:O	1.97	0.81
1:A:337:LEU:O	10:A:526:P15:H131	1.80	0.80
1:A:287:GLN:HG3	7:A:547:EDO:H11	1.61	0.80
1:A:292:ARG:HH22	7:A:514:EDO:H11	1.51	0.76
2:B:68:ARG:NH1	8:B:106:PEG:H22	1.98	0.75
2:B:68:ARG:HD3	8:B:106:PEG:H11	1.67	0.74
8:B:106:PEG:H21	7:B:107:EDO:H22	1.69	0.73
1:A:413:PHE:HB2	7:B:101:EDO:H11	1.72	0.72
1:A:293:SER:HG	7:A:554:EDO:HO2	1.31	0.71
3:C:3:ILE:HG23	3:C:5:GLU:H	1.56	0.70
1:A:293:SER:N	7:A:554:EDO:H12	2.05	0.70
2:B:29:ARG:HH21	13:B:110:EDT:H041	1.55	0.70
7:A:507:EDO:H11	4:D:44:GLU:HG2	1.74	0.70
1:A:417[B]:GLU:HA	7:A:535:EDO:H12	1.75	0.69
2:B:29:ARG:NH2	13:B:110:EDT:H041	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432[A]:ARG:HE	7:A:541:EDO:H21	1.57	0.68
1:A:380:ALA:HB1	17:A:811:HOH:O	1.93	0.68
1:A:105[B]:ARG:HG2	7:A:511:EDO:H11	1.75	0.68
1:A:208[A]:GLU:CG	1:A:379:SER:O	2.42	0.67
1:A:420:ASP:OD2	7:A:535:EDO:H11	1.94	0.67
1:A:417[A]:GLU:HA	7:A:535:EDO:H12	1.78	0.66
1:A:245:ASN:HD21	11:A:533:DTT:C2	2.07	0.66
1:A:167:GLU:OE1	8:A:531:PEG:H42	1.95	0.65
1:A:371:LYS:CD	7:A:507:EDO:H22	2.24	0.64
1:A:376[B]:SER:OG	1:A:379:SER:HB3	1.96	0.64
1:A:105[A]:ARG:HH11	12:A:543:PGE:H6	1.63	0.64
1:A:109:GLN:HE22	12:A:543:PGE:H62	1.62	0.63
2:B:2:ALA:N	17:B:203:HOH:O	2.31	0.63
2:B:22:ARG:HD2	7:B:103:EDO:H12	1.80	0.63
1:A:207:ASN:HD22	1:A:381:CYS:N	1.97	0.63
6:A:503:GOL:H12	2:B:34[A]:ARG:NH2	2.08	0.63
4:D:108:TRP:CZ2	4:D:128:GLU:HG3	2.34	0.62
1:A:142:TYR:CE1	1:A:228:TYR:HE2	2.17	0.62
1:A:290:GLY:O	7:A:554:EDO:H11	2.00	0.61
1:A:245:ASN:ND2	11:A:533:DTT:H2	2.09	0.61
1:A:270:ILE:HG22	7:A:546:EDO:H12	1.83	0.60
1:A:390:TYR:CG	7:A:510:EDO:H12	2.37	0.60
4:D:51:SER:H	7:D:202:EDO:H11	1.65	0.60
1:A:340:VAL:H	10:A:526:P15:H133	1.66	0.60
4:D:50:GLY:HA2	7:D:201:EDO:H12	1.84	0.60
17:A:628:HOH:O	7:D:201:EDO:H11	2.02	0.59
1:A:109:GLN:HE22	12:A:543:PGE:H5	1.66	0.59
1:A:239[A]:LYS:HE2	17:A:654:HOH:O	2.02	0.59
1:A:292:ARG:HH22	7:A:514:EDO:C1	2.15	0.58
12:A:534:PGE:H6	17:A:607:HOH:O	2.02	0.58
1:A:340:VAL:O	10:A:526:P15:H122	2.03	0.58
3:C:14:GLN:O	7:C:304:EDO:H21	2.03	0.58
1:A:292:ARG:NH1	7:A:514:EDO:H12	2.19	0.58
8:A:518:PEG:H22	17:A:841:HOH:O	2.04	0.58
1:A:270:ILE:CG2	7:A:546:EDO:H12	2.34	0.57
1:A:340:VAL:H	10:A:526:P15:C13	2.18	0.57
4:D:134:VAL:HG13	17:D:338:HOH:O	2.05	0.57
1:A:225:ARG:NH1	6:A:505:GOL:O1	2.28	0.57
1:A:435:GLU:HG3	6:A:504:GOL:H32	1.87	0.57
3:C:38:ASP:OD2	15:C:302:MES:H32	2.04	0.57
1:A:142:TYR:OH	1:A:228:TYR:OH	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HD11	1:A:377:SER:HB2	1.88	0.55
11:A:533:DTT:O2	8:A:550:PEG:H32	2.06	0.55
1:A:208[B]:GLU:OE2	1:A:389:SER:OG	2.19	0.55
3:C:41:GLU:HB2	7:C:304:EDO:H11	1.88	0.55
4:D:112:LYS:HG2	16:D:203:1PE:H222	1.89	0.55
4:D:133:PRO:HA	4:D:136:LEU:HG	1.88	0.55
4:D:108:TRP:HZ2	4:D:128:GLU:HG3	1.69	0.55
1:A:175:TYR:HD2	8:A:531:PEG:C1	2.19	0.55
1:A:142:TYR:CE1	1:A:228:TYR:CE2	2.95	0.54
1:A:118:PRO:HB2	7:A:517:EDO:H11	1.89	0.54
1:A:425:LYS:NZ	7:A:530:EDO:H21	2.23	0.54
1:A:349:HIS:H	7:A:552:EDO:C2	2.16	0.54
1:A:330:ILE:HD12	12:A:534:PGE:H1	1.88	0.54
1:A:349:HIS:N	7:A:552:EDO:H21	2.18	0.54
1:A:401:LEU:HD21	10:A:526:P15:H51	1.89	0.53
1:A:104:GLU:O	7:A:517:EDO:H22	2.09	0.53
4:D:151:ALA:O	4:D:155:LEU:HD13	2.09	0.53
1:A:330:ILE:CD1	12:A:534:PGE:H1	2.39	0.52
1:A:68:PRO:HG3	7:B:101:EDO:H22	1.90	0.52
1:A:175:TYR:HD2	8:A:531:PEG:H11	1.74	0.52
2:B:42:GLU:HB2	8:B:104:PEG:H11	1.91	0.52
1:A:221:ILE:HG12	6:A:505:GOL:H12	1.92	0.52
1:A:349:HIS:ND1	12:A:534:PGE:O2	2.43	0.52
