Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 10:13 AM EDT

PDB ID	:	8TVT
Title	:	Structure of human Cysteine desulfurase Nfs1 with L-propargylglycine bound to active site PLP in complex with ISD11, Acp1 and ISCU2
Authors	:	Cygler, M.; Boniecki, M.T.
Deposited on	:	2023-08-18
Resolution	:	2.00 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:

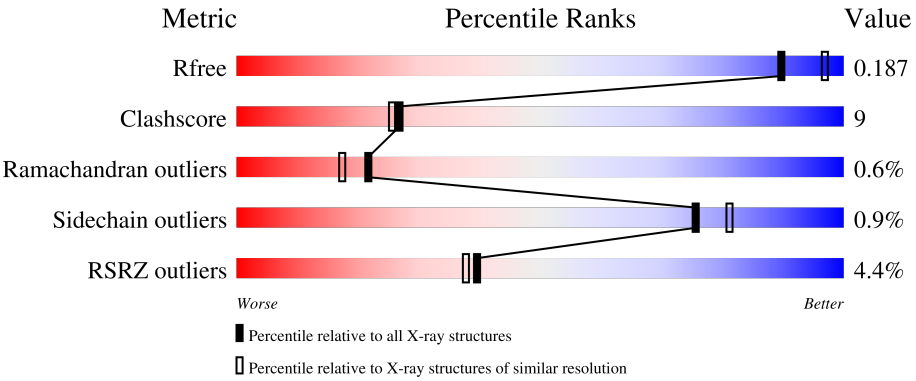
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	403	3% 82% 17% ·
2	B	91	3% 82% 8% · 8%
3	C	76	11% 86% 9% · ·
4	D	135	5% 70% 21% · 7%

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
14	EDT	B	108	-	-	X	-
5	EDO	A	501	-	X	-	-
5	EDO	A	508	-	-	X	-
7	LPH	A	504	-	-	X	-
9	PEG	A	524	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 6126 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	3154	1990	550	593	21	0	18	0

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
			Total	C	N	O	S			
2	B	84	728	458	145	124	1	0	7	0

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
			Total	C	N	O	S			
3	C	74	529	331	83	114	1	0	0	0

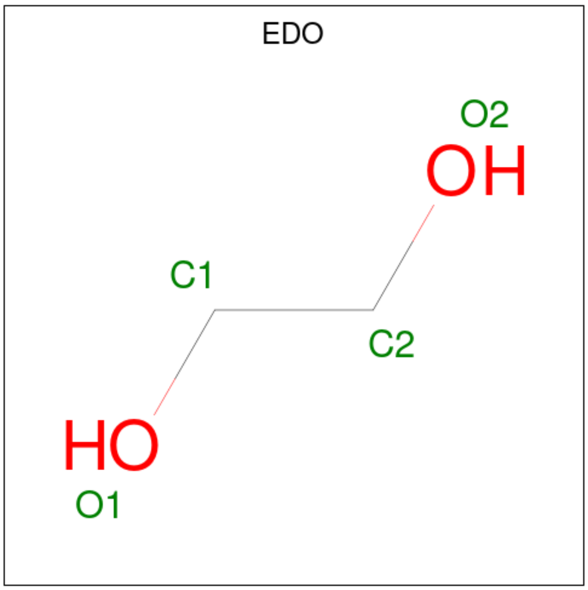
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	126	938	594	157	180	7	0	4	0

There are 2 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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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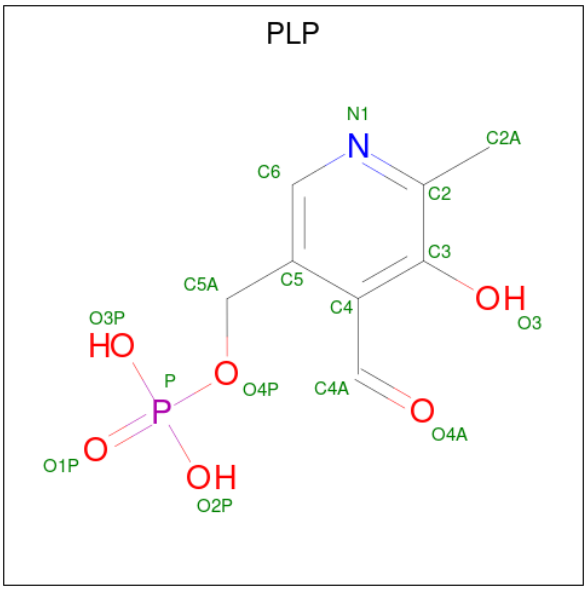
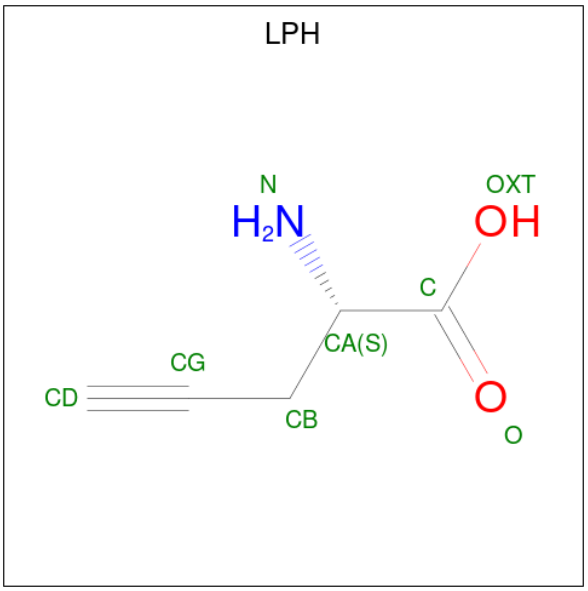
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



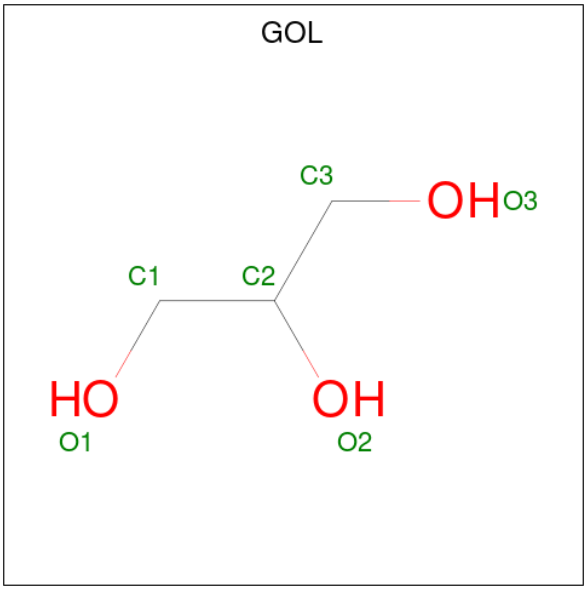
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 7 is L-Propargylglycine (three-letter code: LPH) (formula: $C_5H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



