Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 05:51 PM EDT

PDB ID	:	6W1D
Title	:	Structure of human mitochondrial complex Nfs1-ISCU2 (WT)-ISD11 with E.coli ACP1 at 1.8 A resolution (NIAU)2
Authors	:	Boniecki, M.T.; Cygler, M.
Deposited on	:	2020-03-04
Resolution	:	1.79 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 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:

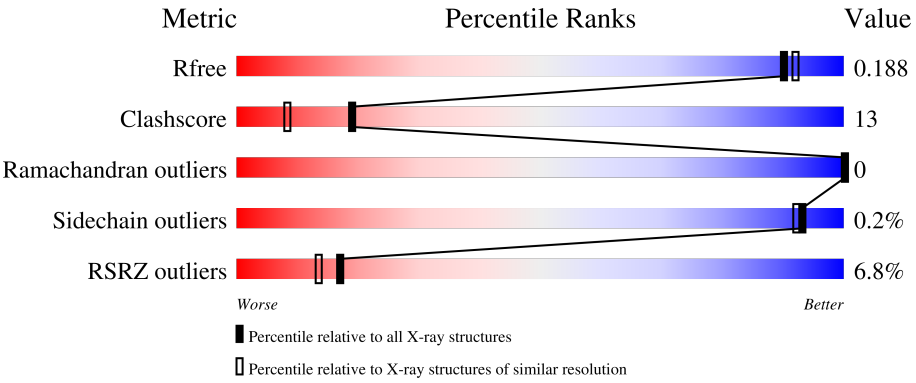
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

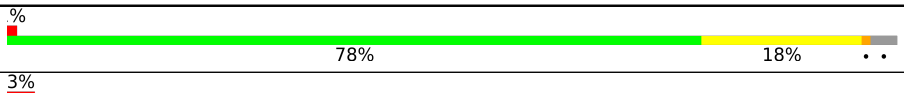
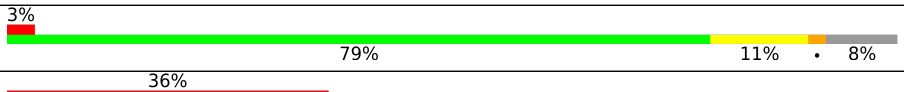
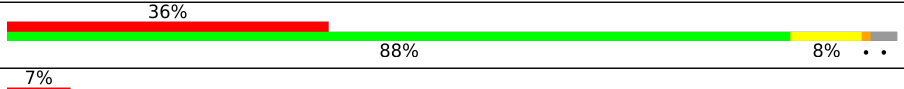
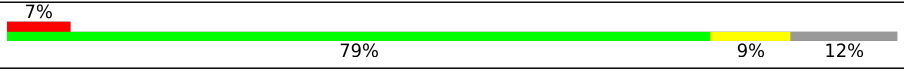
The reported resolution of this entry is 1.79 Å.

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	P15	A	526	-	-	X	-
11	DTT	A	533	-	-	X	-
12	PGE	A	534	-	-	X	-
12	PGE	A	543	-	-	X	-
6	GOL	A	551	-	-	-	X
7	EDO	A	507	-	X	X	-
7	EDO	A	514	-	-	X	-
7	EDO	A	528	-	-	-	X
7	EDO	A	529	-	-	-	X
7	EDO	A	535	-	-	-	X
7	EDO	A	554	-	-	X	-
8	PEG	A	531	-	-	X	-
8	PEG	B	104	-	-	X	-
8	PEG	B	106	-	-	X	-

2 Entry composition (i)

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			

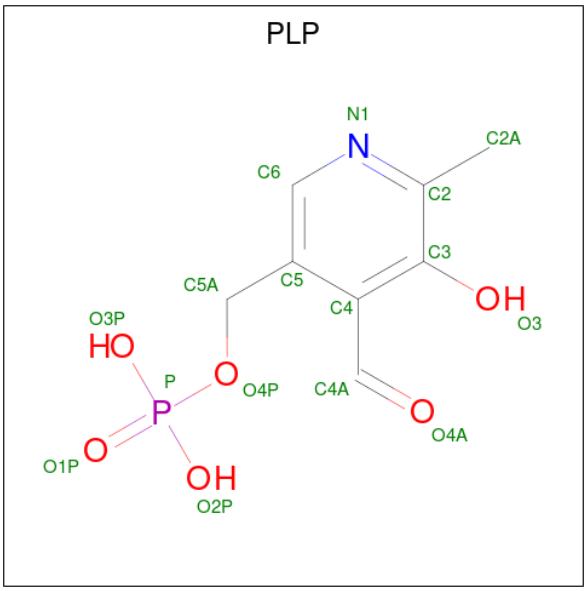
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	126	965	612	159	186	8	0	6	0

There are 10 discrepancies between the modelled and reference sequences:

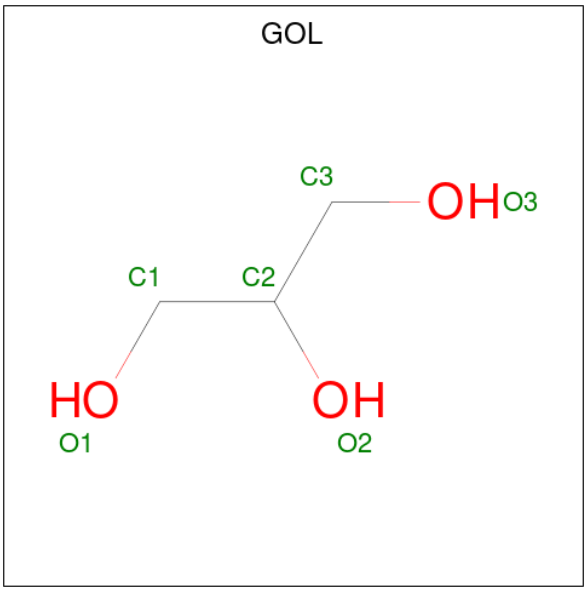
Chain	Residue	Modelled	Actual	Comment	Reference
D	33	MET	-	initiating methionine	UNP Q9H1K1
D	34	ALA	-	expression tag	UNP Q9H1K1
D	168	LEU	-	expression tag	UNP Q9H1K1
D	169	GLU	-	expression tag	UNP Q9H1K1
D	170	HIS	-	expression tag	UNP Q9H1K1
D	171	HIS	-	expression tag	UNP Q9H1K1
D	172	HIS	-	expression 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: $C_8H_{10}NO_6P$).



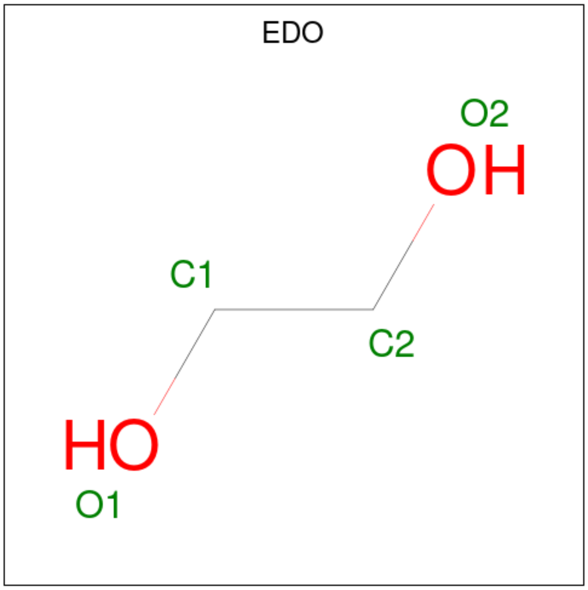
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	15	8	1	5	1	0	0

- 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 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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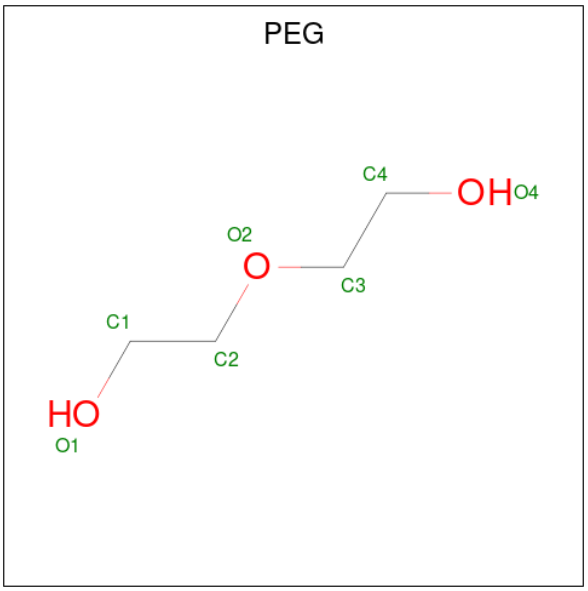
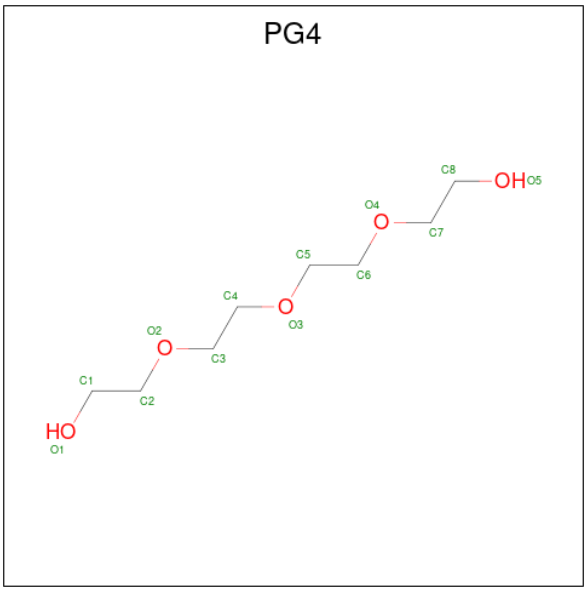
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total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