3:C:5:GLU:N	3:C:5:GLU:OE2	2.43	0.51
12:A:543:PGE:H2	17:B:260:HOH:O	2.09	0.51
3:C:3:ILE:O	3:C:6:ARG:HG3	2.11	0.50
1:A:109:GLN:HE22	12:A:543:PGE:C6	2.24	0.50
1:A:400:ASP:HB2	7:A:522:EDO:H11	1.94	0.50
12:A:543:PGE:H12	2:B:61[B]:ARG:NH1	2.27	0.50
1:A:388:PRO:O	1:A:388:PRO:HD2	2.11	0.49
2:B:34[B]:ARG:NE	17:B:207:HOH:O	2.44	0.49
1:A:105[B]:ARG:CG	7:A:511:EDO:H11	2.40	0.49
1:A:109:GLN:HE22	12:A:543:PGE:C5	2.26	0.49
2:B:67:ARG:HB3	8:B:106:PEG:H41	1.95	0.49
1:A:248:LYS:HE3	7:A:523:EDO:H22	1.94	0.48
1:A:292:ARG:NH2	7:A:514:EDO:H11	2.23	0.48
1:A:293:SER:OG	7:A:554:EDO:O2	2.09	0.48
2:B:29:ARG:HG2	13:B:110:EDT:H091	1.95	0.48
1:A:292:ARG:HH12	7:A:514:EDO:H12	1.79	0.47
1:A:331:GLN:NE2	17:A:611:HOH:O	2.47	0.47
1:A:376[B]:SER:OG	1:A:379:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:515:EDO:C2	8:B:104:PEG:H12	2.45	0.47
8:B:106:PEG:C2	7:B:107:EDO:H22	2.41	0.47
1:A:179:GLN:NE2	17:A:610:HOH:O	2.47	0.47
1:A:175:TYR:CD2	8:A:531:PEG:H11	2.49	0.47
1:A:331:GLN:OE1	8:A:532:PEG:H42	2.14	0.47
8:B:106:PEG:H21	7:B:107:EDO:C2	2.41	0.47
1:A:207:ASN:HD22	1:A:381:CYS:H	1.61	0.46
12:A:534:PGE:H5	17:A:602:HOH:O	2.16	0.46
1:A:108:GLN:HB2	7:A:517:EDO:H22	1.97	0.46
1:A:292:ARG:NH2	7:A:514:EDO:C1	2.76	0.46
2:B:69:GLN:OE1	2:B:72[B]:ILE:HD11	2.15	0.46
1:A:320:LYS:HG3	17:A:764:HOH:O	2.15	0.46
1:A:69[A]:LEU:HD13	1:A:74:LEU:HB2	1.98	0.45
4:D:51:SER:H	7:D:202:EDO:C1	2.30	0.45
1:A:454:TRP:O	1:A:455:THR:HB	2.16	0.45
3:C:41:GLU:HG2	8:C:305:PEG:H22	1.98	0.45
1:A:283:SER:HA	8:A:549:PEG:H41	1.98	0.45
7:A:507:EDO:H12	4:D:43:TYR:CE2	2.52	0.44
1:A:277:ARG:HD2	1:A:277:ARG:HA	1.85	0.44
1:A:156:HIS:NE2	1:A:381:CYS:SG	2.87	0.44
1:A:208[A]:GLU:CD	1:A:379:SER:O	2.55	0.44
1:A:350:TYR:CD1	1:A:351:PRO:HD2	2.53	0.44
1:A:417[A]:GLU:OE1	6:A:503:GOL:H2	2.17	0.44
2:B:41:ARG:HH11	2:B:41:ARG:HD3	1.67	0.44
1:A:280:ALA:HB1	7:A:554:EDO:O1	2.18	0.44
1:A:181:SER:HB2	1:A:345:ASP:HB2	2.00	0.43
1:A:351:PRO:HB3	12:A:534:PGE:H3	2.00	0.43
1:A:381:CYS:HA	1:A:407:ARG:HH12	1.84	0.43
6:A:502:GOL:O1	7:A:509:EDO:H11	2.18	0.43
7:A:515:EDO:H22	8:B:104:PEG:H12	1.99	0.43
4:D:36[A]:HIS:CE1	4:D:38:LYS:HG3	2.53	0.43
1:A:323:SER:OG	12:A:534:PGE:H62	2.18	0.43
1:A:413:PHE:HB3	2:B:27[A]:ASN:HB3	1.99	0.43
7:B:111:EDO:H11	17:B:251:HOH:O	2.18	0.43
1:A:340:VAL:HB	10:A:526:P15:H133	2.00	0.43
1:A:122:ILE:HD11	1:A:291[A]:MET:HE3	2.01	0.43
1:A:292:ARG:CZ	7:A:514:EDO:H12	2.48	0.43
10:A:526:P15:H111	17:A:729:HOH:O	2.19	0.43
1:A:293:SER:H	7:A:554:EDO:C1	2.23	0.42
1:A:367:LEU:HD11	1:A:377:SER:CB	2.49	0.42
1:A:250:ASP:HB3	1:A:276:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HA	1:A:269:TYR:O	2.19	0.42
1:A:371:LYS:HB3	7:A:507:EDO:C2	2.49	0.42
7:C:303:EDO:O1	17:C:401:HOH:O	2.20	0.42
4:D:54:LYS:H	4:D:54:LYS:HE2	1.84	0.42
8:B:104:PEG:H22	17:B:245:HOH:O	2.19	0.42
1:A:339:ASP:N	10:A:526:P15:H132	2.34	0.42
10:A:526:P15:H32	17:A:615:HOH:O	2.20	0.42
1:A:442:MET:HG3	8:A:548:PEG:H32	2.02	0.42
2:B:69:GLN:HA	2:B:72[B]:ILE:HG12	2.01	0.42
7:A:506:EDO:H22	7:A:507:EDO:H11	2.02	0.42
4:D:77:ILE:CD1	4:D:150:LEU:HD23	2.49	0.42
4:D:77:ILE:HD13	4:D:150:LEU:HD23	2.02	0.41
1:A:55:SER:HB2	17:A:770:HOH:O	2.19	0.41
9:A:519:PG4:H71	17:A:745:HOH:O	2.18	0.41
1:A:120:GLU:OE2	11:A:533:DTT:S1	2.78	0.41
4:D:112:LYS:NZ	16:D:203:1PE:H142	2.36	0.41
1:A:146:LYS:HG2	1:A:196:ASP:HA	2.03	0.41
1:A:272:ARG:NH1	7:A:524:EDO:H21	2.36	0.41
4:D:54:LYS:H	4:D:54:LYS:CD	2.32	0.41