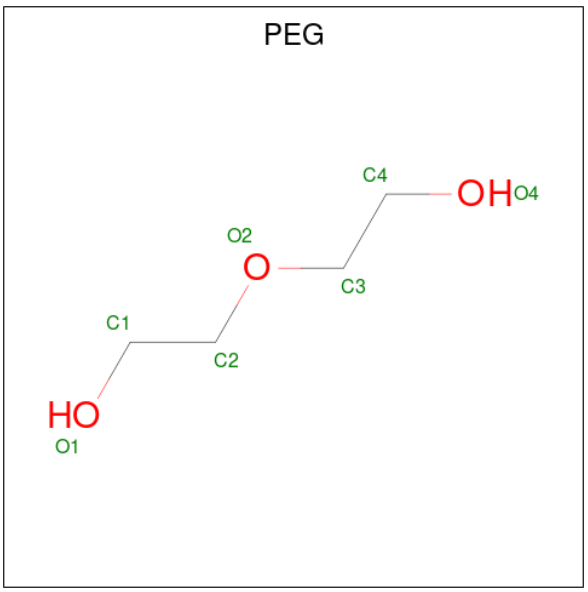
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 8 5 1 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



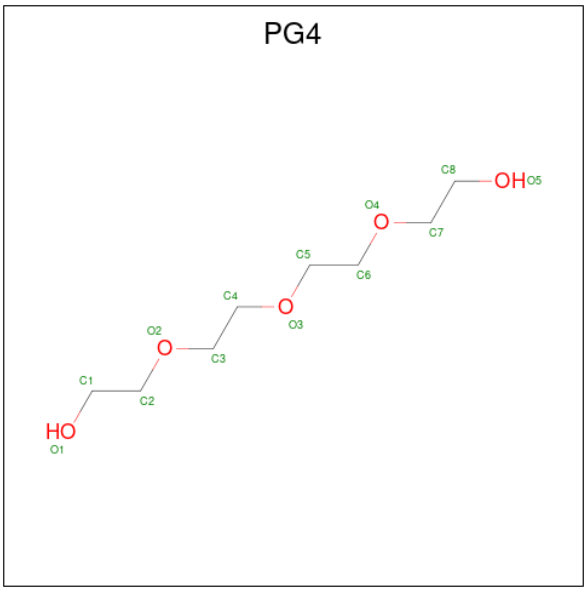
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



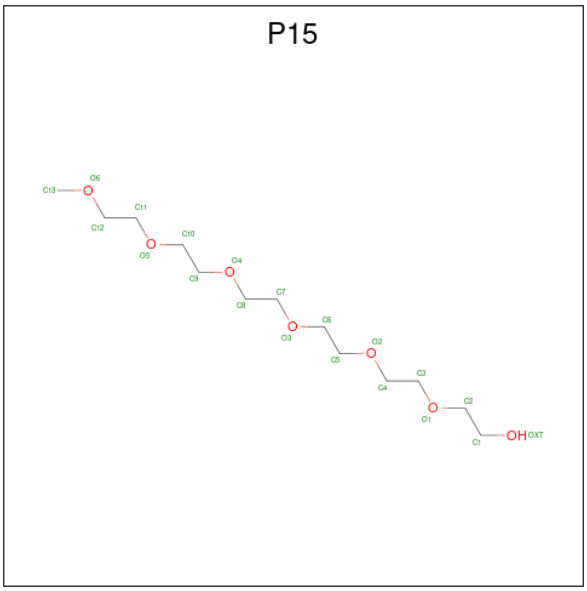
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



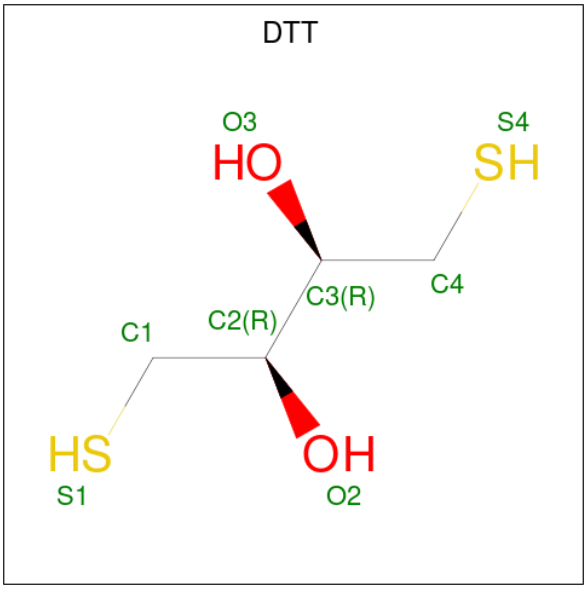
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 13 8 5	0	0
10	A	1	Total C O 13 8 5	0	0

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



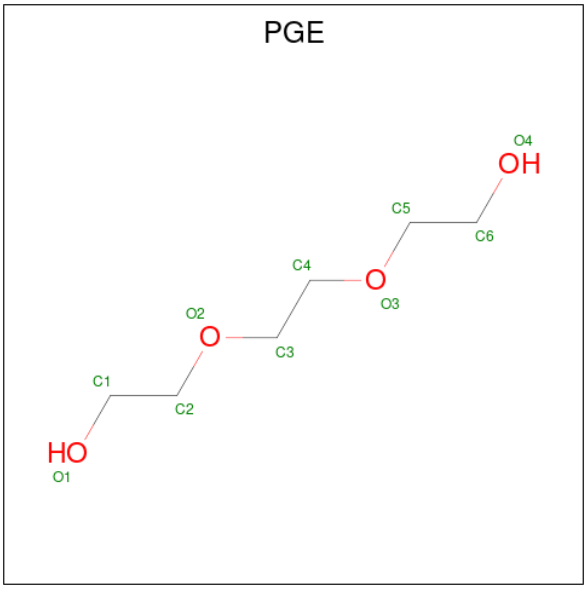
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 20 13 7	0	0

- Molecule 12 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



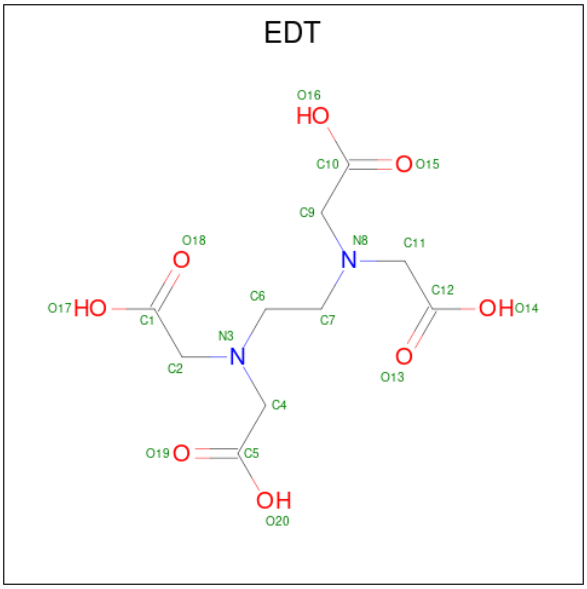
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
12	A	1	8	4	2	2	0	0