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



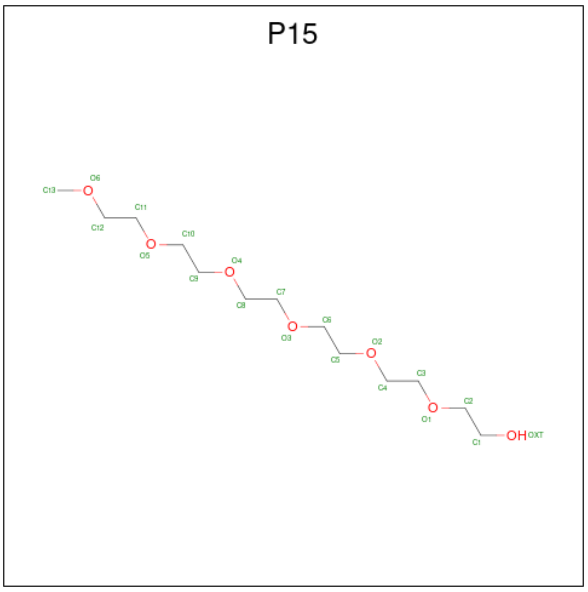
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0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

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



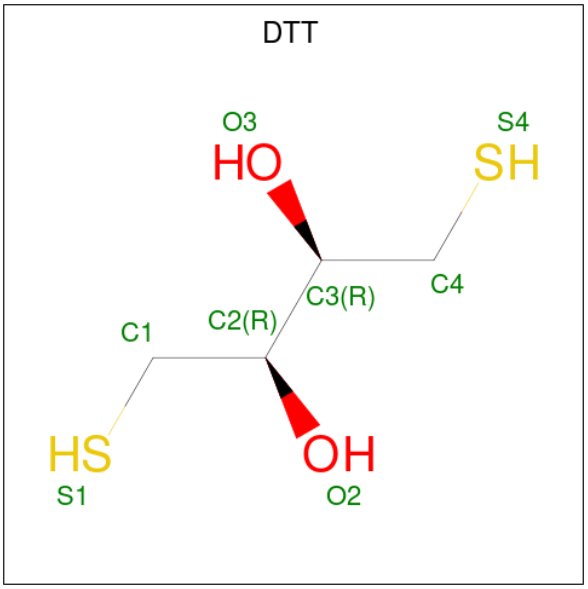
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 13 8 5	0	0
9	A	1	Total C O 13 8 5	0	0

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



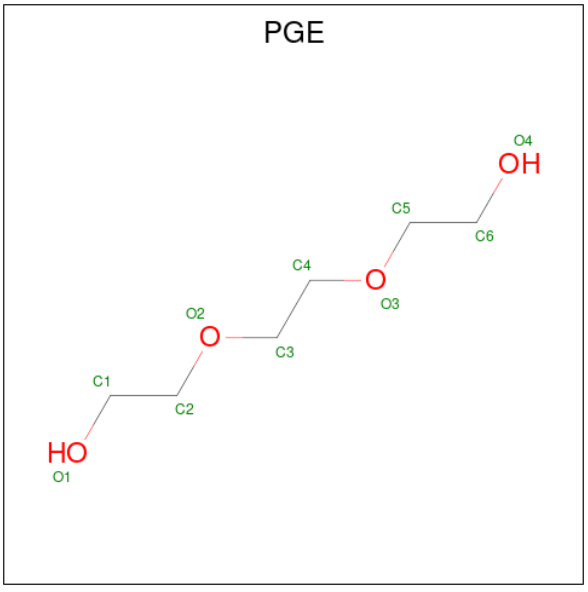
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 20 13 7	0	0

- 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
			Total	C	O	S		
11	A	1	8	4	2	2	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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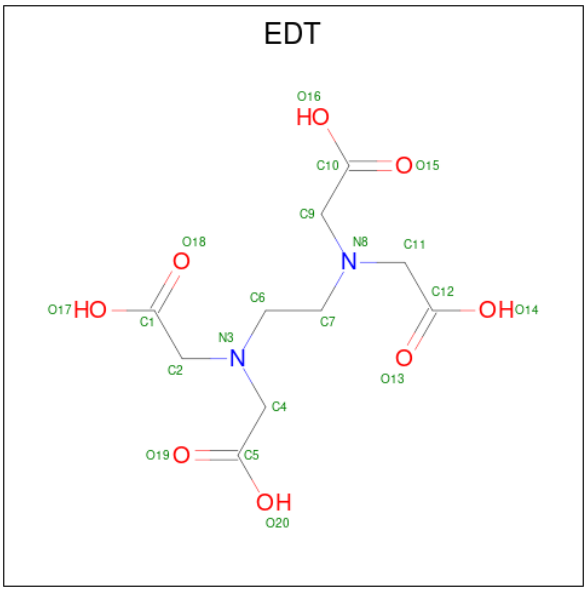
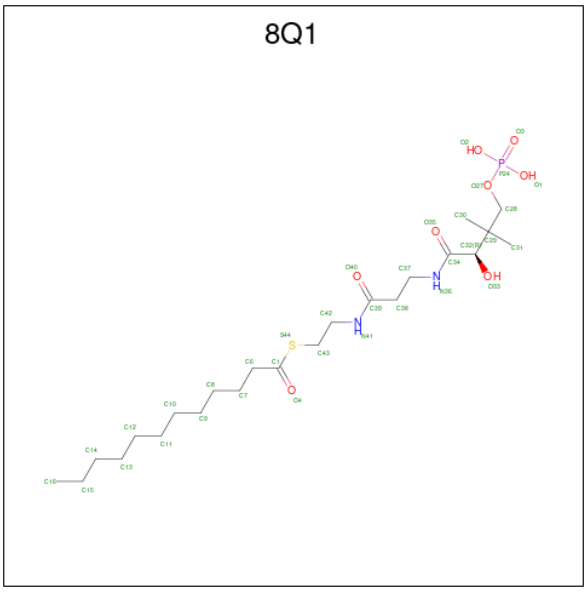
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 10 6 4	0	0
12	A	1	Total C O 10 6 4	0	0

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



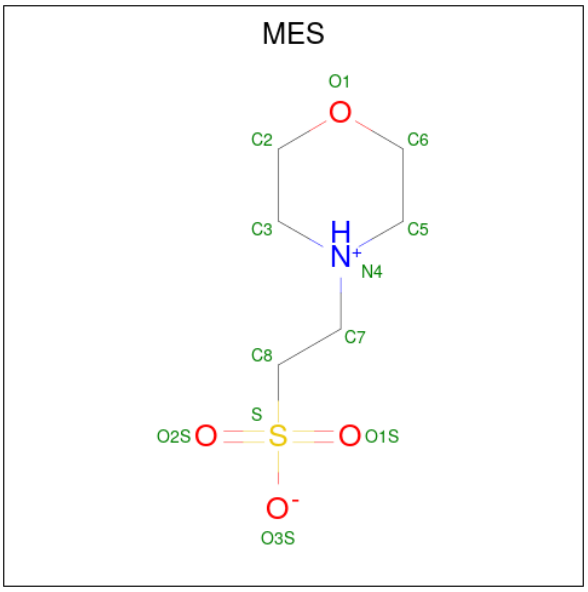
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 20 10 2 8	0	0

- 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: $C_{23}H_{45}N_2O_8PS$).



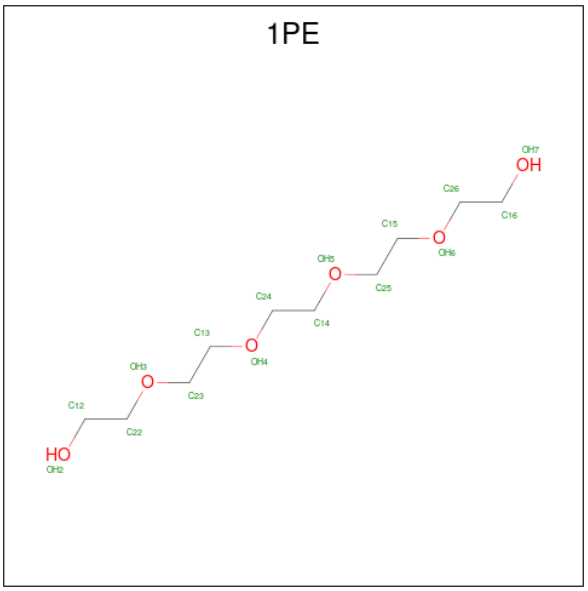
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	S	0	0
			34	23	2	7	1	1		

- 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	0	0
			12	6	1	4	1		

- 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 16 10 6	0	0

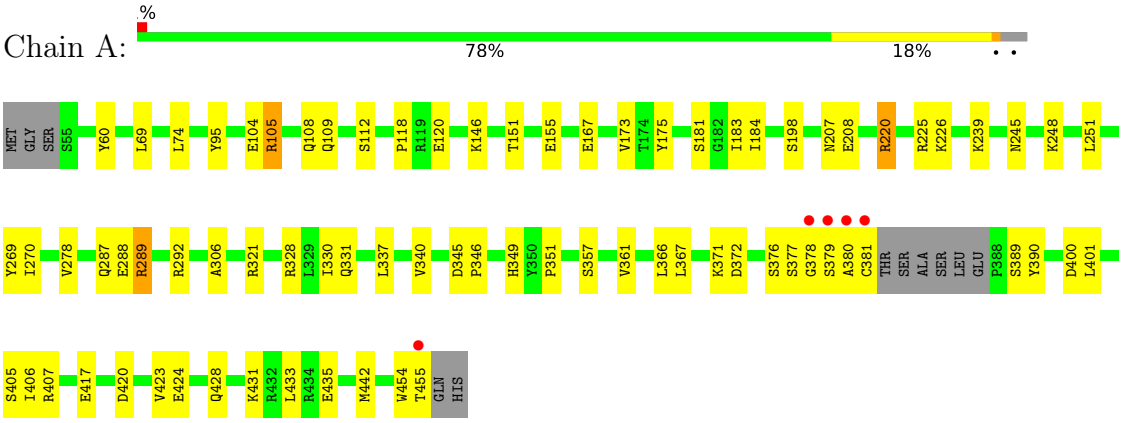
- Molecule 17 is water.