1:A:105[A]:ARG:HA	7:A:511:EDO:H11	2.01	0.41
4:D:87:ASP:HA	4:D:110:LYS:HD3	2.01	0.41
1:A:175:TYR:HD2	8:A:531:PEG:H12	1.85	0.41
9:A:519:PG4:H61	9:A:519:PG4:H81	1.92	0.41
1:A:105[B]:ARG:HA	7:A:511:EDO:H11	2.01	0.41
8:B:106:PEG:H31	8:B:106:PEG:H12	1.66	0.40
4:D:112:LYS:CG	16:D:203:1PE:H222	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	413/406 (102%)	403 (98%)	10 (2%)	0	100	100
2	B	91/91 (100%)	89 (98%)	2 (2%)	0	100	100
3	C	73/77 (95%)	70 (96%)	2 (3%)	1 (1%)	11	2
4	D	130/143 (91%)	128 (98%)	0	2 (2%)	10	1
All	All	707/717 (99%)	690 (98%)	14 (2%)	3 (0%)	41	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	35[A]	TYR
4	D	35[B]	TYR
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	345/346 (100%)	344 (100%)	1 (0%)	92	86
2	B	76/80 (95%)	75 (99%)	1 (1%)	69	48
3	C	49/66 (74%)	49 (100%)	0	100	100
4	D	103/118 (87%)	102 (99%)	1 (1%)	76	59
All	All	573/610 (94%)	570 (100%)	3 (0%)	86	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	CYS
2	B	41	ARG
4	D	47	ARG

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

79 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	A	516	-	3,3,3	0.51	0	2,2,2	0.19	0
8	PEG	A	548	-	6,6,6	0.49	0	5,5,5	0.35	0
7	EDO	D	201	-	3,3,3	0.47	0	2,2,2	0.24	0
7	EDO	B	107	-	3,3,3	0.46	0	2,2,2	0.21	0
9	PG4	A	520	-	12,12,12	0.55	0	11,11,11	0.40	0
7	EDO	A	523	-	3,3,3	0.51	0	2,2,2	0.51	0
8	PEG	A	527	-	6,6,6	0.49	0	5,5,5	0.35	0
7	EDO	A	538	-	3,3,3	0.51	0	2,2,2	0.40	0
7	EDO	A	509	-	3,3,3	0.67	0	2,2,2	0.99	0
7	EDO	A	535	-	3,3,3	0.45	0	2,2,2	0.51	0
7	EDO	B	111	-	3,3,3	0.41	0	2,2,2	0.29	0
7	EDO	A	506	-	3,3,3	0.40	0	2,2,2	0.21	0
7	EDO	B	102	-	3,3,3	0.49	0	2,2,2	0.73	0
7	EDO	A	536	-	3,3,3	0.42	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	206	-	3,3,3	0.48	0	2,2,2	0.48	0
7	EDO	A	524	-	3,3,3	0.45	0	2,2,2	0.49	0
7	EDO	A	547	-	3,3,3	0.45	0	2,2,2	0.48	0
7	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.39	0
11	DTT	A	533	-	7,7,7	0.64	0	4,8,8	0.94	0
7	EDO	A	542	-	3,3,3	0.52	0	2,2,2	0.30	0
16	1PE	D	203	-	15,15,15	0.53	0	14,14,14	0.25	0
8	PEG	B	104	-	6,6,6	0.53	0	5,5,5	0.27	0
6	GOL	D	205	-	5,5,5	0.55	0	5,5,5	0.29	0
6	GOL	A	505	-	5,5,5	0.86	0	5,5,5	0.61	0
7	EDO	B	101	-	3,3,3	0.87	0	2,2,2	1.18	0
7	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.44	0
7	EDO	D	207	-	3,3,3	0.44	0	2,2,2	0.47	0
7	EDO	B	105	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	A	507	-	3,3,3	1.96	1 (33%)	2,2,2	1.64	1 (50%)
12	PGE	A	544	-	9,9,9	0.37	0	8,8,8	0.23	0
14	8Q1	C	301	3	27,33,34	2.43	9 (33%)	32,40,43	1.19	2 (6%)
7	EDO	A	529	-	3,3,3	0.49	0	2,2,2	0.29	0
7	EDO	A	512	-	3,3,3	0.42	0	2,2,2	0.77	0
8	PEG	A	532	-	6,6,6	0.50	0	5,5,5	0.61	0
7	EDO	A	515	-	3,3,3	0.52	0	2,2,2	0.16	0
8	PEG	B	106	-	6,6,6	0.63	0	5,5,5	0.83	0
12	PGE	A	534	-	9,9,9	0.47	0	8,8,8	1.00	1 (12%)
8	PEG	A	518	-	6,6,6	0.58	0	5,5,5	0.63	0
7	EDO	A	553	-	3,3,3	0.44	0	2,2,2	0.31	0
7	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.26	0
7	EDO	B	108	-	3,3,3	0.46	0	2,2,2	0.38	0
8	PEG	C	305	-	6,6,6	0.49	0	5,5,5	0.24	0
7	EDO	A	545	-	3,3,3	0.47	0	2,2,2	0.25	0
6	GOL	A	502	-	5,5,5	0.40	0	5,5,5	1.27	1 (20%)
7	EDO	A	541	-	3,3,3	0.43	0	2,2,2	0.18	0
7	EDO	B	112	-	3,3,3	0.48	0	2,2,2	0.19	0
7	EDO	C	304	-	3,3,3	0.51	0	2,2,2	0.55	0
7	EDO	A	513	-	3,3,3	0.43	0	2,2,2	0.47	0
7	EDO	A	530	-	3,3,3	0.52	0	2,2,2	0.27	0
7	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.28	0
12	PGE	A	543	-	9,9,9	0.26	0	8,8,8	0.59	0
7	EDO	A	539	-	3,3,3	0.47	0	2,2,2	0.33	0