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



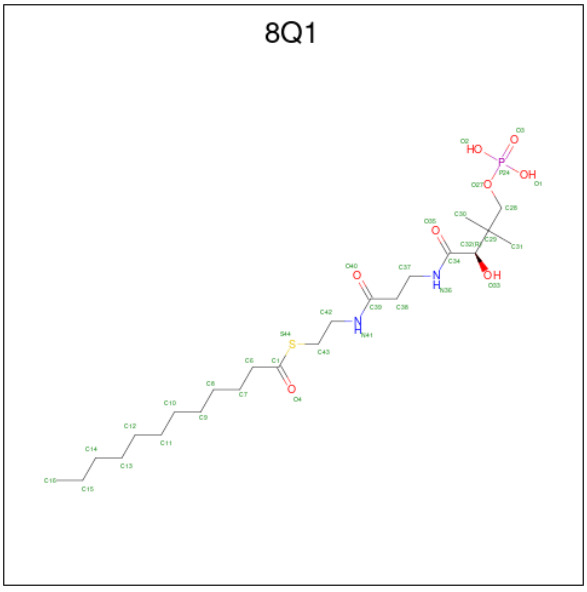
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	A	1	10	6	4	0	0

- Molecule 14 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



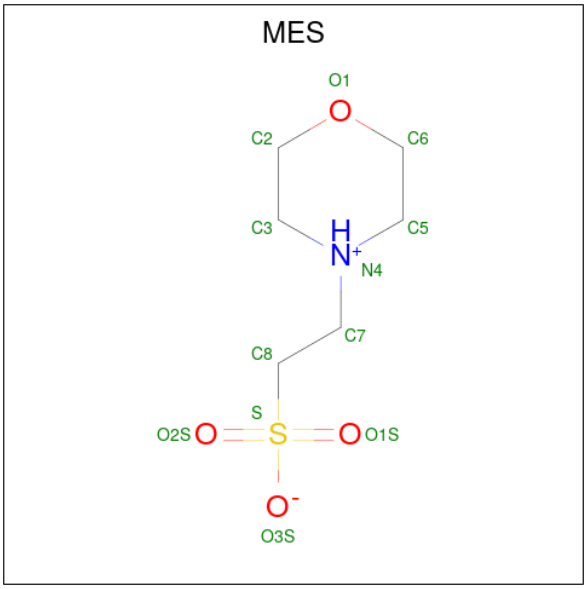
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C N O 20 10 2 8	0	0

- Molecule 15 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



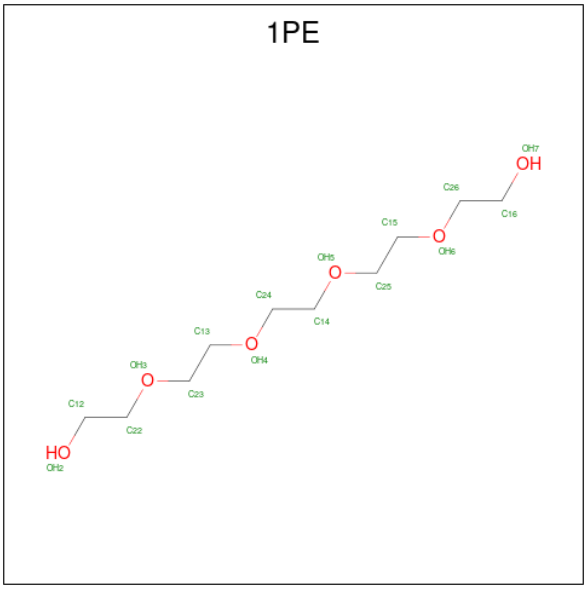
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C N O P S 34 23 2 7 1 1	0	0

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 17 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

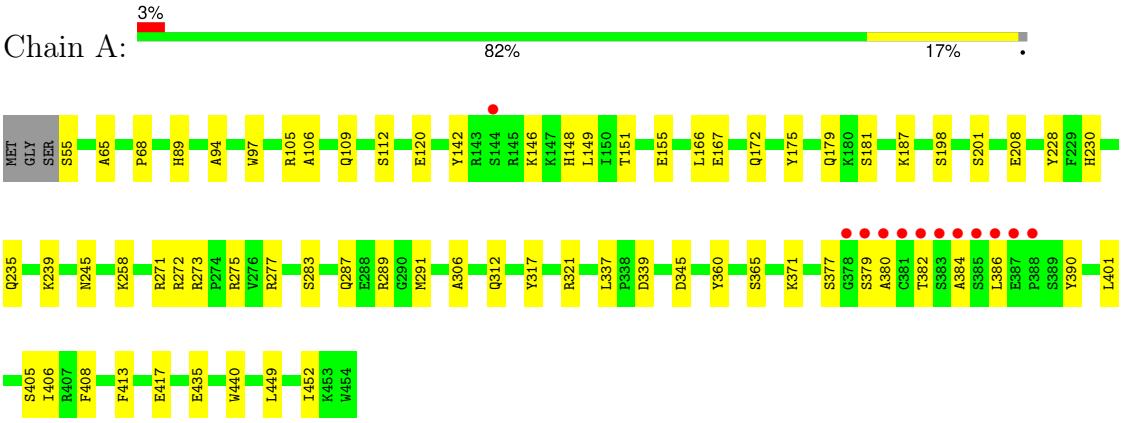
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	286	Total O 286 286	0	0
18	B	64	Total O 64 64	0	0
18	C	24	Total O 24 24	0	0
18	D	40	Total O 40 40	0	0

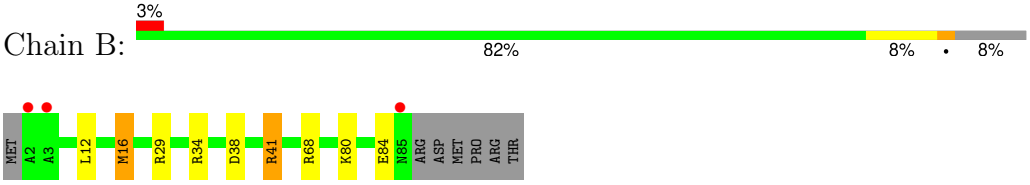
3 Residue-property plots (i)

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.