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

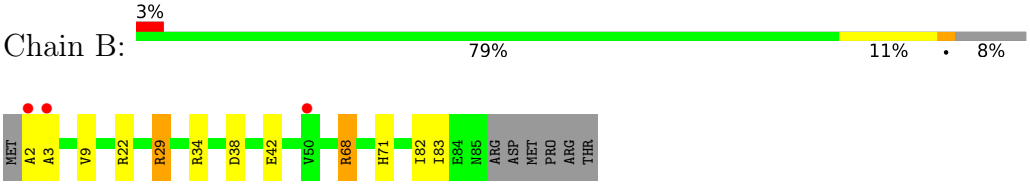
3 Residue-property plots (i)

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.

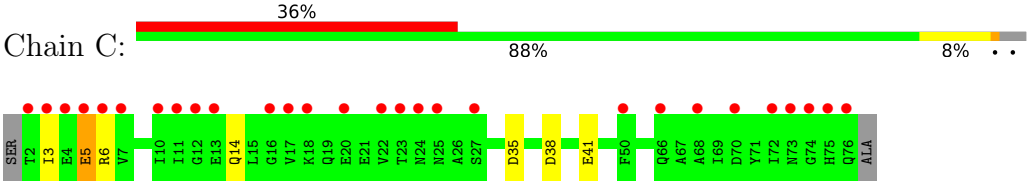
• Molecule 1: Cysteine desulfurase, mitochondrial



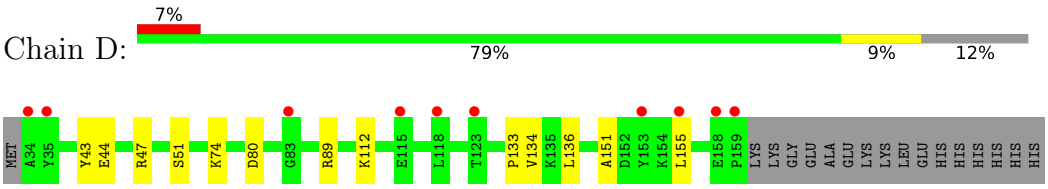
• Molecule 2: LYR motif-containing protein 4



• 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	86.35Å 86.35Å 245.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 1.79 48.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-1.79) 100.0 (48.93-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.159 , 0.189 0.159 , 0.188	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)	0.36 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	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.*

[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, EDO, PGE, PG4, PLP, PEG, P15, 8Q1, MES, EDT, DTT, GOL

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	0.98	4/3289 (0.1%)	0.86	4/4452 (0.1%)
2	B	0.91	0/756	0.86	3/1014 (0.3%)
3	C	0.56	0/539	0.67	1/735 (0.1%)
4	D	0.74	1/986 (0.1%)	0.77	2/1336 (0.1%)
All	All	0.90	5/5570 (0.1%)	0.83	10/7537 (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	1
3	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105[A]	ARG	CZ-NH1	-5.83	1.25	1.33
1	A	105[B]	ARG	CZ-NH1	-5.83	1.25	1.33
1	A	95	TYR	CG-CD2	5.63	1.46	1.39
1	A	423	VAL	CB-CG1	5.52	1.64	1.52
4	D	74	LYS	CD-CE	5.46	1.64	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220[A]	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	A	220[B]	ARG	NE-CZ-NH1	-6.37	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	29	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	B	29	ARG	NE-CZ-NH1	5.92	123.26	120.30
4	D	80	ASP	CB-CG-OD1	5.70	123.42	118.30
4	D	89	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	372	ASP	CB-CG-OD1	5.27	123.05	118.30
2	B	68	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	C	35	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	289	ARG	CG-CD-NE	-5.16	100.97	111.80

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 (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	3170	0	3192	94	0
2	B	723	0	764	20	0
3	C	535	0	472	7	0
4	D	965	0	956	11	0
5	A	15	0	7	0	0
6	A	30	0	39	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	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.

All (155) 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
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
1:A:287:GLN:HG3	7:A:547:EDO:H11	1.56	0.88
1:A:104:GLU:O	7:A:517:EDO:H22	1.78	0.84
9:A:519:PG4:H12	17:A:772:HOH:O	1.76	0.84
2:B:29:ARG:HH21	13:B:108:EDT:H061	1.42	0.83
4:D:51:SER:H	7:D:201:EDO:H11	1.43	0.83
1:A:105[A]:ARG:HG2	7:A:511:EDO:H11	1.62	0.80
1:A:337:LEU:O	10:A:526:P15:H131	1.85	0.76
7:A:507:EDO:H11	4:D:44:GLU:HG2	1.69	0.75
1:A:349:HIS:H	7:A:552:EDO:H21	1.52	0.74
2:B:68:ARG:NH1	8:B:106:PEG:H22	2.02	0.73
1:A:357[B]:SER:HG	1:A:405[B]:SER:HG	1.18	0.72
1:A:109:GLN:HE22	12:A:543:PGE:H5	1.54	0.71
1:A:175:TYR:CD1	8:A:531:PEG:H11	2.23	0.70
1:A:245:ASN:ND2	11:A:533:DTT:H2	2.02	0.70
2:B:68:ARG:HD3	8:B:106:PEG:H11	1.74	0.69
1:A:239[A]:LYS:HE2	17:A:673:HOH:O	1.92	0.69
1:A:340:VAL:O	10:A:526:P15:H122	1.94	0.68
1:A:330:ILE:HD12	12:A:534:PGE:H1	1.76	0.68
1:A:270:ILE:HD13	1:A:278[B]:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:OD2	7:A:535:EDO:H11	1.95	0.66
2:B:3:ALA:HA	7:B:110:EDO:H11	1.78	0.66
17:A:783:HOH:O	7:B:101:EDO:H12	1.95	0.65
1:A:417[B]:GLU:HA	7:A:535:EDO:H12	1.80	0.63
1:A:118:PRO:HB2	7:A:517:EDO:H11	1.80	0.63
1:A:371:LYS:HB3	7:A:507:EDO:H22	1.81	0.63
2:B:29:ARG:NH2	13:B:108:EDT:H041	2.14	0.63
1:A:208[B]:GLU:OE2	1:A:389:SER:OG	2.17	0.62
1:A:371:LYS:HD3	7:A:507:EDO:H22	1.82	0.62
2:B:29:ARG:HH21	13:B:108:EDT:H041	1.63	0.62
1:A:351:PRO:HA	12:A:534:PGE:H2	1.82	0.61
1:A:109:GLN:HE22	12:A:543:PGE:C5	2.14	0.61
1:A:109:GLN:HE22	12:A:543:PGE:C6	2.13	0.61
3:C:3:ILE:HG23	3:C:5:GLU:H	1.65	0.61
1:A:248:LYS:HE3	7:A:523:EDO:H22	1.83	0.60
1:A:292:ARG:HH22	7:A:514:EDO:C1	2.15	0.60
1:A:225:ARG:NH1	6:A:505:GOL:O1	2.29	0.59
3:C:38:ASP:OD2	15:C:302:MES:H32	2.02	0.59
1:A:167:GLU:OE1	8:A:531:PEG:H42	2.01	0.59
1:A:108:GLN:HB2	7:A:517:EDO:H21	1.84	0.58
1:A:417[A]:GLU:HA	7:A:535:EDO:H12	1.85	0.58
4:D:151:ALA:O	4:D:155:LEU:HD13	2.04	0.57
1:A:105[A]:ARG:CG	7:A:511:EDO:H11	2.32	0.57
1:A:377:SER:HB2	1:A:406[B]:ILE:HG22	1.86	0.57
1:A:109:GLN:HE22	12:A:543:PGE:H62	1.69	0.57
1:A:292:ARG:HH22	7:A:514:EDO:H11	1.69	0.57