9	PG4	A	519	-	12,12,12	0.53	0	11,11,11	0.48	0
7	EDO	A	540	-	3,3,3	0.46	0	2,2,2	0.43	0
7	EDO	A	511	-	3,3,3	0.57	0	2,2,2	0.66	0
7	EDO	A	517	-	3,3,3	0.07	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	525	-	3,3,3	0.47	0	2,2,2	0.42	0
15	MES	C	302	-	12,12,12	1.92	4 (33%)	14,16,16	2.24	4 (28%)
13	EDT	B	110	-	7,19,19	0.60	0	12,24,24	2.49	3 (25%)
7	EDO	A	537	-	3,3,3	0.45	0	2,2,2	0.29	0
5	PLP	A	501	1	15,15,16	1.09	1 (6%)	20,22,23	1.06	0
8	PEG	A	550	-	6,6,6	0.48	0	5,5,5	0.29	0
7	EDO	A	546	-	3,3,3	0.78	0	2,2,2	1.40	0
7	EDO	A	554	-	3,3,3	0.48	0	2,2,2	0.41	0
7	EDO	B	103	-	3,3,3	0.43	0	2,2,2	0.33	0
8	PEG	A	549	-	6,6,6	0.48	0	5,5,5	0.33	0
7	EDO	B	109	-	3,3,3	0.50	0	2,2,2	0.45	0
7	EDO	D	204	-	3,3,3	0.48	0	2,2,2	0.28	0
8	PEG	A	531	-	6,6,6	0.54	0	5,5,5	0.86	0
7	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.69	0
7	EDO	A	552	-	3,3,3	0.47	0	2,2,2	0.76	0
6	GOL	A	551	-	5,5,5	0.47	0	5,5,5	0.51	0
7	EDO	A	514	-	3,3,3	1.28	0	2,2,2	0.83	0
7	EDO	A	522	-	3,3,3	0.74	0	2,2,2	0.76	0
8	PEG	A	521	-	6,6,6	0.48	0	5,5,5	0.94	0
7	EDO	A	528	-	3,3,3	0.54	0	2,2,2	0.27	0
6	GOL	A	503	-	5,5,5	0.45	0	5,5,5	0.51	0
10	P15	A	526	-	19,19,19	0.64	0	18,18,18	0.76	0
6	GOL	A	504	-	5,5,5	0.56	0	5,5,5	0.28	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	A	516	-	-	1/1/1/1	-
8	PEG	A	548	-	-	4/4/4/4	-
7	EDO	D	201	-	-	0/1/1/1	-
7	EDO	B	107	-	-	0/1/1/1	-
9	PG4	A	520	-	-	5/10/10/10	-
7	EDO	A	523	-	-	1/1/1/1	-
8	PEG	A	527	-	-	1/4/4/4	-
7	EDO	A	538	-	-	0/1/1/1	-
7	EDO	A	509	-	-	0/1/1/1	-
7	EDO	A	535	-	-	1/1/1/1	-
7	EDO	B	111	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	506	-	-	1/1/1/1	-
7	EDO	B	102	-	-	1/1/1/1	-
7	EDO	A	536	-	-	1/1/1/1	-
7	EDO	D	206	-	-	1/1/1/1	-
7	EDO	A	524	-	-	1/1/1/1	-
7	EDO	A	547	-	-	1/1/1/1	-
7	EDO	D	202	-	-	1/1/1/1	-
11	DTT	A	533	-	-	2/8/8/8	-
7	EDO	A	542	-	-	0/1/1/1	-
16	1PE	D	203	-	-	7/13/13/13	-
8	PEG	B	104	-	-	3/4/4/4	-
6	GOL	D	205	-	-	1/4/4/4	-
6	GOL	A	505	-	-	2/4/4/4	-
7	EDO	B	101	-	-	0/1/1/1	-
7	EDO	C	303	-	-	1/1/1/1	-
7	EDO	D	207	-	-	0/1/1/1	-
7	EDO	B	105	-	-	1/1/1/1	-
7	EDO	A	507	-	-	0/1/1/1	-
12	PGE	A	544	-	-	3/7/7/7	-
14	8Q1	C	301	3	-	2/38/40/41	-
7	EDO	A	529	-	-	1/1/1/1	-
7	EDO	A	512	-	-	1/1/1/1	-
8	PEG	A	532	-	-	0/4/4/4	-
7	EDO	A	515	-	-	1/1/1/1	-
8	PEG	B	106	-	-	3/4/4/4	-
12	PGE	A	534	-	-	5/7/7/7	-
8	PEG	A	518	-	-	1/4/4/4	-
7	EDO	A	553	-	-	1/1/1/1	-
7	EDO	A	508	-	-	0/1/1/1	-
7	EDO	B	108	-	-	1/1/1/1	-
8	PEG	C	305	-	-	4/4/4/4	-
7	EDO	A	545	-	-	1/1/1/1	-
6	GOL	A	502	-	-	0/4/4/4	-
7	EDO	A	541	-	-	1/1/1/1	-
7	EDO	B	112	-	-	1/1/1/1	-
7	EDO	C	304	-	-	1/1/1/1	-
7	EDO	A	513	-	-	1/1/1/1	-
7	EDO	A	530	-	-	1/1/1/1	-
7	EDO	C	306	-	-	1/1/1/1	-
12	PGE	A	543	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	539	-	-	0/1/1/1	-
9	PG4	A	519	-	-	5/10/10/10	-
7	EDO	A	540	-	-	1/1/1/1	-
7	EDO	A	511	-	-	0/1/1/1	-
7	EDO	A	517	-	-	1/1/1/1	-
7	EDO	A	525	-	-	1/1/1/1	-
15	MES	C	302	-	-	3/6/14/14	0/1/1/1
13	EDT	B	110	-	-	8/13/21/21	-
7	EDO	A	537	-	-	0/1/1/1	-
5	PLP	A	501	1	-	0/6/6/8	0/1/1/1
8	PEG	A	550	-	-	2/4/4/4	-
7	EDO	A	546	-	-	1/1/1/1	-
7	EDO	A	554	-	-	1/1/1/1	-
7	EDO	B	103	-	-	0/1/1/1	-
8	PEG	A	549	-	-	2/4/4/4	-
7	EDO	B	109	-	-	0/1/1/1	-
7	EDO	D	204	-	-	0/1/1/1	-
8	PEG	A	531	-	-	2/4/4/4	-
7	EDO	A	510	-	-	1/1/1/1	-
7	EDO	A	552	-	-	0/1/1/1	-
6	GOL	A	551	-	-	4/4/4/4	-
7	EDO	A	514	-	-	1/1/1/1	-
7	EDO	A	522	-	-	0/1/1/1	-
8	PEG	A	521	-	-	1/4/4/4	-
7	EDO	A	528	-	-	1/1/1/1	-
6	GOL	A	503	-	-	4/4/4/4	-