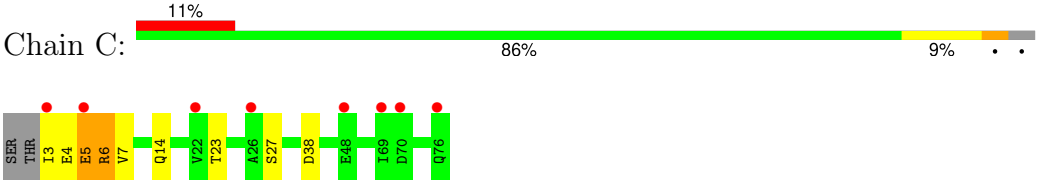
• Molecule 1: Cysteine desulfurase



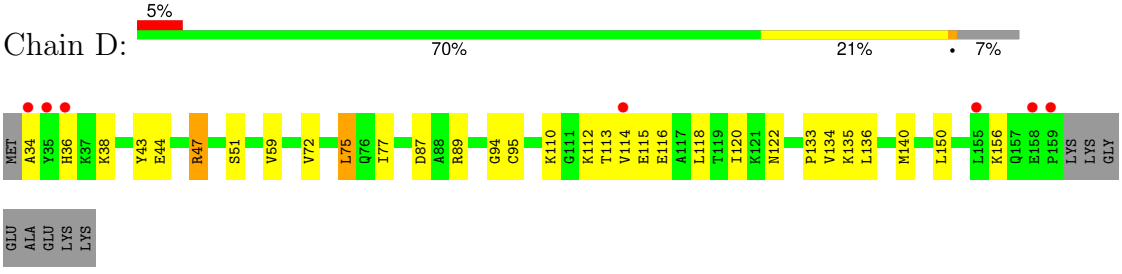
• Molecule 2: LYR motif-containing protein 4



• Molecule 3: Acyl carrier protein



• Molecule 4: Iron-sulfur cluster assembly enzyme ISCU



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.27Å 86.27Å 246.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.00 48.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-2.00) 100.0 (48.95-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.150 , 0.186 0.151 , 0.187	Depositor DCC
R_{free} test set	3199 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6126	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: LPH, PEG, EDT, PGE, PLP, 1PE, 8Q1, P15, PG4, GOL, MES, EDO, 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	0.88	0/3253	0.85	1/4406 (0.0%)
2	B	0.88	0/755	0.90	1/1013 (0.1%)
3	C	0.53	0/533	0.78	0/727
4	D	0.68	1/961 (0.1%)	0.83	2/1303 (0.2%)
All	All	0.82	1/5502 (0.0%)	0.85	4/7449 (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	2
2	B	0	1
3	C	0	1
4	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	72	VAL	CB-CG1	5.62	1.64	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	75	LEU	CB-CG-CD2	-5.66	101.38	111.00
4	D	77	ILE	CG1-CB-CG2	-5.53	99.24	111.40
1	A	235	GLN	CA-CB-CG	-5.15	102.08	113.40
2	B	16	MET	N-CA-CB	-5.09	101.43	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	ARG	Sidechain
1	A	321[A]	ARG	Sidechain
2	B	41[A]	ARG	Sidechain
3	C	6	ARG	Sidechain
4	D	47	ARG	Sidechain

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	3154	0	3156	58	0
2	B	728	0	765	11	0
3	C	529	0	468	7	0
4	D	938	0	937	20	0
5	A	80	0	119	8	0
5	B	24	0	36	2	0
5	C	8	0	12	0	0
5	D	8	0	12	3	0
6	A	15	0	6	4	0
7	A	8	0	5	4	0
8	A	12	0	16	3	0
8	D	6	0	8	0	0
9	A	42	0	60	7	0
9	B	14	0	20	5	0
10	A	26	0	36	3	0
11	A	20	0	28	4	0
12	A	8	0	10	2	0
13	A	10	0	14	4	0
14	B	20	0	12	7	0
15	C	34	0	0	0	0
16	C	12	0	12	1	0
17	D	16	0	22	2	0
18	A	286	0	0	6	0
18	B	64	0	0	0	0
18	C	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	40	0	0	2	0
All	All	6126	0	5754	104	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 9.