7:A:554:EDO:H21	17:A:650:HOH:O	2.04	0.57
1:A:381:CYS:HA	1:A:407:ARG:NH1	2.12	0.57
8:A:518:PEG:H22	17:A:838:HOH:O	2.04	0.56
1:A:340:VAL:H	10:A:526:P15:C13	2.19	0.56
1:A:366:LEU:HD23	1:A:406[A]:ILE:HG13	1.88	0.56
3:C:41:GLU:HG2	8:C:305:PEG:H22	1.87	0.56
10:A:526:P15:H111	17:A:737:HOH:O	2.06	0.55
1:A:431:LYS:HE2	7:A:554:EDO:H12	1.87	0.55
1:A:330:ILE:CD1	12:A:534:PGE:H1	2.36	0.55
1:A:340:VAL:HB	10:A:526:P15:H133	1.88	0.55
1:A:400:ASP:HB2	7:A:522:EDO:H11	1.89	0.55
1:A:208[A]:GLU:HG2	1:A:379:SER:O	2.07	0.54
1:A:351:PRO:HB3	12:A:534:PGE:H3	1.90	0.54
12:A:534:PGE:O1	17:A:601:HOH:O	2.11	0.54
1:A:371:LYS:HB3	7:A:507:EDO:C2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HD21	10:A:526:P15:H51	1.89	0.54
7:A:506:EDO:H22	7:A:507:EDO:H11	1.88	0.54
1:A:109:GLN:NE2	12:A:543:PGE:H5	2.23	0.53
1:A:349:HIS:CE1	12:A:534:PGE:H22	2.44	0.52
1:A:346:PRO:HG3	8:A:532:PEG:H11	1.91	0.52
11:A:533:DTT:O2	8:A:550:PEG:H32	2.08	0.52
2:B:34[B]:ARG:NE	17:B:204:HOH:O	2.43	0.52
4:D:51:SER:N	7:D:201:EDO:H11	2.21	0.51
4:D:134:VAL:HG13	17:D:339:HOH:O	2.10	0.51
1:A:435:GLU:HG3	6:A:504:GOL:H32	1.92	0.51
2:B:68:ARG:HH11	8:B:106:PEG:C2	2.08	0.51
1:A:146:LYS:HB3	1:A:198[A]:SER:HB3	1.93	0.50
1:A:292:ARG:NH1	7:A:514:EDO:H12	2.25	0.50
1:A:390:TYR:CG	7:A:510:EDO:H12	2.47	0.49
2:B:2:ALA:N	17:B:205:HOH:O	2.44	0.49
1:A:292:ARG:NH2	7:A:514:EDO:H12	2.28	0.49
12:A:534:PGE:H5	17:A:601:HOH:O	2.12	0.49
1:A:151:THR:OG1	1:A:155:GLU:HG3	2.13	0.48
1:A:340:VAL:H	10:A:526:P15:H133	1.78	0.48
1:A:376[A]:SER:OG	1:A:379:SER:HB3	2.12	0.48
1:A:207:ASN:HD22	1:A:381:CYS:N	2.11	0.48
2:B:34[B]:ARG:HG2	17:B:204:HOH:O	2.12	0.48
9:A:519:PG4:H62	9:A:519:PG4:H31	1.95	0.48
4:D:133:PRO:HA	4:D:136:LEU:HG	1.95	0.48
7:A:538:EDO:H12	17:A:752:HOH:O	2.13	0.48
3:C:14:GLN:O	7:C:304:EDO:H21	2.13	0.48
1:A:321[B]:ARG:HH12	6:A:503:GOL:HO2	1.62	0.47
1:A:367:LEU:HD11	1:A:377:SER:HB3	1.96	0.47
2:B:38:ASP:HB3	8:B:104:PEG:C2	2.45	0.47
1:A:181:SER:HB2	1:A:345:ASP:HB2	1.96	0.47
1:A:60:TYR:HB3	7:B:101:EDO:H21	1.96	0.47
12:A:534:PGE:H6	17:A:603:HOH:O	2.13	0.47
13:B:108:EDT:O18	13:B:108:EDT:H042	2.10	0.47
1:A:69[A]:LEU:HD13	1:A:74:LEU:HB2	1.96	0.47
1:A:428:GLN:OE1	7:A:530:EDO:O1	2.32	0.47
2:B:22:ARG:HD2	7:B:103:EDO:H12	1.97	0.47
3:C:41:GLU:HB2	7:C:304:EDO:H11	1.95	0.47
1:A:349:HIS:H	7:A:552:EDO:C2	2.22	0.47
6:A:504:GOL:O1	7:A:554:EDO:H22	2.15	0.46
1:A:442:MET:HG3	8:A:548:PEG:H32	1.95	0.46
2:B:29:ARG:NH2	13:B:108:EDT:H061	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ARG:HG2	13:B:108:EDT:H091	1.97	0.46
1:A:349:HIS:ND1	12:A:534:PGE:O2	2.48	0.46
12:A:543:PGE:H2	17:B:260:HOH:O	2.16	0.46
7:A:515:EDO:C2	8:B:104:PEG:H12	2.45	0.46
1:A:248:LYS:HA	7:A:513:EDO:H11	1.98	0.45
7:A:507:EDO:H12	4:D:43:TYR:CD2	2.51	0.45
1:A:306:ALA:HB2	12:A:543:PGE:H52	1.98	0.45
2:B:38:ASP:HB3	8:B:104:PEG:H22	1.99	0.45
1:A:331:GLN:NE2	17:A:612:HOH:O	2.50	0.45
1:A:292:ARG:CZ	7:A:514:EDO:H12	2.47	0.45
1:A:306:ALA:CB	12:A:543:PGE:H52	2.47	0.44
8:A:549:PEG:H42	17:A:696:HOH:O	2.18	0.44
1:A:207:ASN:HD22	1:A:381:CYS:H	1.65	0.44
1:A:357[B]:SER:OG	1:A:405[B]:SER:OG	2.00	0.44
1:A:289:ARG:H	7:A:553:EDO:C2	2.30	0.44
1:A:431:LYS:CE	7:A:554:EDO:H12	2.48	0.44
1:A:292:ARG:NH2	7:A:514:EDO:C1	2.79	0.43
8:A:532:PEG:H11	8:A:532:PEG:H32	1.67	0.43
1:A:220[B]:ARG:HB3	6:A:505:GOL:H31	1.99	0.43
2:B:71[B]:HIS:CE1	17:B:203:HOH:O	2.72	0.43
1:A:146:LYS:HB3	1:A:198[B]:SER:HB2	2.01	0.43
1:A:288:GLU:N	7:A:553:EDO:H21	2.34	0.43
1:A:328:ARG:HG3	9:A:520:PG4:H11	2.00	0.43
3:C:14:GLN:HB3	7:C:304:EDO:O1	2.19	0.42
1:A:454:TRP:O	1:A:455:THR:HB	2.19	0.42
3:C:3:ILE:O	3:C:6:ARG:HG3	2.19	0.42
4:D:112:LYS:HE3	16:D:202:1PE:H252	2.00	0.42
1:A:173:VAL:O	8:A:531:PEG:H22	2.20	0.42
1:A:183[B]:ILE:HG22	1:A:184:ILE:O	2.19	0.42
1:A:220[A]:ARG:HB3	6:A:505:GOL:H31	2.02	0.42
7:A:515:EDO:H21	8:B:104:PEG:H12	2.02	0.41
1:A:226:LYS:HA	6:A:551:GOL:H12	2.02	0.41
4:D:51:SER:H	7:D:201:EDO:C1	2.23	0.41
1:A:361[B]:VAL:HG23	1:A:433:LEU:HB3	2.02	0.41
7:A:507:EDO:H12	4:D:43:TYR:CE2	2.55	0.41
7:B:109:EDO:H11	17:B:248:HOH:O	2.20	0.41
4:D:112:LYS:CG	16:D:202:1PE:H222	2.50	0.41
1:A:120:GLU:OE1	11:A:533:DTT:S4	2.76	0.41
1:A:424:GLU:OE1	7:A:537:EDO:H12	2.21	0.41
2:B:82:ILE:HG23	2:B:83:ILE:HG23	2.03	0.41
1:A:380:ALA:HB1	17:A:784:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLU:HB2	8:B:104:PEG:H11	2.01	0.41
10:A:526:P15:H32	17:A:616:HOH:O	2.21	0.40
1:A:292:ARG:HH12	7:A:514:EDO:H12	1.85	0.40
1:A:251:LEU:HA	1:A:269:TYR:O	2.21	0.40
7:A:516:EDO:H12	17:A:630:HOH:O	2.21	0.40
7:A:552:EDO:H22	17:A:603:HOH:O	2.22	0.40
1:A:340:VAL:H	10:A:526:P15:H132	1.85	0.40