10	P15	A	526	-	-	10/17/17/17	-
6	GOL	A	504	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	O4-C1	-6.02	1.11	1.21
14	C	301	8Q1	C39-N41	4.68	1.44	1.33
14	C	301	8Q1	O40-C39	-4.67	1.13	1.23
15	C	302	MES	C8-S	4.08	1.83	1.77
14	C	301	8Q1	O35-C34	-4.08	1.15	1.23
14	C	301	8Q1	O33-C32	-3.85	1.35	1.42
14	C	301	8Q1	C34-N36	3.72	1.41	1.33
14	C	301	8Q1	C12-C13	-3.14	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	507	EDO	O1-C1	-3.07	1.26	1.42
14	C	301	8Q1	O27-C28	-2.72	1.38	1.44
14	C	301	8Q1	C15-C14	-2.59	1.33	1.51
15	C	302	MES	O1S-S	2.53	1.52	1.45
15	C	302	MES	C7-N4	2.53	1.53	1.47
5	A	501	PLP	C3-C2	-2.13	1.38	1.40
15	C	302	MES	O2S-S	2.00	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	110	EDT	C11-N8-C9	5.56	120.45	110.72
15	C	302	MES	O1S-S-C8	5.52	113.56	106.92
13	B	110	EDT	C10-C9-N8	5.15	120.82	113.48
15	C	302	MES	O3S-S-O2S	-3.90	101.73	111.27
13	B	110	EDT	C11-N8-C7	3.49	118.66	111.29
14	C	301	8Q1	C42-N41-C39	-2.59	118.03	122.84
15	C	302	MES	O2S-S-C8	2.46	109.87	106.92
15	C	302	MES	O3S-S-C8	2.42	109.68	105.77
7	A	507	EDO	O2-C2-C1	-2.31	95.31	111.91
6	A	502	GOL	C3-C2-C1	-2.26	102.93	111.70
12	A	534	PGE	O1-C1-C2	-2.10	99.63	111.81
14	C	301	8Q1	C37-N36-C34	-2.07	118.89	122.59

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	505	GOL	O1-C1-C2-C3
6	A	504	GOL	C1-C2-C3-O3
15	C	302	MES	C8-C7-N4-C3
15	C	302	MES	N4-C7-C8-S
6	A	551	GOL	C1-C2-C3-O3
6	A	551	GOL	O2-C2-C3-O3
6	A	503	GOL	O1-C1-C2-C3
6	A	503	GOL	C1-C2-C3-O3
11	A	533	DTT	C2-C3-C4-S4
13	B	110	EDT	C1-C2-N3-C4
13	B	110	EDT	C10-C9-N8-C11
8	B	106	PEG	C1-C2-O2-C3
9	A	519	PG4	C3-C4-O3-C5
10	A	526	P15	O5-C11-C12-O6

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Mol	Chain	Res	Type	Atoms
16	D	203	1PE	OH6-C15-C25-OH5
9	A	520	PG4	O2-C3-C4-O3
10	A	526	P15	O5-C10-C9-O4
16	D	203	1PE	OH4-C13-C23-OH3
8	B	106	PEG	O1-C1-C2-O2
8	C	305	PEG	O1-C1-C2-O2
10	A	526	P15	O1-C3-C4-O2
6	A	551	GOL	O1-C1-C2-O2
6	A	503	GOL	O2-C2-C3-O3
9	A	520	PG4	O1-C1-C2-O2
8	A	518	PEG	O1-C1-C2-O2
10	A	526	P15	OXT-C1-C2-O1
9	A	520	PG4	C3-C4-O3-C5
8	A	548	PEG	O1-C1-C2-O2
8	A	548	PEG	O2-C3-C4-O4
8	A	549	PEG	O1-C1-C2-O2
8	A	549	PEG	O2-C3-C4-O4
12	A	534	PGE	O3-C5-C6-O4
9	A	519	PG4	O3-C5-C6-O4
16	D	203	1PE	OH5-C14-C24-OH4
6	A	504	GOL	O1-C1-C2-C3
6	A	551	GOL	O1-C1-C2-C3
16	D	203	1PE	OH7-C16-C26-OH6
8	B	104	PEG	O2-C3-C4-O4
9	A	520	PG4	O4-C7-C8-O5
12	A	534	PGE	O1-C1-C2-O2
6	A	504	GOL	O1-C1-C2-O2
6	A	504	GOL	O2-C2-C3-O3
6	A	503	GOL	O1-C1-C2-O2
7	B	111	EDO	O1-C1-C2-O2
7	B	102	EDO	O1-C1-C2-O2
7	D	202	EDO	O1-C1-C2-O2
7	C	303	EDO	O1-C1-C2-O2
7	A	529	EDO	O1-C1-C2-O2
7	A	545	EDO	O1-C1-C2-O2
7	B	112	EDO	O1-C1-C2-O2
7	A	513	EDO	O1-C1-C2-O2
7	A	530	EDO	O1-C1-C2-O2
7	C	306	EDO	O1-C1-C2-O2
7	A	525	EDO	O1-C1-C2-O2
7	A	512	EDO	O1-C1-C2-O2
7	A	554	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	553	EDO	O1-C1-C2-O2
7	A	510	EDO	O1-C1-C2-O2
7	A	528	EDO	O1-C1-C2-O2
10	A	526	P15	O2-C5-C6-O3
14	C	301	8Q1	C6-C7-C8-C9
12	A	543	PGE	O1-C1-C2-O2
8	A	531	PEG	O2-C3-C4-O4
9	A	519	PG4	O2-C3-C4-O3
13	B	110	EDT	C7-C6-N3-C2
8	A	550	PEG	O1-C1-C2-O2
13	B	110	EDT	C10-C9-N8-C7
15	C	302	MES	C8-C7-N4-C5
6	A	505	GOL	O1-C1-C2-O2
7	A	506	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2
16	D	203	1PE	C15-C25-OH5-C14
8	B	104	PEG	C1-C2-O2-C3
8	A	548	PEG	C1-C2-O2-C3
8	B	104	PEG	C4-C3-O2-C2
8	A	527	PEG	C1-C2-O2-C3
16	D	203	1PE	C14-C24-OH4-C13
9	A	520	PG4	C6-C5-O3-C4
10	A	526	P15	C10-C9-O4-C8