All (104) 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)
5:A:501:EDO:H21	18:A:756:HOH:O	1.68	0.91
1:A:312:GLN:HE22	10:A:517:PG4:H32	1.41	0.86
2:B:29:ARG:HH21	14:B:108:EDT:H061	1.38	0.86
4:D:95:CYS:SG	4:D:135:LYS:NZ	2.50	0.84
2:B:68:ARG:HD3	9:B:105:PEG:H12	1.68	0.76
1:A:379:SER:HB2	1:A:384:ALA:HB2	1.68	0.75
9:A:516:PEG:H41	9:B:105:PEG:H11	1.70	0.74
1:A:175:TYR:HD2	9:A:524:PEG:H12	1.55	0.70
3:C:3:ILE:HG22	3:C:5:GLU:H	1.56	0.70
1:A:413:PHE:HB2	5:B:101:EDO:H11	1.73	0.70
5:A:508:EDO:H11	4:D:44:GLU:HG2	1.75	0.69
1:A:245:ASN:HD22	1:A:271:ARG:HH22	1.42	0.66
1:A:68:PRO:HG3	5:B:101:EDO:H22	1.78	0.66
4:D:112:LYS:HG2	17:D:202:1PE:H222	1.77	0.66
2:B:29:ARG:NH2	14:B:108:EDT:H041	2.13	0.64
2:B:29:ARG:HG2	14:B:108:EDT:H091	1.80	0.64
2:B:29:ARG:HH21	14:B:108:EDT:H041	1.63	0.64
1:A:272:ARG:O	1:A:273:ARG:HD3	1.99	0.62
1:A:337:LEU:O	11:A:521:P15:H131	1.99	0.62
4:D:134:VAL:HG13	18:D:337:HOH:O	2.00	0.60
6:A:503:PLP:C4A	7:A:504:LPH:CG	2.78	0.60
1:A:258:LYS:HZ1	6:A:503:PLP:C4A	2.16	0.59
4:D:51:SER:O	5:D:201:EDO:H21	2.03	0.58
1:A:112:SER:OG	10:A:517:PG4:H11	2.04	0.58
8:A:505:GOL:H12	2:B:34:ARG:HH21	1.68	0.57
1:A:390:TYR:CG	5:A:510:EDO:H12	2.40	0.57
1:A:306:ALA:HB2	13:A:530:PGE:H52	1.87	0.56
1:A:377:SER:O	1:A:384:ALA:HB1	2.05	0.56
1:A:106:ALA:HA	1:A:109:GLN:HE21	1.70	0.56
3:C:4:GLU:C	3:C:6:ARG:H	2.10	0.55
1:A:142:TYR:HH	1:A:228:TYR:HH	1.54	0.55
1:A:208:GLU:HG2	1:A:379:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:HA	11:A:521:P15:H101	1.89	0.54
4:D:120:ILE:HG12	17:D:202:1PE:H252	1.90	0.54
4:D:133:PRO:HA	4:D:136:LEU:HG	1.89	0.53
1:A:371:LYS:HD3	5:A:508:EDO:H22	1.89	0.53
12:A:525:DTT:S1	12:A:525:DTT:S4	3.07	0.53
13:A:530:PGE:H62	18:A:668:HOH:O	2.08	0.52
4:D:59:VAL:O	4:D:156:LYS:NZ	2.36	0.52
1:A:435:GLU:HG3	8:A:506:GOL:H32	1.92	0.52
4:D:34:ALA:N	18:D:302:HOH:O	2.42	0.52
4:D:89:ARG:HE	5:D:201:EDO:H22	1.76	0.51
1:A:317:TYR:CD2	9:B:103:PEG:H21	2.46	0.51
1:A:179:GLN:NE2	18:A:612:HOH:O	2.44	0.50
1:A:449:LEU:HA	1:A:452:ILE:HD13	1.92	0.50
3:C:4:GLU:O	3:C:7:VAL:HG23	2.11	0.49
1:A:181:SER:HB2	1:A:345:ASP:HB2	1.94	0.49
1:A:175:TYR:H	9:A:524:PEG:C1	2.25	0.49
1:A:109:GLN:OE1	13:A:530:PGE:H5	2.12	0.49
1:A:105[B]:ARG:HG2	5:A:511:EDO:H11	1.95	0.49
1:A:406:ILE:HD11	1:A:408:PHE:CZ	2.48	0.49
4:D:36:HIS:CE1	4:D:38:LYS:HG3	2.48	0.49
1:A:258:LYS:NZ	6:A:503:PLP:C4	2.76	0.48
1:A:401:LEU:HD21	11:A:521:P15:H42	1.95	0.48
1:A:65:ALA:HA	7:A:504:LPH:H3	1.94	0.48
4:D:113:THR:OG1	4:D:116:GLU:HG3	2.13	0.48
4:D:114:VAL:HG13	4:D:150:LEU:HD22	1.95	0.48
10:A:518:PG4:H32	10:A:518:PG4:H52	1.59	0.48
2:B:12:LEU:O	2:B:16:MET:HB2	2.13	0.47
1:A:417[A]:GLU:OE1	8:A:505:GOL:H2	2.14	0.47
2:B:80:LYS:HB3	2:B:84:GLU:OE2	2.15	0.47
4:D:87:ASP:HA	4:D:110:LYS:HD3	1.96	0.47
1:A:89:HIS:CE1	1:A:287:GLN:HG2	2.49	0.47
5:A:508:EDO:H12	4:D:43:TYR:CE2	2.49	0.47
1:A:283:SER:HA	9:A:534:PEG:H41	1.97	0.46
1:A:239:LYS:HE2	18:A:683:HOH:O	2.16	0.46
4:D:122:ASN:HD22	4:D:140:MET:HG2	1.80	0.46
1:A:151:THR:OG1	1:A:155:GLU:HG3	2.16	0.46
1:A:187:LYS:NZ	18:A:616:HOH:O	2.48	0.46
3:C:4:GLU:C	3:C:6:ARG:N	2.68	0.46
1:A:371:LYS:CD	5:A:508:EDO:H22	2.46	0.46
1:A:105[B]:ARG:CG	5:A:511:EDO:H11	2.46	0.45
1:A:105[A]:ARG:HE	13:A:530:PGE:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:MET:HE3	1:A:291:MET:HA	2.00	0.44
14:B:108:EDT:O18	14:B:108:EDT:H042	2.09	0.44
3:C:14:GLN:HB3	18:C:415:HOH:O	2.19	0.43
1:A:167:GLU:OE2	9:A:524:PEG:H31	2.19	0.43
1:A:201:SER:HA	1:A:230:HIS:O	2.19	0.43
1:A:146:LYS:HB3	1:A:198[A]:SER:HB3	2.01	0.42
3:C:38:ASP:OD1	16:C:302:MES:H52	2.19	0.42
4:D:115:GLU:O	4:D:118:LEU:HB2	2.19	0.42
1:A:94:ALA:HA	1:A:97:TRP:CE3	2.54	0.42
4:D:75:LEU:C	4:D:75:LEU:HD23	2.40	0.42
1:A:142:TYR:OH	1:A:228:TYR:OH	2.25	0.42
1:A:175:TYR:CD2	9:A:524:PEG:H32	2.55	0.42
1:A:277:ARG:HA	1:A:277:ARG:HD2	1.87	0.42
1:A:175:TYR:CD1	9:A:522:PEG:H41	2.55	0.41
2:B:29:ARG:NH2	14:B:108:EDT:H061	2.19	0.41
3:C:4:GLU:O	3:C:6:ARG:N	2.53	0.41
1:A:275:ARG:HD3	1:A:277:ARG:HD3	2.03	0.41
1:A:55:SER:HB2	18:A:786:HOH:O	2.21	0.41
1:A:148:HIS:HA	1:A:172:GLN:O	2.21	0.41
1:A:149:LEU:HD11	1:A:166:LEU:HD13	2.03	0.41
2:B:38:ASP:HB3	9:B:103:PEG:C2	2.51	0.41
2:B:29:ARG:HH21	14:B:108:EDT:C4	2.31	0.41
1:A:258:LYS:HZ1	7:A:504:LPH:CD	2.34	0.40
4:D:89:ARG:HE	5:D:201:EDO:C2	2.34	0.40
1:A:317:TYR:CE2	9:B:103:PEG:H21	2.56	0.40
1:A:365:SER:HB3	4:D:94:GLY:O	2.22	0.40
1:A:120:GLU:OE2	12:A:525:DTT:S4	2.80	0.40
1:A:245:ASN:ND2	1:A:271:ARG:HH22	2.15	0.40
1:A:360:TYR:CD2	1:A:440:TRP:HE3	2.39	0.40
6:A:503:PLP:O3P	7:A:504:LPH:H1	2.21	0.40
11:A:521:P15:H62	11:A:521:P15:H81	1.90	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	416/403 (103%)	399 (96%)	14 (3%)	3 (1%)	19 14
2	B	89/91 (98%)	87 (98%)	2 (2%)	0	100 100
3	C	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9 4
4	D	128/135 (95%)	128 (100%)	0	0	100 100
All	All	705/705 (100%)	683 (97%)	18 (3%)	4 (1%)	22 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ALA
1	A	386	LEU
1	A	382	THR
3	C	5	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/343 (99%)	339 (99%)	2 (1%)	84 88
2	B	77/80 (96%)	75 (97%)	2 (3%)	41 44
3	C	49/66 (74%)	47 (96%)	2 (4%)	26 25
4	D	98/110 (89%)	97 (99%)	1 (1%)	73 78
All	All	565/599 (94%)	558 (99%)	7 (1%)	75 73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405[A]	SER
1	A	405[B]	SER
2	B	41[A]	ARG
2	B	41[B]	ARG