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
3	C	49/66 (74%)	49 (100%)	0	100	100
4	D	100/118 (85%)	99 (99%)	1 (1%)	76	71
All	All	574/610 (94%)	573 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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)

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	A	542	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.55	0
7	EDO	A	539	-	3,3,3	0.47	0	2,2,2	0.23	0
5	PLP	A	501	1	15,15,16	1.42	2 (13%)	20,22,23	1.09	2 (10%)
7	EDO	A	530	-	3,3,3	0.43	0	2,2,2	0.47	0
7	EDO	A	528	-	3,3,3	0.77	0	2,2,2	0.70	0
8	PEG	B	104	-	6,6,6	0.58	0	5,5,5	0.33	0
7	EDO	B	103	-	3,3,3	0.43	0	2,2,2	0.24	0
8	PEG	A	518	-	6,6,6	0.61	0	5,5,5	0.81	0
7	EDO	A	529	-	3,3,3	0.49	0	2,2,2	0.25	0
7	EDO	A	523	-	3,3,3	0.49	0	2,2,2	0.27	0
7	EDO	C	304	-	3,3,3	0.37	0	2,2,2	0.14	0
15	MES	C	302	-	12,12,12	2.07	4 (33%)	14,16,16	2.35	4 (28%)
10	P15	A	526	-	19,19,19	0.64	0	18,18,18	0.74	0
7	EDO	A	514	-	3,3,3	1.32	0	2,2,2	0.69	0
6	GOL	A	503	-	5,5,5	0.41	0	5,5,5	0.59	0
6	GOL	A	504	-	5,5,5	0.52	0	5,5,5	0.39	0
7	EDO	A	545	-	3,3,3	0.45	0	2,2,2	0.28	0
7	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.24	0
12	PGE	A	544	-	9,9,9	0.34	0	8,8,8	0.42	0
7	EDO	A	552	-	3,3,3	0.54	0	2,2,2	0.71	0
7	EDO	A	554	-	3,3,3	0.49	0	2,2,2	0.03	0
7	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.47	0
6	GOL	A	551	-	5,5,5	0.47	0	5,5,5	0.69	0
12	PGE	A	543	-	9,9,9	0.25	0	8,8,8	0.59	0
7	EDO	A	511	-	3,3,3	0.50	0	2,2,2	0.73	0
7	EDO	B	101	-	3,3,3	0.82	0	2,2,2	0.35	0
8	PEG	B	106	-	6,6,6	0.90	0	5,5,5	0.71	0
7	EDO	A	516	-	3,3,3	0.47	0	2,2,2	0.36	0
7	EDO	A	522	-	3,3,3	0.79	0	2,2,2	0.83	0
7	EDO	A	508	-	3,3,3	0.50	0	2,2,2	0.10	0
11	DTT	A	533	-	7,7,7	0.64	0	4,8,8	1.29	0
8	PEG	A	550	-	6,6,6	0.47	0	5,5,5	0.17	0
7	EDO	B	111	-	3,3,3	0.50	0	2,2,2	0.19	0
7	EDO	A	536	-	3,3,3	0.53	0	2,2,2	1.07	0
7	EDO	B	110	-	3,3,3	0.53	0	2,2,2	0.02	0
7	EDO	B	109	-	3,3,3	0.43	0	2,2,2	0.24	0
8	PEG	A	548	-	6,6,6	0.50	0	5,5,5	0.51	0
6	GOL	D	204	-	5,5,5	0.70	0	5,5,5	0.35	0
9	PG4	A	520	-	12,12,12	0.59	0	11,11,11	0.57	0
8	PEG	A	527	-	6,6,6	0.52	0	5,5,5	0.53	0
7	EDO	A	512	-	3,3,3	0.42	0	2,2,2	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	541	-	3,3,3	0.51	0	2,2,2	0.39	0
7	EDO	A	547	-	3,3,3	0.47	0	2,2,2	0.73	0
8	PEG	A	549	-	6,6,6	0.51	0	5,5,5	0.28	0
7	EDO	A	535	-	3,3,3	0.42	0	2,2,2	0.58	0
7	EDO	A	515	-	3,3,3	0.59	0	2,2,2	0.26	0
7	EDO	A	509	-	3,3,3	0.74	0	2,2,2	1.33	0
7	EDO	B	102	-	3,3,3	0.50	0	2,2,2	0.83	0
8	PEG	C	305	-	6,6,6	0.51	0	5,5,5	0.36	0
13	EDT	B	108	-	19,19,19	1.29	1 (5%)	24,24,24	1.41	3 (12%)
7	EDO	A	546	-	3,3,3	0.83	0	2,2,2	1.05	0
7	EDO	D	201	-	3,3,3	0.53	0	2,2,2	0.68	0
7	EDO	A	507	-	3,3,3	1.73	1 (33%)	2,2,2	1.46	1 (50%)
8	PEG	A	531	-	6,6,6	0.51	0	5,5,5	0.52	0
7	EDO	A	524	-	3,3,3	0.44	0	2,2,2	0.42	0
6	GOL	A	502	-	5,5,5	0.64	0	5,5,5	1.84	1 (20%)
7	EDO	B	107	-	3,3,3	0.52	0	2,2,2	0.27	0
6	GOL	A	505	-	5,5,5	0.96	0	5,5,5	0.81	0
12	PGE	A	534	-	9,9,9	0.47	0	8,8,8	0.64	0
7	EDO	A	513	-	3,3,3	0.51	0	2,2,2	0.56	0
7	EDO	A	553	-	3,3,3	0.39	0	2,2,2	0.36	0
7	EDO	A	517	-	3,3,3	0.28	0	2,2,2	0.40	0
7	EDO	B	105	-	3,3,3	0.45	0	2,2,2	0.35	0
8	PEG	A	521	-	6,6,6	0.48	0	5,5,5	0.67	0
7	EDO	D	203	-	3,3,3	0.52	0	2,2,2	0.16	0
7	EDO	D	206	-	3,3,3	0.43	0	2,2,2	0.53	0
7	EDO	A	506	-	3,3,3	0.43	0	2,2,2	0.19	0
7	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.20	0
7	EDO	A	537	-	3,3,3	0.44	0	2,2,2	0.14	0
14	8Q1	C	301	3	27,33,34	2.03	6 (22%)	32,40,43	1.84	7 (21%)
9	PG4	A	519	-	12,12,12	0.52	0	11,11,11	0.53	0
7	EDO	A	540	-	3,3,3	0.47	0	2,2,2	0.40	0
16	1PE	D	202	-	15,15,15	0.53	0	14,14,14	0.30	0
7	EDO	A	525	-	3,3,3	0.47	0	2,2,2	0.19	0
7	EDO	A	538	-	3,3,3	0.56	0	2,2,2	0.48	0
8	PEG	A	532	-	6,6,6	0.48	0	5,5,5	0.59	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	542	-	-	1/1/1/1	-
7	EDO	D	205	-	-	0/1/1/1	-
7	EDO	A	539	-	-	1/1/1/1	-
5	PLP	A	501	1	-	0/6/6/8	0/1/1/1
7	EDO	A	530	-	-	0/1/1/1	-
7	EDO	A	528	-	-	1/1/1/1	-
8	PEG	B	104	-	-	3/4/4/4	-
7	EDO	B	103	-	-	1/1/1/1	-
8	PEG	A	518	-	-	1/4/4/4	-
7	EDO	A	529	-	-	1/1/1/1	-
7	EDO	A	523	-	-	1/1/1/1	-
7	EDO	C	304	-	-	1/1/1/1	-
15	MES	C	302	-	-	3/6/14/14	0/1/1/1
10	P15	A	526	-	-	10/17/17/17	-
7	EDO	A	514	-	-	1/1/1/1	-
6	GOL	A	503	-	-	4/4/4/4	-
6	GOL	A	504	-	-	4/4/4/4	-
7	EDO	A	545	-	-	1/1/1/1	-
7	EDO	C	303	-	-	1/1/1/1	-
12	PGE	A	544	-	-	3/7/7/7	-
7	EDO	A	552	-	-	0/1/1/1	-
7	EDO	A	554	-	-	0/1/1/1	-
7	EDO	A	510	-	-	1/1/1/1	-
6	GOL	A	551	-	-	4/4/4/4	-
12	PGE	A	543	-	-	4/7/7/7	-
7	EDO	A	511	-	-	0/1/1/1	-
7	EDO	B	101	-	-	1/1/1/1	-
8	PEG	B	106	-	-	2/4/4/4	-
7	EDO	A	516	-	-	1/1/1/1	-
7	EDO	A	522	-	-	0/1/1/1	-
7	EDO	A	508	-	-	1/1/1/1	-
11	DTT	A	533	-	-	3/8/8/8	-
8	PEG	A	550	-	-	1/4/4/4	-
7	EDO	B	111	-	-	0/1/1/1	-
7	EDO	A	536	-	-	1/1/1/1	-
7	EDO	B	110	-	-	1/1/1/1	-
7	EDO	B	109	-	-	1/1/1/1	-
8	PEG	A	548	-	-	2/4/4/4	-
6	GOL	D	204	-	-	0/4/4/4	-
9	PG4	A	520	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	A	527	-	-	1/4/4/4	-
7	EDO	A	512	-	-	1/1/1/1	-
7	EDO	A	541	-	-	0/1/1/1	-
7	EDO	A	547	-	-	1/1/1/1	-
8	PEG	A	549	-	-	3/4/4/4	-
7	EDO	A	535	-	-	1/1/1/1	-
7	EDO	A	515	-	-	1/1/1/1	-
7	EDO	A	509	-	-	0/1/1/1	-
7	EDO	B	102	-	-	1/1/1/1	-
8	PEG	C	305	-	-	1/4/4/4	-
13	EDT	B	108	-	-	12/21/21/21	-
7	EDO	A	546	-	-	0/1/1/1	-
7	EDO	D	201	-	-	1/1/1/1	-
7	EDO	A	507	-	-	1/1/1/1	-
8	PEG	A	531	-	-	2/4/4/4	-
7	EDO	A	524	-	-	1/1/1/1	-
6	GOL	A	502	-	-	1/4/4/4	-
7	EDO	B	107	-	-	0/1/1/1	-
6	GOL	A	505	-	-	4/4/4/4	-
12	PGE	A	534	-	-	6/7/7/7	-
7	EDO	A	513	-	-	1/1/1/1	-
7	EDO	A	553	-	-	1/1/1/1	-
7	EDO	A	517	-	-	1/1/1/1	-
7	EDO	B	105	-	-	0/1/1/1	-
8	PEG	A	521	-	-	1/4/4/4	-
7	EDO	D	203	-	-	1/1/1/1	-
7	EDO	D	206	-	-	0/1/1/1	-
7	EDO	A	506	-	-	1/1/1/1	-
7	EDO	C	306	-	-	1/1/1/1	-
7	EDO	A	537	-	-	0/1/1/1	-
14	8Q1	C	301	3	-	1/38/40/41	-
9	PG4	A	519	-	-	4/10/10/10	-
7	EDO	A	540	-	-	1/1/1/1	-
16	1PE	D	202	-	-	11/13/13/13	-
7	EDO	A	525	-	-	1/1/1/1	-
7	EDO	A	538	-	-	0/1/1/1	-
8	PEG	A	532	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	C39-N41	5.21	1.45	1.33
14	C	301	8Q1	C34-N36	5.06	1.44	1.33
15	C	302	MES	C8-S	4.59	1.84	1.77
5	A	501	PLP	C3-C2	-3.68	1.37	1.40
14	C	301	8Q1	C6-C1	3.22	1.54	1.50
15	C	302	MES	O1S-S	2.73	1.53	1.45
15	C	302	MES	C7-N4	2.72	1.53	1.47
14	C	301	8Q1	C12-C13	-2.69	1.36	1.51
14	C	301	8Q1	C1-S44	2.56	1.82	1.76
7	A	507	EDO	O1-C1	-2.56	1.28	1.42
5	A	501	PLP	C6-N1	2.32	1.39	1.34
14	C	301	8Q1	C15-C14	-2.16	1.36	1.51
13	B	108	EDT	C11-C12	2.07	1.55	1.51
15	C	302	MES	C7-C8	2.03	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	302	MES	O1S-S-C8	6.01	114.15	106.92
14	C	301	8Q1	C42-N41-C39	-4.71	114.10	122.84
14	C	301	8Q1	C37-N36-C34	-4.43	114.69	122.59
13	B	108	EDT	C11-N8-C9	3.91	120.38	111.54
15	C	302	MES	O3S-S-O2S	-3.56	102.58	111.27
6	A	502	GOL	C3-C2-C1	-3.50	98.11	111.70
14	C	301	8Q1	C38-C37-N36	-3.37	105.10	111.90
14	C	301	8Q1	C8-C7-C6	-3.28	101.41	113.19
14	C	301	8Q1	C30-C29-C32	3.12	114.22	108.82
15	C	302	MES	C2-C3-N4	3.07	114.76	110.10
5	A	501	PLP	C6-C5-C4	2.56	120.17	118.16
5	A	501	PLP	C5A-C5-C6	-2.49	115.28	119.37
14	C	301	8Q1	C31-C29-C32	2.40	112.98	108.82
15	C	302	MES	O3S-S-C8	2.34	109.55	105.77
13	B	108	EDT	O14-C12-O13	-2.32	117.52	123.30
14	C	301	8Q1	O40-C39-N41	-2.21	118.84	123.01
13	B	108	EDT	C11-N8-C7	2.11	117.08	111.94
7	A	507	EDO	O2-C2-C1	-2.04	97.23	111.91