8	C	305	PEG	C4-C3-O2-C2
8	C	305	PEG	O2-C3-C4-O4
13	B	110	EDT	C7-C6-N3-C4
8	A	521	PEG	O2-C3-C4-O4
7	B	105	EDO	O1-C1-C2-O2
7	A	546	EDO	O1-C1-C2-O2
10	A	526	P15	C5-C6-O3-C7
8	C	305	PEG	C1-C2-O2-C3
11	A	533	DTT	O3-C3-C4-S4
10	A	526	P15	C8-C7-O3-C6
9	A	519	PG4	O1-C1-C2-O2
7	A	524	EDO	O1-C1-C2-O2
7	B	108	EDO	O1-C1-C2-O2
7	A	541	EDO	O1-C1-C2-O2
7	A	540	EDO	O1-C1-C2-O2
13	B	110	EDT	C5-C4-N3-C2
12	A	543	PGE	C3-C4-O3-C5
8	A	531	PEG	C1-C2-O2-C3
8	A	548	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
13	B	110	EDT	C5-C4-N3-C6
10	A	526	P15	C3-C4-O2-C5
8	B	106	PEG	C4-C3-O2-C2
7	D	206	EDO	O1-C1-C2-O2
12	A	534	PGE	C4-C3-O2-C2
12	A	544	PGE	C1-C2-O2-C3
12	A	534	PGE	O2-C3-C4-O3
10	A	526	P15	C11-C12-O6-C13
13	B	110	EDT	C12-C11-N8-C9
7	A	523	EDO	O1-C1-C2-O2
7	A	536	EDO	O1-C1-C2-O2
7	A	547	EDO	O1-C1-C2-O2
12	A	534	PGE	C1-C2-O2-C3
7	A	516	EDO	O1-C1-C2-O2
7	A	517	EDO	O1-C1-C2-O2
7	A	535	EDO	O1-C1-C2-O2
7	C	304	EDO	O1-C1-C2-O2
12	A	544	PGE	O2-C3-C4-O3
14	C	301	8Q1	C12-C13-C14-C15
8	A	550	PEG	C4-C3-O2-C2
16	D	203	1PE	C24-C14-OH5-C25
6	D	205	GOL	C1-C2-C3-O3
12	A	544	PGE	O1-C1-C2-O2
12	A	543	PGE	O3-C5-C6-O4
7	A	515	EDO	O1-C1-C2-O2
9	A	519	PG4	C8-C7-O4-C6

There are no ring outliers.

47 monomers are involved in 123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	548	PEG	1	0
7	D	201	EDO	2	0
7	B	107	EDO	4	0
7	A	523	EDO	1	0
7	A	509	EDO	1	0
7	A	535	EDO	3	0
7	B	111	EDO	1	0
7	A	506	EDO	1	0
7	A	524	EDO	1	0
7	A	547	EDO	1	0
7	D	202	EDO	2	0

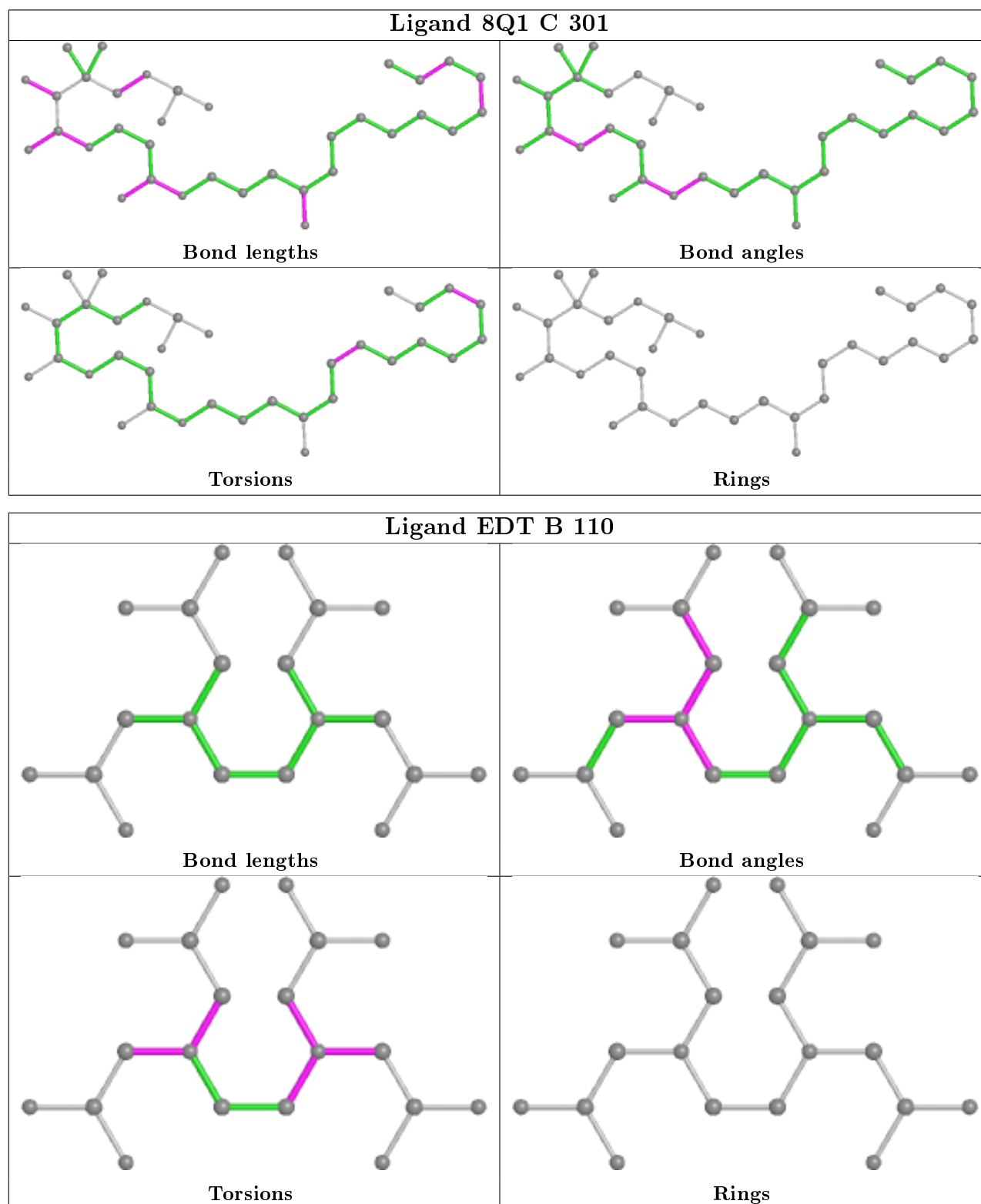
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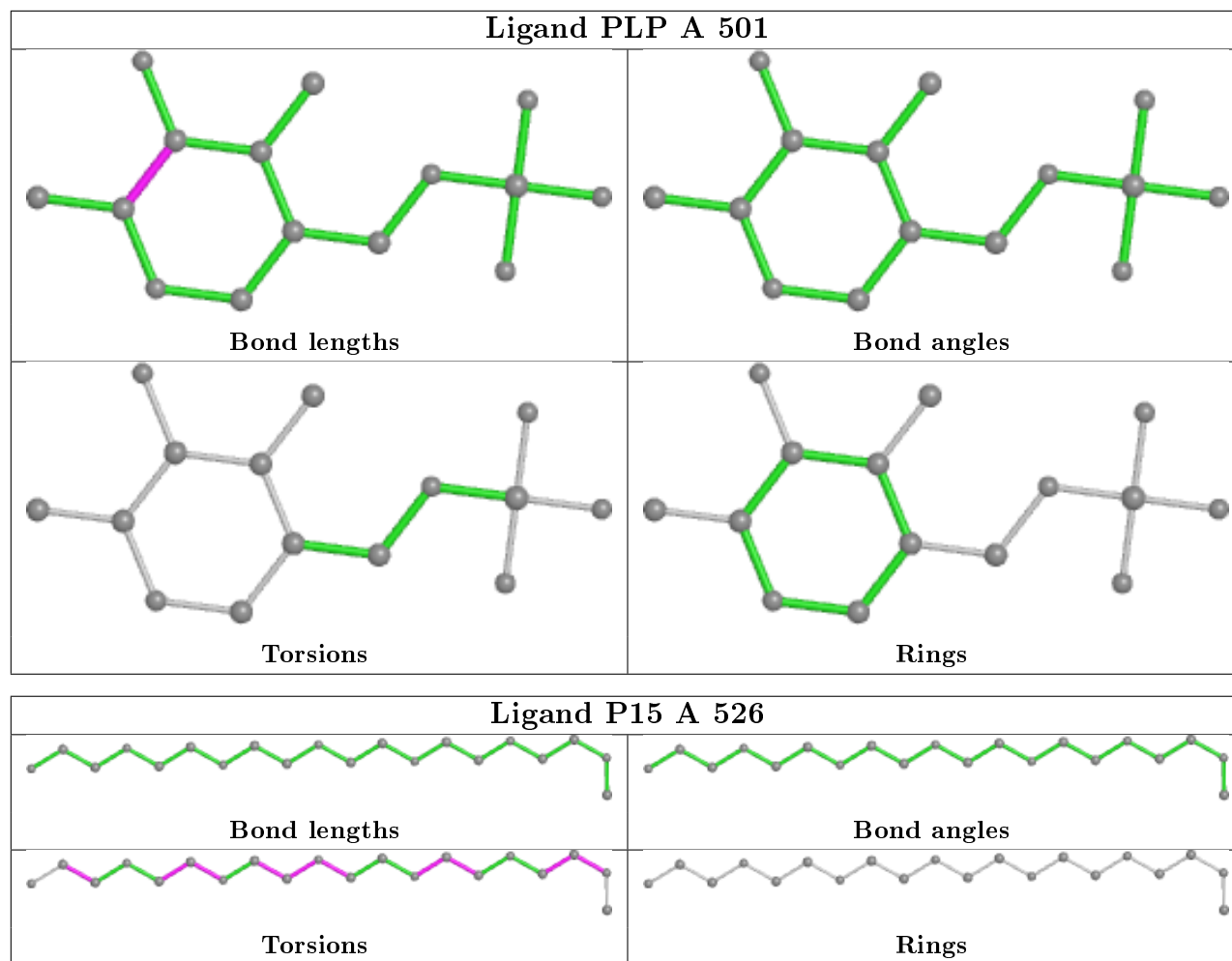
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	533	DTT	5	0
16	D	203	1PE	3	0
8	B	104	PEG	4	0
6	A	505	GOL	2	0
7	B	101	EDO	2	0
7	C	303	EDO	1	0
7	A	507	EDO	6	0
8	A	532	PEG	1	0
7	A	515	EDO	2	0
8	B	106	PEG	8	0
12	A	534	PGE	7	0
8	A	518	PEG	1	0
8	C	305	PEG	1	0
6	A	502	GOL	1	0
7	A	541	EDO	1	0
7	C	304	EDO	2	0
7	A	530	EDO	1	0
12	A	543	PGE	7	0
9	A	519	PG4	4	0
7	A	511	EDO	4	0
7	A	517	EDO	3	0
15	C	302	MES	1	0
13	B	110	EDT	4	0
8	A	550	PEG	1	0
7	A	546	EDO	2	0
7	A	554	EDO	7	0
7	B	103	EDO	1	0
8	A	549	PEG	1	0
8	A	531	PEG	5	0
7	A	510	EDO	1	0
7	A	552	EDO	3	0
7	A	514	EDO	7	0
7	A	522	EDO	1	0
6	A	503	GOL	3	0
10	A	526	P15	9	0
6	A	504	GOL	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

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, 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%)	-0.03	8 (2%) 65 66	13, 20, 45, 89	4 (1%)
2	B	85/91 (93%)	-0.03	4 (4%) 31 31	15, 24, 46, 88	0
3	C	75/77 (97%)	1.90	37 (49%) 0 0	28, 50, 84, 93	0
4	D	126/143 (88%)	0.39	16 (12%) 3 3	18, 34, 56, 97	0
All	All	681/717 (94%)	0.26	65 (9%) 8 8	13, 25, 62, 97	4 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	ALA	9.8
3	C	3	ILE	9.0
4	D	35[A]	TYR	8.2
3	C	2	THR	8.0
3	C	22	VAL	7.4
1	A	378	GLY	6.9
3	C	17	VAL	5.8
4	D	159	PRO	5.7
3	C	76	GLN	4.7
4	D	155	LEU	4.7
1	A	455	THR	4.6
4	D	134	VAL	4.5
3	C	20	GLU	4.4
3	C	23	THR	4.2
2	B	2	ALA	4.2
4	D	158	GLU	4.1
1	A	381	CYS	4.1
3	C	10	ILE	4.1
4	D	118	LEU	3.7
3	C	73	ASN	3.7
3	C	7	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	65	VAL	3.5
4	D	123	THR	3.5
2	B	3	ALA	3.5
3	C	69	ILE	3.5
3	C	74	GLY	3.4
3	C	68	ALA	3.3
3	C	12	GLY	3.1
3	C	19	GLN	3.1
3	C	66	GLN	3.1
3	C	11	ILE	3.1
3	C	72	ILE	3.0
2	B	86	ARG	3.0
3	C	18	LYS	2.9
3	C	25	ASN	2.9
4	D	115	GLU	2.8
1	A	379	SER	2.8
3	C	6	ARG	2.8
4	D	81	GLU	2.8
4	D	34[A]	ALA	2.7