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Mol	Chain	Res	Type
3	C	23	THR
3	C	27	SER
4	D	47	ARG

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

Mol	Chain	Res	Type
1	A	245	ASN
1	A	312	GLN
1	A	313	GLN
1	A	428	GLN
4	D	78	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

52 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	$\#\|Z\| > 2$
5	EDO	A	508	-	3,3,3	0.68	0	2,2,2	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	C	303	-	3,3,3	0.30	0	2,2,2	0.43	0
5	EDO	A	514	-	3,3,3	1.02	0	2,2,2	0.84	0
8	GOL	D	203	-	5,5,5	1.53	1 (20%)	5,5,5	0.85	0
8	GOL	A	506	-	5,5,5	1.09	0	5,5,5	0.73	0
15	8Q1	C	301	3	28,33,34	1.78	4 (14%)	32,40,43	1.47	6 (18%)
13	PGE	A	530	-	9,9,9	0.49	0	8,8,8	1.08	1 (12%)
5	EDO	B	102	-	3,3,3	0.42	0	2,2,2	0.72	0
5	EDO	A	507	-	3,3,3	0.47	0	2,2,2	0.41	0
8	GOL	A	505	-	5,5,5	1.40	1 (20%)	5,5,5	0.77	0
7	LPH	A	504	6	6,7,7	1.75	2 (33%)	2,8,8	2.41	1 (50%)
9	PEG	A	522	-	6,6,6	0.38	0	5,5,5	0.21	0
5	EDO	A	513	-	3,3,3	0.38	0	2,2,2	0.63	0
5	EDO	A	529	-	3,3,3	0.55	0	2,2,2	0.15	0
5	EDO	A	526	-	3,3,3	0.62	0	2,2,2	0.64	0
10	PG4	A	517	-	12,12,12	0.37	0	11,11,11	0.65	0
9	PEG	A	524	-	6,6,6	0.11	0	5,5,5	0.36	0
9	PEG	A	516	-	6,6,6	0.25	0	5,5,5	0.50	0
14	EDT	B	108	-	19,19,19	1.47	1 (5%)	24,24,24	1.45	5 (20%)
16	MES	C	302	-	12,12,12	1.94	1 (8%)	15,16,16	2.33	5 (33%)
9	PEG	B	105	-	6,6,6	0.33	0	5,5,5	0.28	0
12	DTT	A	525	-	7,7,7	0.64	0	4,8,8	1.86	1 (25%)
5	EDO	C	304	-	3,3,3	0.59	0	2,2,2	0.29	0
5	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.66	0
5	EDO	B	106	-	3,3,3	0.53	0	2,2,2	0.14	0
5	EDO	A	501	-	3,3,3	1.71	1 (33%)	2,2,2	1.87	1 (50%)
5	EDO	B	101	-	3,3,3	0.64	0	2,2,2	1.01	0
9	PEG	A	535	-	6,6,6	0.29	0	5,5,5	0.20	0
5	EDO	A	523	-	3,3,3	0.93	0	2,2,2	0.31	0
5	EDO	A	511	-	3,3,3	0.55	0	2,2,2	0.56	0
9	PEG	A	534	-	6,6,6	0.27	0	5,5,5	0.22	0
5	EDO	A	509	-	3,3,3	0.53	0	2,2,2	0.22	0
6	PLP	A	503	7	15,15,16	2.35	4 (26%)	21,22,23	1.88	4 (19%)
5	EDO	A	527	-	3,3,3	0.56	0	2,2,2	0.46	0
9	PEG	A	519	-	6,6,6	0.27	0	5,5,5	0.30	0
5	EDO	A	532	-	3,3,3	0.61	0	2,2,2	1.26	0
5	EDO	B	104	-	3,3,3	0.47	0	2,2,2	0.48	0
5	EDO	A	515	-	3,3,3	0.76	0	2,2,2	0.04	0
5	EDO	A	533	-	3,3,3	0.59	0	2,2,2	0.16	0
5	EDO	D	204	-	3,3,3	0.58	0	2,2,2	0.32	0
5	EDO	A	531	-	3,3,3	0.69	0	2,2,2	0.25	0
11	P15	A	521	-	19,19,19	0.53	0	18,18,18	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	520	-	3,3,3	0.77	0	2,2,2	0.33	0
5	EDO	B	107	-	3,3,3	0.61	0	2,2,2	0.43	0
9	PEG	B	103	-	6,6,6	0.32	0	5,5,5	0.34	0
5	EDO	B	109	-	3,3,3	0.62	0	2,2,2	0.44	0
5	EDO	A	528	-	3,3,3	0.47	0	2,2,2	0.51	0
5	EDO	A	510	-	3,3,3	0.56	0	2,2,2	0.43	0
17	1PE	D	202	-	15,15,15	0.59	0	14,14,14	0.53	0
10	PG4	A	518	-	12,12,12	0.42	0	11,11,11	0.56	0
5	EDO	A	502	-	3,3,3	0.53	0	2,2,2	0.43	0
5	EDO	D	201	-	3,3,3	0.49	0	2,2,2	0.85	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
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	C	303	-	-	1/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-
8	GOL	D	203	-	-	4/4/4/4	-
8	GOL	A	506	-	-	4/4/4/4	-
15	8Q1	C	301	3	-	2/38/40/41	-
13	PGE	A	530	-	-	4/7/7/7	-
5	EDO	B	102	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
8	GOL	A	505	-	-	4/4/4/4	-
7	LPH	A	504	6	-	3/6/7/7	-
9	PEG	A	522	-	-	3/4/4/4	-
5	EDO	A	513	-	-	1/1/1/1	-
5	EDO	A	529	-	-	0/1/1/1	-
5	EDO	A	526	-	-	0/1/1/1	-
10	PG4	A	517	-	-	6/10/10/10	-
9	PEG	A	524	-	-	1/4/4/4	-
9	PEG	A	516	-	-	2/4/4/4	-
14	EDT	B	108	-	-	11/21/21/21	-
16	MES	C	302	-	-	4/6/14/14	0/1/1/1
9	PEG	B	105	-	-	2/4/4/4	-
12	DTT	A	525	-	-	6/8/8/8	-
5	EDO	C	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	512	-	-	1/1/1/1	-
5	EDO	B	106	-	-	0/1/1/1	-
5	EDO	A	501	-	-	1/1/1/1	-
5	EDO	B	101	-	-	0/1/1/1	-
9	PEG	A	535	-	-	2/4/4/4	-
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
9	PEG	A	534	-	-	4/4/4/4	-
5	EDO	A	509	-	-	1/1/1/1	-
6	PLP	A	503	7	-	2/6/6/8	0/1/1/1
5	EDO	A	527	-	-	0/1/1/1	-
9	PEG	A	519	-	-	1/4/4/4	-
5	EDO	A	532	-	-	0/1/1/1	-
5	EDO	B	104	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	533	-	-	1/1/1/1	-
5	EDO	D	204	-	-	0/1/1/1	-
5	EDO	A	531	-	-	1/1/1/1	-
11	P15	A	521	-	-	13/17/17/17	-
5	EDO	A	520	-	-	0/1/1/1	-
5	EDO	B	107	-	-	1/1/1/1	-
9	PEG	B	103	-	-	3/4/4/4	-
5	EDO	B	109	-	-	1/1/1/1	-
5	EDO	A	528	-	-	1/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-
17	1PE	D	202	-	-	5/13/13/13	-
10	PG4	A	518	-	-	6/10/10/10	-
5	EDO	A	502	-	-	0/1/1/1	-
5	EDO	D	201	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	503	PLP	P-O1P	6.55	1.70	1.50
16	C	302	MES	C8-S	-6.31	1.68	1.77
15	C	301	8Q1	C39-N41	5.51	1.46	1.33
15	C	301	8Q1	C34-N36	4.63	1.44	1.33
6	A	503	PLP	P-O3P	-4.37	1.38	1.54
7	A	504	LPH	CB-CG	3.19	1.52	1.47
14	B	108	EDT	C11-C12	2.93	1.57	1.51
15	C	301	8Q1	C6-C1	2.84	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	504	LPH	O-C	2.61	1.29	1.22
8	A	505	GOL	C1-C2	2.41	1.61	1.51
8	D	203	GOL	C1-C2	2.36	1.60	1.51
5	A	501	EDO	O1-C1	2.28	1.53	1.42
6	A	503	PLP	C6-N1	2.18	1.38	1.34
15	C	301	8Q1	O35-C34	-2.07	1.19	1.23
6	A	503	PLP	P-O4P	2.03	1.66	1.60