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	504	GOL	C1-C2-C3-O3
6	A	551	GOL	C1-C2-C3-O3
6	A	551	GOL	O2-C2-C3-O3
7	A	513	EDO	O1-C1-C2-O2
11	A	533	DTT	C1-C2-C3-C4
11	A	533	DTT	C2-C3-C4-S4
13	B	108	EDT	C1-C2-N3-C4
13	B	108	EDT	N8-C11-C12-O14
15	C	302	MES	C8-C7-N4-C3
15	C	302	MES	N4-C7-C8-S
12	A	544	PGE	C3-C4-O3-C5
12	A	544	PGE	C1-C2-O2-C3
13	B	108	EDT	C10-C9-N8-C11
9	A	520	PG4	O1-C1-C2-O2
13	B	108	EDT	N8-C11-C12-O13
9	A	520	PG4	O2-C3-C4-O3
10	A	526	P15	O5-C11-C12-O6
10	A	526	P15	O5-C10-C9-O4
8	A	548	PEG	O1-C1-C2-O2
16	D	202	1PE	OH6-C15-C25-OH5
16	D	202	1PE	OH4-C13-C23-OH3
13	B	108	EDT	O16-C10-C9-N8
12	A	544	PGE	O2-C3-C4-O3
16	D	202	1PE	OH5-C14-C24-OH4
8	A	518	PEG	O1-C1-C2-O2
8	A	531	PEG	O2-C3-C4-O4
8	A	549	PEG	O1-C1-C2-O2
8	A	549	PEG	O2-C3-C4-O4
16	D	202	1PE	OH7-C16-C26-OH6
7	A	517	EDO	O1-C1-C2-O2
8	A	532	PEG	C1-C2-O2-C3
8	A	548	PEG	O2-C3-C4-O4
8	A	550	PEG	O1-C1-C2-O2
8	B	104	PEG	O2-C3-C4-O4
10	A	526	P15	OXT-C1-C2-O1
12	A	534	PGE	O3-C5-C6-O4
9	A	520	PG4	C3-C4-O3-C5
10	A	526	P15	O1-C3-C4-O2
6	A	503	GOL	C1-C2-C3-O3
6	A	504	GOL	O1-C1-C2-C3
6	A	505	GOL	C1-C2-C3-O3
6	A	551	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	B	108	EDT	O18-C1-C2-N3
13	B	108	EDT	O15-C10-C9-N8
6	A	504	GOL	O1-C1-C2-O2
6	A	504	GOL	O2-C2-C3-O3
6	A	551	GOL	O1-C1-C2-O2
7	A	506	EDO	O1-C1-C2-O2
7	A	510	EDO	O1-C1-C2-O2
7	A	516	EDO	O1-C1-C2-O2
7	A	524	EDO	O1-C1-C2-O2
7	A	536	EDO	O1-C1-C2-O2
7	C	303	EDO	O1-C1-C2-O2
7	C	306	EDO	O1-C1-C2-O2
13	B	108	EDT	O17-C1-C2-N3
12	A	543	PGE	O1-C1-C2-O2
8	A	531	PEG	C1-C2-O2-C3
8	B	106	PEG	O1-C1-C2-O2
6	A	503	GOL	O2-C2-C3-O3
7	A	512	EDO	O1-C1-C2-O2
7	A	525	EDO	O1-C1-C2-O2
7	A	528	EDO	O1-C1-C2-O2
10	A	526	P15	C6-C5-O2-C4
15	C	302	MES	C8-C7-N4-C5
12	A	543	PGE	C3-C4-O3-C5
13	B	108	EDT	C7-C6-N3-C2
9	A	520	PG4	O4-C7-C8-O5
7	A	529	EDO	O1-C1-C2-O2
7	A	545	EDO	O1-C1-C2-O2
8	B	104	PEG	C1-C2-O2-C3
9	A	520	PG4	C6-C5-O3-C4
10	A	526	P15	C10-C9-O4-C8
13	B	108	EDT	C7-C6-N3-C4
16	D	202	1PE	C14-C24-OH4-C13
8	A	549	PEG	C4-C3-O2-C2
8	B	104	PEG	C4-C3-O2-C2
8	A	527	PEG	C1-C2-O2-C3
8	B	106	PEG	C4-C3-O2-C2
7	A	535	EDO	O1-C1-C2-O2
7	B	102	EDO	O1-C1-C2-O2
16	D	202	1PE	C15-C25-OH5-C14
11	A	533	DTT	O3-C3-C4-S4
9	A	519	PG4	O1-C1-C2-O2
16	D	202	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
8	A	521	PEG	C4-C3-O2-C2
16	D	202	1PE	C13-C23-OH3-C22
10	A	526	P15	O2-C5-C6-O3
10	A	526	P15	C3-C4-O2-C5
13	B	108	EDT	C10-C9-N8-C7
7	A	508	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2
7	A	515	EDO	O1-C1-C2-O2
7	A	542	EDO	O1-C1-C2-O2
7	B	109	EDO	O1-C1-C2-O2
7	B	110	EDO	O1-C1-C2-O2
8	A	532	PEG	O1-C1-C2-O2
6	A	505	GOL	O2-C2-C3-O3
12	A	534	PGE	O2-C3-C4-O3
10	A	526	P15	C5-C6-O3-C7
12	A	534	PGE	C1-C2-O2-C3
7	A	523	EDO	O1-C1-C2-O2
7	A	539	EDO	O1-C1-C2-O2
7	D	201	EDO	O1-C1-C2-O2
8	C	305	PEG	C1-C2-O2-C3
12	A	534	PGE	O1-C1-C2-O2
7	A	553	EDO	O1-C1-C2-O2
7	B	103	EDO	O1-C1-C2-O2
6	A	505	GOL	O1-C1-C2-C3
10	A	526	P15	C8-C7-O3-C6
9	A	519	PG4	C4-C3-O2-C2
12	A	534	PGE	C6-C5-O3-C4
14	C	301	8Q1	C6-C7-C8-C9
6	A	503	GOL	O1-C1-C2-O2
6	A	505	GOL	O1-C1-C2-O2
9	A	520	PG4	O3-C5-C6-O4
16	D	202	1PE	C16-C26-OH6-C15
12	A	543	PGE	O2-C3-C4-O3
12	A	543	PGE	C1-C2-O2-C3
16	D	202	1PE	C24-C14-OH5-C25
12	A	534	PGE	C4-C3-O2-C2
13	B	108	EDT	C6-C7-N8-C9
7	A	507	EDO	O1-C1-C2-O2
7	A	540	EDO	O1-C1-C2-O2
7	A	547	EDO	O1-C1-C2-O2
7	C	304	EDO	O1-C1-C2-O2
7	D	203	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	502	GOL	O1-C1-C2-C3
16	D	202	1PE	OH2-C12-C22-OH3
7	B	101	EDO	O1-C1-C2-O2
9	A	519	PG4	C5-C6-O4-C7
9	A	519	PG4	O3-C5-C6-O4

There are no ring outliers.

47 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	530	EDO	1	0
8	B	104	PEG	5	0
7	B	103	EDO	1	0
8	A	518	PEG	1	0
7	A	523	EDO	1	0
7	C	304	EDO	3	0
15	C	302	MES	1	0
10	A	526	P15	9	0
7	A	514	EDO	7	0
6	A	503	GOL	1	0
6	A	504	GOL	2	0
7	A	552	EDO	3	0
7	A	554	EDO	4	0
7	A	510	EDO	1	0
6	A	551	GOL	1	0
12	A	543	PGE	8	0
7	A	511	EDO	2	0
7	B	101	EDO	2	0
8	B	106	PEG	4	0
7	A	516	EDO	1	0
7	A	522	EDO	1	0
11	A	533	DTT	4	0
8	A	550	PEG	1	0
7	B	110	EDO	1	0
7	B	109	EDO	1	0
8	A	548	PEG	1	0
9	A	520	PG4	1	0
7	A	547	EDO	1	0
8	A	549	PEG	1	0
7	A	535	EDO	3	0
7	A	515	EDO	2	0
8	C	305	PEG	1	0

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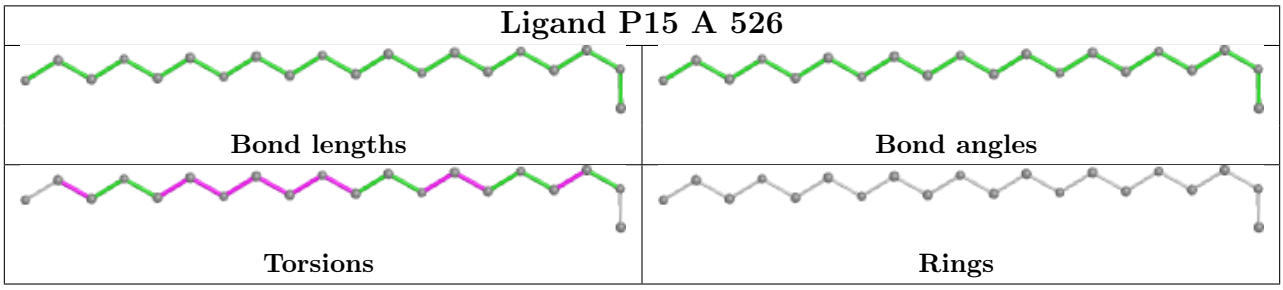
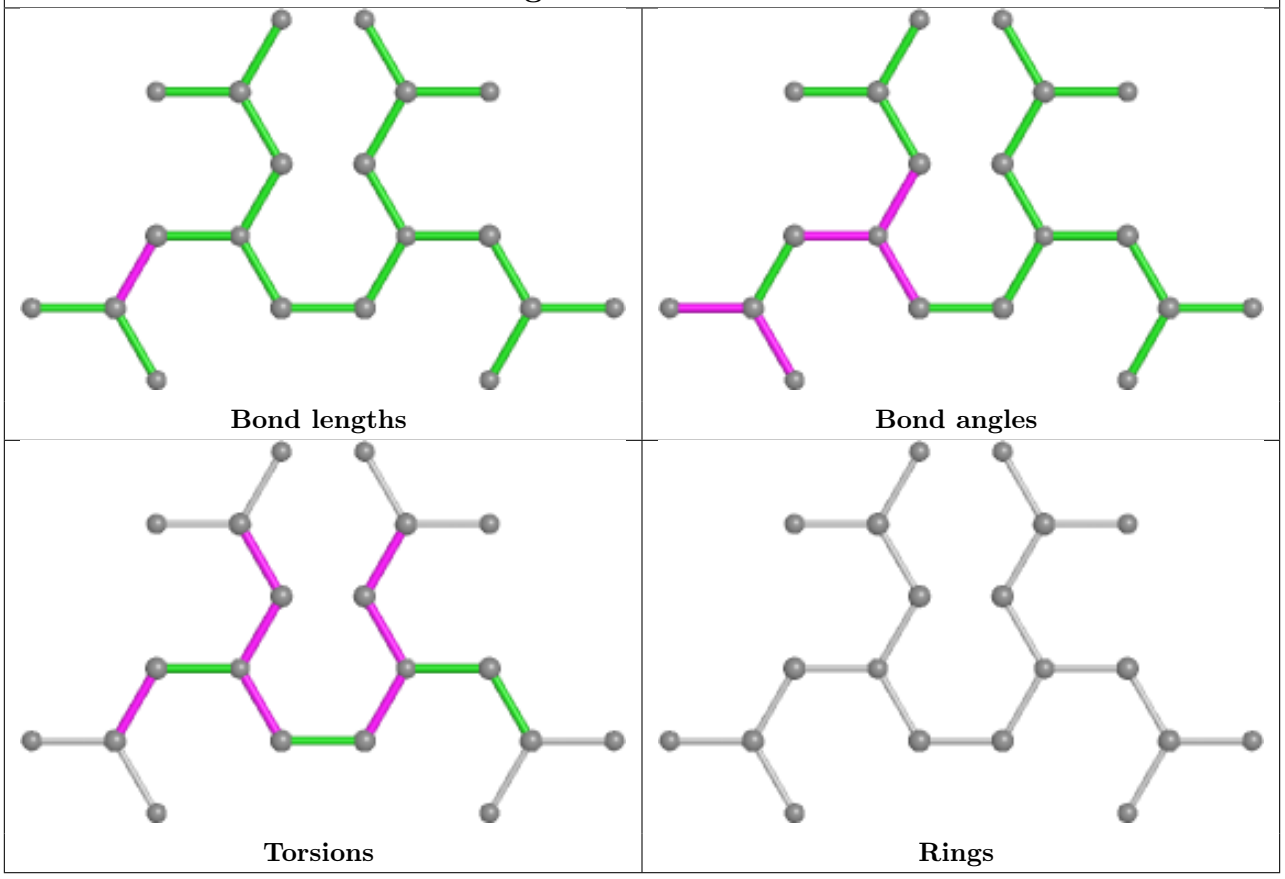
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	108	EDT	6	0
7	D	201	EDO	3	0
7	A	507	EDO	7	0
8	A	531	PEG	4	0
6	A	505	GOL	3	0
12	A	534	PGE	9	0
7	A	513	EDO	1	0
7	A	553	EDO	2	0
7	A	517	EDO	3	0
7	A	506	EDO	1	0
7	A	537	EDO	1	0
9	A	519	PG4	3	0
16	D	202	1PE	2	0
7	A	538	EDO	1	0
8	A	532	PEG	2	0