1	A	144	SER	2.7
3	C	50	PHE	2.7
3	C	24	ASN	2.6
3	C	70	ASP	2.6
4	D	83	GLY	2.6
2	B	50	VAL	2.5
3	C	71	TYR	2.5
3	C	75	HIS	2.5
3	C	5	GLU	2.4
1	A	388	PRO	2.4
4	D	113	THR	2.4
3	C	13	GLU	2.4
3	C	49	GLU	2.4
4	D	36[A]	HIS	2.3
3	C	52	THR	2.3
3	C	16	GLY	2.3
3	C	31	ASP	2.2
3	C	4	GLU	2.2
1	A	237[A]	VAL	2.1
4	D	154	LYS	2.1
3	C	27	SER	2.1
3	C	21	GLU	2.0
3	C	64	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	119	THR	2.0
4	D	151	ALA	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
7	EDO	A	515	4/4	0.48	0.17	58,59,60,63	0
8	PEG	A	527	7/7	0.49	0.24	61,71,77,80	0
7	EDO	B	108	4/4	0.53	0.26	88,90,91,92	0
13	EDT	B	110	20/20	0.56	0.28	35,65,91,96	20
7	EDO	C	306	4/4	0.57	0.28	53,67,67,68	0
8	PEG	A	548	7/7	0.57	0.19	79,82,87,87	0
7	EDO	A	529	4/4	0.60	0.29	84,85,87,87	0
7	EDO	D	201	4/4	0.61	0.31	83,87,88,88	0
12	PGE	A	544	10/10	0.62	0.20	84,91,95,95	0
8	PEG	A	532	7/7	0.63	0.16	69,72,77,83	0
9	PG4	A	519	13/13	0.65	0.27	36,61,71,75	13
7	EDO	B	111	4/4	0.65	0.25	73,74,78,84	0
8	PEG	A	550	7/7	0.66	0.21	74,75,77,79	0
7	EDO	A	525	4/4	0.67	0.20	73,74,75,77	0
8	PEG	C	305	7/7	0.67	0.19	57,71,76,76	0
7	EDO	A	542	4/4	0.69	0.34	42,53,63,69	4
7	EDO	A	540	4/4	0.69	0.25	76,77,78,80	0
7	EDO	B	103	4/4	0.70	0.21	65,67,74,81	0
16	1PE	D	203	16/16	0.71	0.16	54,63,71,76	0
7	EDO	B	112	4/4	0.71	0.24	57,61,69,72	0
7	EDO	A	539	4/4	0.72	0.16	65,66,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	530	4/4	0.72	0.35	46,51,56,59	4
7	EDO	A	535	4/4	0.72	0.42	43,50,53,56	4
7	EDO	A	528	4/4	0.72	0.36	32,44,45,46	4
7	EDO	A	545	4/4	0.73	0.16	54,63,69,77	0
7	EDO	B	107	4/4	0.73	0.25	18,24,29,41	4
9	PG4	A	520	13/13	0.73	0.31	33,65,81,82	0
7	EDO	A	510	4/4	0.74	0.18	47,56,57,59	0
7	EDO	A	553	4/4	0.74	0.31	87,88,90,91	0
7	EDO	A	508	4/4	0.76	0.20	47,51,55,59	0
8	PEG	B	104	7/7	0.76	0.23	36,58,79,80	0
7	EDO	D	204	4/4	0.76	0.25	63,66,72,75	0
7	EDO	B	102	4/4	0.77	0.14	48,49,58,59	0
8	PEG	A	549	7/7	0.77	0.27	43,73,80,80	0
7	EDO	B	105	4/4	0.77	0.15	63,66,67,69	0
8	PEG	A	518	7/7	0.79	0.12	33,41,54,61	0
7	EDO	B	109	4/4	0.79	0.16	64,67,73,79	0
7	EDO	A	536	4/4	0.80	0.26	41,51,64,65	0
6	GOL	A	551	6/6	0.81	0.30	36,71,92,98	0
7	EDO	D	207	4/4	0.81	0.17	70,71,76,82	0
7	EDO	A	523	4/4	0.82	0.14	40,45,47,49	0
7	EDO	A	511	4/4	0.82	0.18	36,36,37,37	4
7	EDO	A	506	4/4	0.83	0.11	45,47,52,54	0
8	PEG	B	106	7/7	0.83	0.18	18,40,51,56	7
7	EDO	A	537	4/4	0.83	0.20	55,59,71,79	0
7	EDO	A	554	4/4	0.83	0.65	58,64,74,81	0
7	EDO	A	513	4/4	0.84	0.14	40,56,57,60	0
7	EDO	A	547	4/4	0.84	0.19	43,56,68,76	0
7	EDO	A	546	4/4	0.84	0.15	26,28,32,39	4
11	DTT	A	533	8/8	0.84	0.24	47,75,81,85	8
7	EDO	A	538	4/4	0.85	0.26	61,63,74,75	0
7	EDO	A	517	4/4	0.85	0.24	13,20,34,35	4
12	PGE	A	534	10/10	0.85	0.18	27,42,48,49	10
7	EDO	A	512	4/4	0.86	0.16	37,37,39,43	4
7	EDO	A	541	4/4	0.86	0.25	42,60,66,70	0
10	P15	A	526	20/20	0.86	0.21	20,74,88,90	0
7	EDO	A	552	4/4	0.86	0.20	38,43,46,54	0
7	EDO	A	524	4/4	0.87	0.22	57,59,63,64	4
12	PGE	A	543	10/10	0.87	0.16	25,45,58,61	10
7	EDO	B	101	4/4	0.88	0.11	23,29,31,42	4
6	GOL	D	205	6/6	0.88	0.12	35,39,43,47	6
7	EDO	D	206	4/4	0.89	0.38	55,61,61,70	4
6	GOL	A	504	6/6	0.89	0.20	35,49,56,66	6

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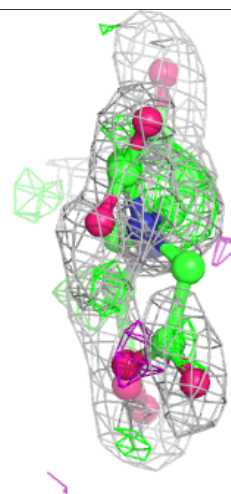
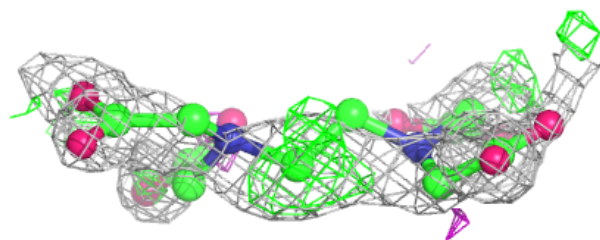
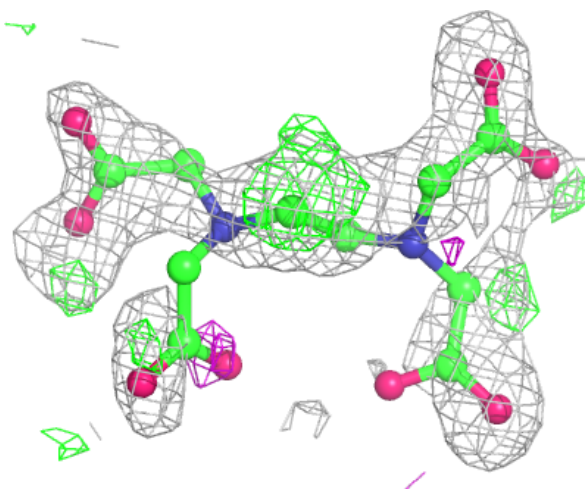
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	A	531	7/7	0.90	0.24	23,38,66,70	7