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	503	PLP	C4A-C4-C3	-5.81	110.83	120.52
16	C	302	MES	C5-N4-C3	5.53	120.75	108.84
16	C	302	MES	C7-N4-C5	3.74	121.20	111.24
16	C	302	MES	O1S-S-C8	3.65	112.25	106.73
12	A	525	DTT	C3-C4-S4	-3.48	104.71	114.43
15	C	301	8Q1	C42-N41-C39	-3.42	116.45	122.82
7	A	504	LPH	OXT-C-O	-3.40	116.36	124.08
15	C	301	8Q1	C38-C37-N36	-2.79	106.06	112.00
6	A	503	PLP	C2A-C2-N1	2.78	122.88	117.64
6	A	503	PLP	C4A-C4-C5	-2.68	118.17	120.94
5	A	501	EDO	O2-C2-C1	2.65	132.57	112.39
14	B	108	EDT	C10-C9-N8	2.59	121.97	113.77
13	A	530	PGE	O3-C5-C6	2.45	120.89	110.11
16	C	302	MES	C7-N4-C3	2.38	117.58	111.24
14	B	108	EDT	C12-C11-N8	2.37	121.28	113.77
15	C	301	8Q1	C37-C38-C39	2.35	116.31	112.39
15	C	301	8Q1	C8-C7-C6	-2.33	104.55	113.13
6	A	503	PLP	C2A-C2-C3	-2.30	118.11	120.80
14	B	108	EDT	O17-C1-O18	2.27	129.17	123.33
16	C	302	MES	C6-C5-N4	-2.23	106.73	110.12
15	C	301	8Q1	O4-C1-S44	-2.19	119.90	122.68
15	C	301	8Q1	C37-N36-C34	-2.13	118.72	122.55
14	B	108	EDT	O15-C10-C9	-2.06	113.78	122.38
14	B	108	EDT	C11-N8-C7	2.02	116.78	111.91

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	505	GOL	C1-C2-C3-O3
8	A	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	A	506	GOL	C1-C2-C3-O3
8	D	203	GOL	O1-C1-C2-C3
8	D	203	GOL	C1-C2-C3-O3
12	A	525	DTT	C1-C2-C3-O3
12	A	525	DTT	C1-C2-C3-C4
12	A	525	DTT	O2-C2-C3-O3
12	A	525	DTT	O2-C2-C3-C4
12	A	525	DTT	C2-C3-C4-S4
12	A	525	DTT	O3-C3-C4-S4
14	B	108	EDT	C1-C2-N3-C4
14	B	108	EDT	O17-C1-C2-N3
14	B	108	EDT	O16-C10-C9-N8
16	C	302	MES	C8-C7-N4-C3
16	C	302	MES	C7-C8-S-O2S
16	C	302	MES	C7-C8-S-O3S
10	A	517	PG4	C4-C3-O2-C2
10	A	518	PG4	C3-C4-O3-C5
11	A	521	P15	C8-C7-O3-C6
14	B	108	EDT	O18-C1-C2-N3
14	B	108	EDT	O15-C10-C9-N8
10	A	518	PG4	O3-C5-C6-O4
11	A	521	P15	O1-C3-C4-O2
10	A	518	PG4	O2-C3-C4-O3
11	A	521	P15	O3-C7-C8-O4
9	A	534	PEG	O2-C3-C4-O4
9	B	103	PEG	O1-C1-C2-O2
11	A	521	P15	OXT-C1-C2-O1
5	A	509	EDO	O1-C1-C2-O2
14	B	108	EDT	N3-C6-C7-N8
9	A	534	PEG	O1-C1-C2-O2
9	A	535	PEG	O1-C1-C2-O2
10	A	517	PG4	O4-C7-C8-O5
10	A	518	PG4	O4-C7-C8-O5
17	D	202	1PE	OH4-C13-C23-OH3
8	A	505	GOL	O1-C1-C2-C3
9	A	516	PEG	O2-C3-C4-O4
10	A	518	PG4	O1-C1-C2-O2
17	D	202	1PE	OH7-C16-C26-OH6
17	D	202	1PE	OH6-C15-C25-OH5
8	A	506	GOL	O1-C1-C2-O2
8	A	506	GOL	O2-C2-C3-O3
5	A	510	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	512	EDO	O1-C1-C2-O2
5	C	303	EDO	O1-C1-C2-O2
14	B	108	EDT	N8-C11-C12-O13
11	A	521	P15	O5-C10-C9-O4
14	B	108	EDT	N8-C11-C12-O14
9	A	522	PEG	O1-C1-C2-O2
9	A	522	PEG	O2-C3-C4-O4
8	A	505	GOL	O2-C2-C3-O3
8	D	203	GOL	O1-C1-C2-O2
9	B	103	PEG	O2-C3-C4-O4
11	A	521	P15	O5-C11-C12-O6
5	A	513	EDO	O1-C1-C2-O2
5	A	523	EDO	O1-C1-C2-O2
5	A	531	EDO	O1-C1-C2-O2
5	B	107	EDO	O1-C1-C2-O2
8	D	203	GOL	O2-C2-C3-O3
11	A	521	P15	C9-C10-O5-C11
5	A	533	EDO	O1-C1-C2-O2
14	B	108	EDT	C5-C4-N3-C2
16	C	302	MES	C7-C8-S-O1S
11	A	521	P15	C7-C8-O4-C9
11	A	521	P15	C4-C3-O1-C2
17	D	202	1PE	C25-C15-OH6-C26
9	A	522	PEG	C4-C3-O2-C2
13	A	530	PGE	C4-C3-O2-C2
10	A	518	PG4	C8-C7-O4-C6
11	A	521	P15	C12-C11-O5-C10
5	A	514	EDO	O1-C1-C2-O2
6	A	503	PLP	C4-C5-C5A-O4P
9	A	524	PEG	O1-C1-C2-O2
8	A	505	GOL	O1-C1-C2-O2
7	A	504	LPH	OXT-C-CA-CB
11	A	521	P15	C6-C5-O2-C4
11	A	521	P15	C1-C2-O1-C3
9	A	519	PEG	C1-C2-O2-C3
14	B	108	EDT	C10-C9-N8-C11
9	B	105	PEG	C1-C2-O2-C3
13	A	530	PGE	C3-C4-O3-C5
9	A	534	PEG	C1-C2-O2-C3
14	B	108	EDT	C12-C11-N8-C9
9	A	535	PEG	O2-C3-C4-O4
10	A	517	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	504	LPH	O-C-CA-CB
9	B	105	PEG	O1-C1-C2-O2
5	B	102	EDO	O1-C1-C2-O2
9	B	103	PEG	C4-C3-O2-C2
15	C	301	8Q1	C12-C13-C14-C15
9	A	534	PEG	C4-C3-O2-C2
6	A	503	PLP	C6-C5-C5A-O4P
17	D	202	1PE	C14-C24-OH4-C13
5	A	501	EDO	O1-C1-C2-O2
10	A	517	PG4	C8-C7-O4-C6
15	C	301	8Q1	C6-C7-C8-C9
5	A	507	EDO	O1-C1-C2-O2
5	B	109	EDO	O1-C1-C2-O2
5	D	201	EDO	O1-C1-C2-O2
13	A	530	PGE	O3-C5-C6-O4
10	A	517	PG4	O2-C3-C4-O3
13	A	530	PGE	C6-C5-O3-C4
10	A	517	PG4	C5-C6-O4-C7
9	A	516	PEG	C4-C3-O2-C2
11	A	521	P15	C3-C4-O2-C5
5	A	528	EDO	O1-C1-C2-O2
7	A	504	LPH	OXT-C-CA-N