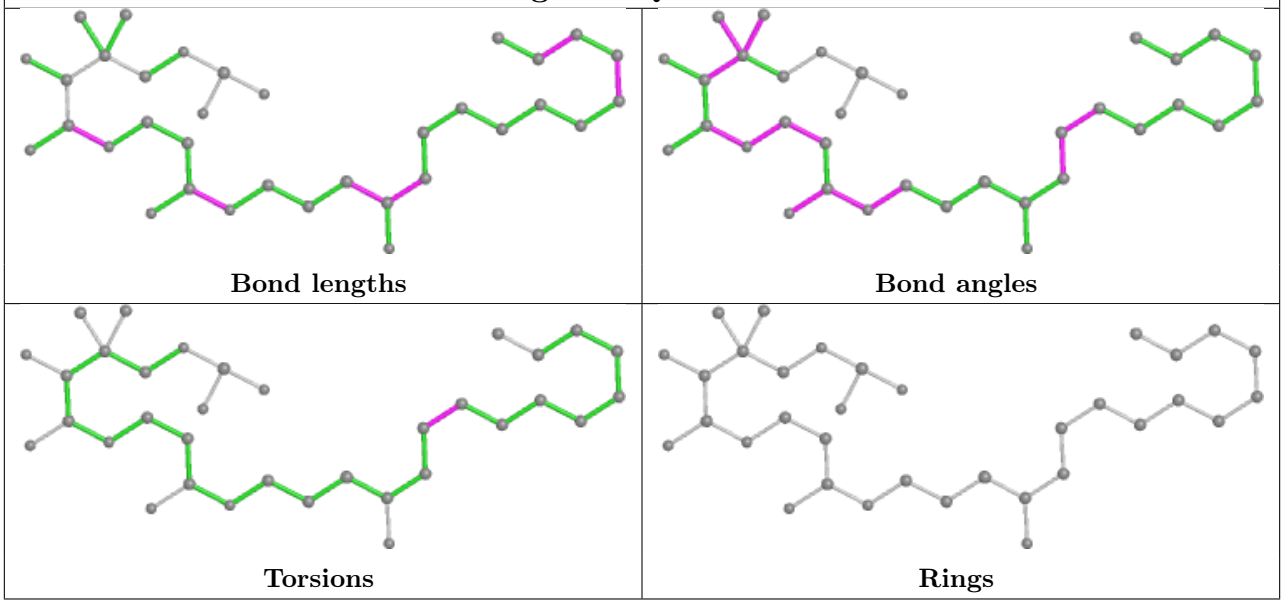
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 EDT B 108



Ligand 8Q1 C 301



5.7 Other polymers

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	395/406 (97%)	-0.23	5 (1%) 77 74	11, 18, 45, 90	7 (1%)
2	B	84/91 (92%)	-0.26	3 (3%) 42 37	13, 22, 45, 63	0
3	C	75/77 (97%)	1.56	28 (37%) 0 0	27, 50, 79, 98	0
4	D	126/143 (88%)	0.26	10 (7%) 12 9	17, 34, 59, 110	0
All	All	680/717 (94%)	0.06	46 (6%) 17 13	11, 23, 60, 110	7 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35[A]	TYR	6.6
3	C	17	VAL	6.1
1	A	381	CYS	5.7
3	C	2	THR	5.6
1	A	380	ALA	5.3
4	D	159	PRO	4.9
3	C	3	ILE	4.6
2	B	3	ALA	4.5
3	C	72	ILE	4.5
3	C	22	VAL	4.4
3	C	20	GLU	4.3
3	C	7	VAL	4.3
4	D	155	LEU	4.3
4	D	34[A]	ALA	4.1
3	C	23	THR	4.0
3	C	73	ASN	4.0
1	A	455	THR	3.9
3	C	66	GLN	3.9
3	C	12	GLY	3.6
3	C	11	ILE	3.5
3	C	68	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	10	ILE	3.4
3	C	50	PHE	3.3
4	D	123	THR	3.1
1	A	379	SER	3.1
3	C	6	ARG	3.1
2	B	2	ALA	3.1
4	D	153	TYR	2.9
3	C	24	ASN	2.9
3	C	76	GLN	2.8
3	C	16	GLY	2.7
4	D	118	LEU	2.7
3	C	74	GLY	2.7
4	D	158	GLU	2.5
2	B	50	VAL	2.5
1	A	378	GLY	2.4
3	C	25	ASN	2.4
3	C	18	LYS	2.4
4	D	115	GLU	2.4
3	C	75	HIS	2.4
3	C	5	GLU	2.3
3	C	13	GLU	2.2
3	C	4	GLU	2.2
4	D	83	GLY	2.1
3	C	70	ASP	2.1
3	C	27	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
7	EDO	C	306	4/4	0.51	0.27	65,69,69,69	0
8	PEG	C	305	7/7	0.57	0.27	65,71,73,73	0
13	EDT	B	108	20/20	0.58	0.35	47,57,71,72	20
7	EDO	A	529	4/4	0.60	0.46	84,85,87,87	0
7	EDO	D	203	4/4	0.62	0.33	57,61,63,66	0
7	EDO	B	109	4/4	0.62	0.27	74,75,76,77	0
7	EDO	A	553	4/4	0.62	0.37	69,69,73,76	0
7	EDO	A	540	4/4	0.65	0.21	71,73,76,78	0
8	PEG	A	527	7/7	0.66	0.20	61,64,67,68	0
8	PEG	A	550	7/7	0.67	0.27	69,73,75,76	0
7	EDO	A	554	4/4	0.68	0.30	85,85,85,85	0
9	PG4	A	519	13/13	0.70	0.30	31,51,58,61	13
12	PGE	A	544	10/10	0.70	0.19	78,80,82,82	0
7	EDO	A	539	4/4	0.70	0.17	61,62,63,65	0
7	EDO	A	515	4/4	0.71	0.20	54,55,56,57	0
7	EDO	A	528	4/4	0.71	0.44	31,33,36,37	4
8	PEG	A	548	7/7	0.72	0.24	69,71,79,81	0
7	EDO	B	110	4/4	0.72	0.20	57,60,61,63	0
7	EDO	B	103	4/4	0.72	0.22	72,73,76,79	0
7	EDO	B	107	4/4	0.73	0.17	57,60,61,64	0
9	PG4	A	520	13/13	0.73	0.34	36,59,67,67	13
8	PEG	B	104	7/7	0.74	0.23	34,51,68,70	0
6	GOL	A	551	6/6	0.74	0.42	41,65,76,81	0
7	EDO	A	525	4/4	0.76	0.22	56,57,57,59	0
7	EDO	A	547	4/4	0.78	0.27	48,55,60,62	0
7	EDO	A	535	4/4	0.78	0.45	32,37,38,38	4
8	PEG	A	518	7/7	0.79	0.15	35,44,49,53	0
7	EDO	A	538	4/4	0.79	0.25	59,62,65,67	0
16	1PE	D	202	16/16	0.79	0.15	59,64,69,70	0
7	EDO	A	542	4/4	0.80	0.34	53,58,62,67	0
7	EDO	B	105	4/4	0.80	0.20	70,71,73,73	0
7	EDO	A	536	4/4	0.80	0.22	29,32,33,33	4
7	EDO	A	530	4/4	0.81	0.38	52,58,60,61	4
8	PEG	A	532	7/7	0.82	0.18	56,64,67,68	0
7	EDO	D	206	4/4	0.82	0.14	62,62,63,63	0
6	GOL	A	504	6/6	0.83	0.30	38,57,61,67	0
8	PEG	A	549	7/7	0.83	0.26	42,66,73,73	0
7	EDO	A	537	4/4	0.85	0.25	60,64,67,70	0
7	EDO	A	541	4/4	0.85	0.27	44,52,55,56	0
10	P15	A	526	20/20	0.85	0.27	18,69,74,74	0
12	PGE	A	534	10/10	0.85	0.21	29,39,45,45	10
7	EDO	A	517	4/4	0.85	0.36	16,22,28,34	4
7	EDO	B	111	4/4	0.85	0.13	61,62,62,63	0