6	GOL	A	502	6/6	0.90	0.15	13,25,25,30	6
7	EDO	C	303	4/4	0.91	0.14	39,39,42,43	4
6	GOL	A	505	6/6	0.92	0.16	34,47,48,55	6
15	MES	C	302	12/12	0.93	0.15	52,60,66,69	0
7	EDO	A	522	4/4	0.93	0.21	22,31,37,38	4
8	PEG	A	521	7/7	0.93	0.11	44,45,54,69	0
7	EDO	A	516	4/4	0.94	0.17	23,24,33,40	4
7	EDO	C	304	4/4	0.94	0.36	33,45,48,49	4
6	GOL	A	503	6/6	0.94	0.10	28,65,66,67	0
7	EDO	A	509	4/4	0.94	0.16	31,36,38,47	4
14	8Q1	C	301	34/35	0.94	0.09	23,29,41,42	0
7	EDO	D	202	4/4	0.95	0.10	29,35,50,59	4
7	EDO	A	507	4/4	0.95	0.18	18,19,20,33	4
7	EDO	A	514	4/4	0.95	0.16	22,25,26,34	4
5	PLP	A	501	15/16	0.97	0.07	14,16,25,26	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.

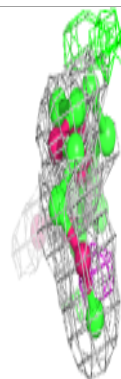
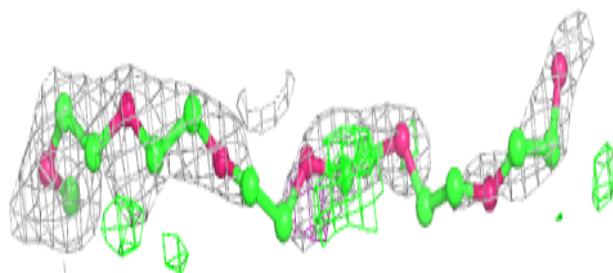
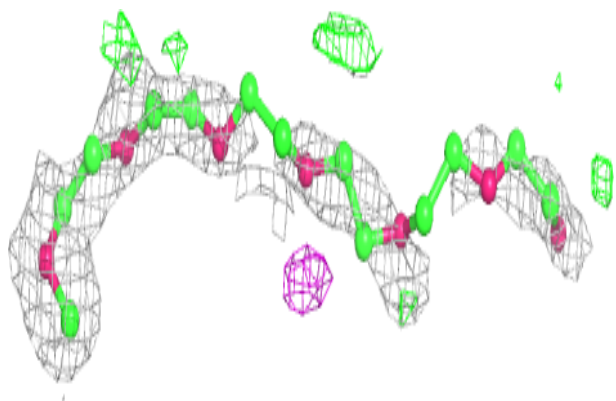
Electron density around EDT B 110:

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

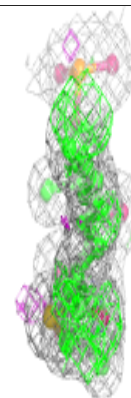
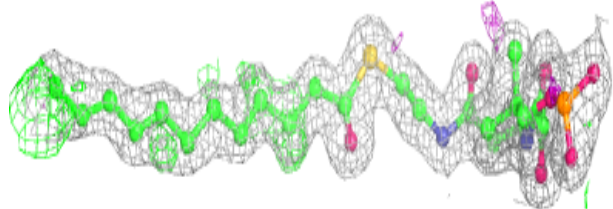
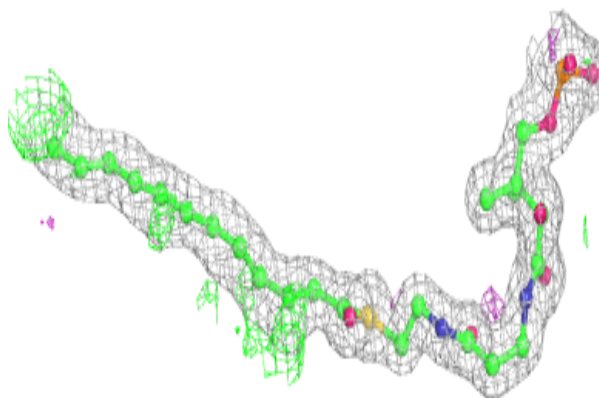


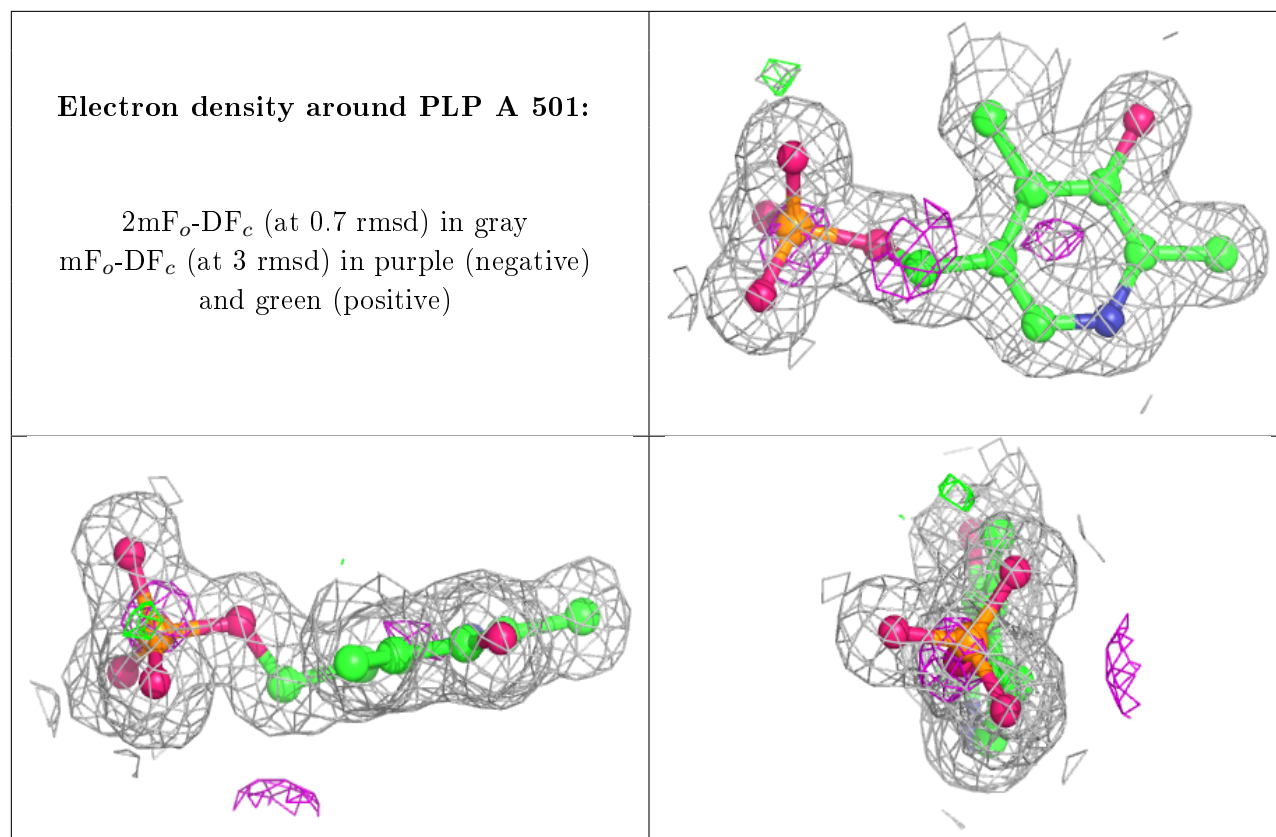
Electron density around P15 A 526:

$2mF_o-DF_c$ (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.