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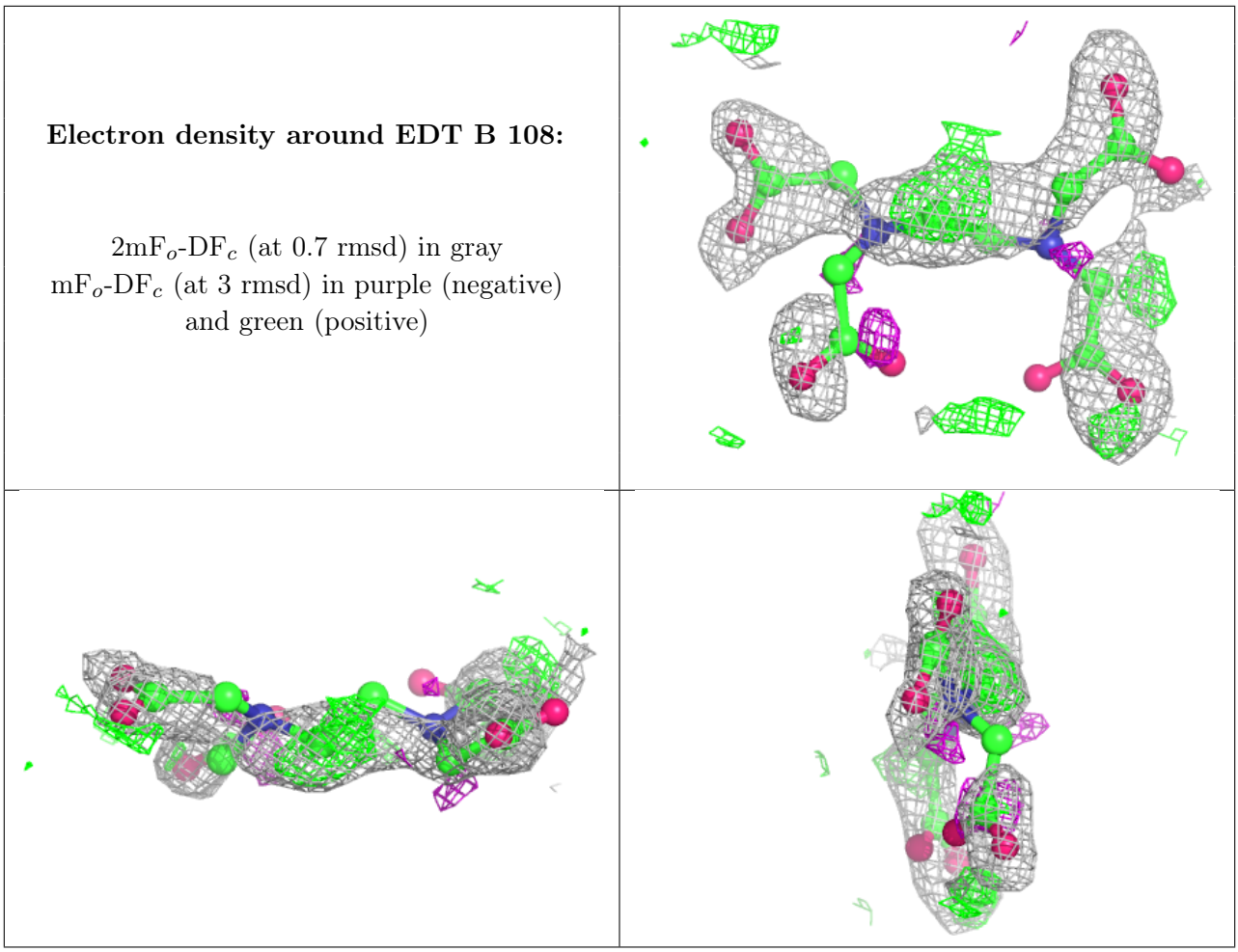
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	524	4/4	0.85	0.24	54,54,54,55	4
7	EDO	A	511	4/4	0.86	0.20	34,34,36,37	4
7	EDO	A	508	4/4	0.86	0.19	48,50,51,53	0
7	EDO	A	546	4/4	0.86	0.19	26,32,33,38	4
6	GOL	A	503	6/6	0.87	0.15	32,55,60,61	0
8	PEG	A	531	7/7	0.87	0.28	23,42,66,70	7
7	EDO	B	102	4/4	0.87	0.11	44,49,50,53	0
12	PGE	A	543	10/10	0.88	0.19	23,41,51,52	10
7	EDO	D	205	4/4	0.88	0.20	41,43,45,52	4
7	EDO	A	545	4/4	0.88	0.15	51,59,65,69	0
7	EDO	A	510	4/4	0.88	0.15	48,51,53,56	0
7	EDO	A	512	4/4	0.89	0.21	35,36,38,39	4
8	PEG	A	521	7/7	0.89	0.11	39,48,56,61	0
6	GOL	A	502	6/6	0.89	0.20	9,20,25,28	6
8	PEG	B	106	7/7	0.89	0.21	18,29,37,42	7
15	MES	C	302	12/12	0.89	0.15	60,62,64,66	0
11	DTT	A	533	8/8	0.89	0.24	45,60,65,70	8
7	EDO	C	304	4/4	0.90	0.45	28,32,33,36	4
7	EDO	A	552	4/4	0.90	0.22	39,41,42,44	0
7	EDO	A	506	4/4	0.91	0.17	39,39,43,43	4
7	EDO	A	523	4/4	0.91	0.17	28,32,33,35	4
7	EDO	C	303	4/4	0.92	0.23	37,37,39,39	4
6	GOL	D	204	6/6	0.92	0.13	30,35,39,43	6
7	EDO	A	516	4/4	0.92	0.20	11,12,15,20	4
7	EDO	A	509	4/4	0.93	0.17	23,27,30,31	4
7	EDO	A	522	4/4	0.93	0.29	19,24,35,36	4
7	EDO	A	514	4/4	0.94	0.16	14,15,18,25	4
7	EDO	B	101	4/4	0.94	0.21	19,24,26,27	4
6	GOL	A	505	6/6	0.94	0.19	23,32,36,37	6
7	EDO	A	513	4/4	0.94	0.17	35,42,42,44	4
7	EDO	D	201	4/4	0.95	0.12	26,26,35,40	4
7	EDO	A	507	4/4	0.97	0.19	9,11,12,19	4
14	8Q1	C	301	34/35	0.97	0.09	19,29,39,40	0
5	PLP	A	501	15/16	0.99	0.09	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.

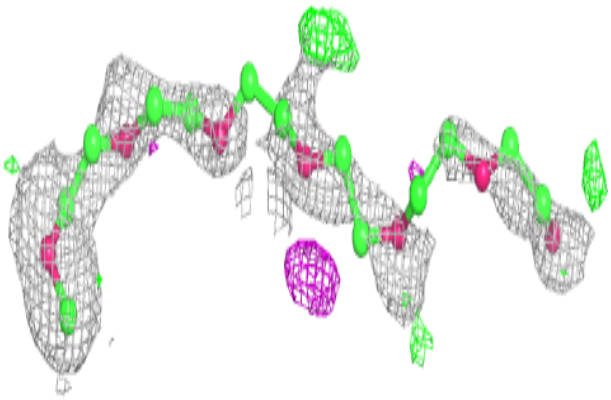
Electron density around EDT B 108:

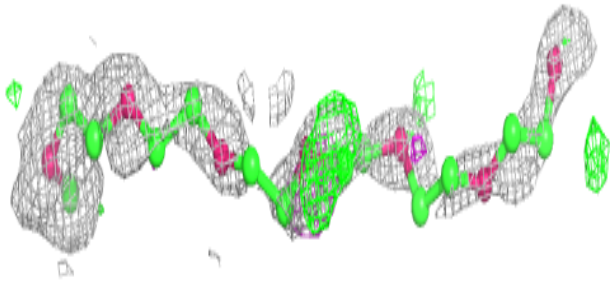
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

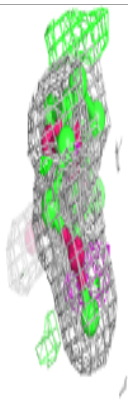


Electron density around P15 A 526:

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

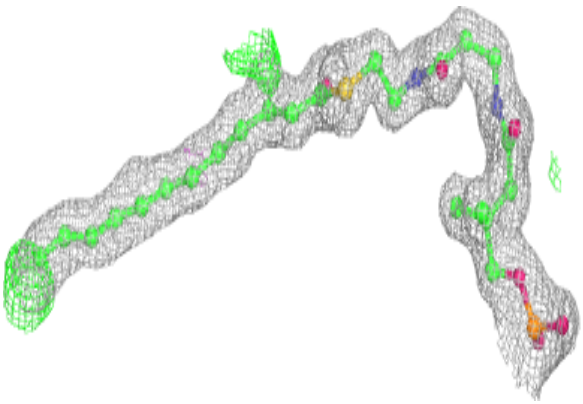


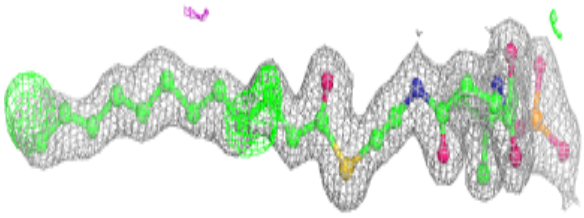


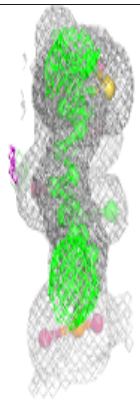


Electron density around 8Q1 C 301:

$2mF_o$-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.