There are no ring outliers.

24 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	EDO	4	0
8	A	506	GOL	1	0
13	A	530	PGE	4	0
8	A	505	GOL	2	0
7	A	504	LPH	4	0
9	A	522	PEG	1	0
10	A	517	PG4	2	0
9	A	524	PEG	4	0
9	A	516	PEG	1	0
14	B	108	EDT	7	0
16	C	302	MES	1	0
9	B	105	PEG	2	0
12	A	525	DTT	2	0
5	A	501	EDO	1	0
5	B	101	EDO	2	0

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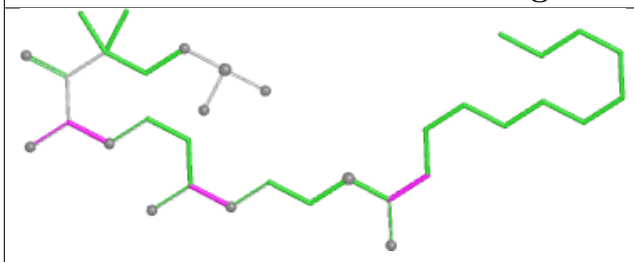
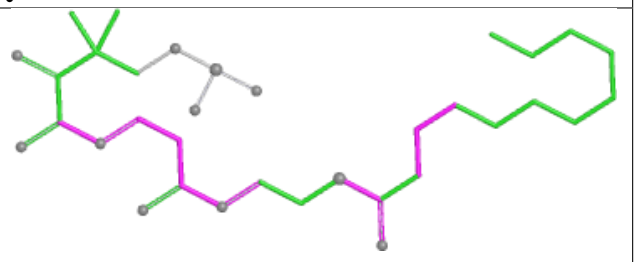
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	511	EDO	2	0
9	A	534	PEG	1	0
6	A	503	PLP	4	0
11	A	521	P15	4	0
9	B	103	PEG	3	0
5	A	510	EDO	1	0
17	D	202	1PE	2	0
10	A	518	PG4	1	0
5	D	201	EDO	3	0

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

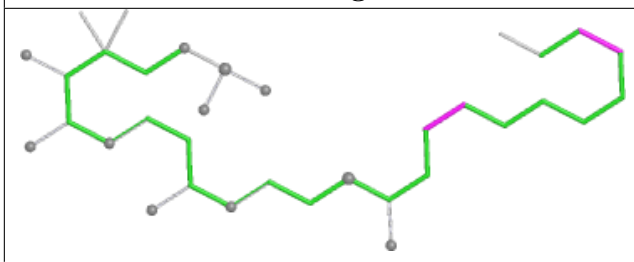
Ligand 8Q1 C 301



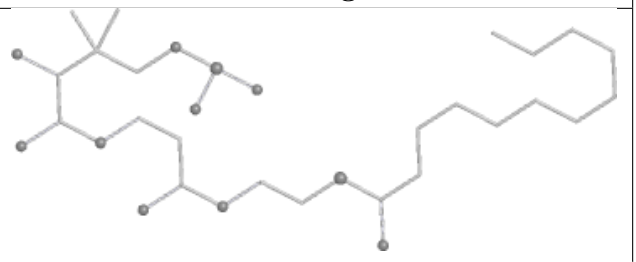
Bond lengths



Bond angles

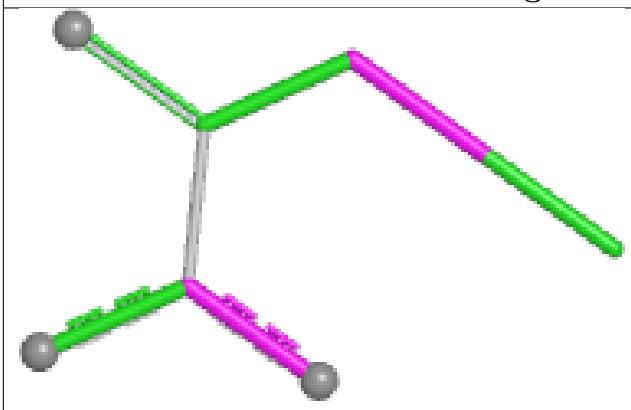


Torsions

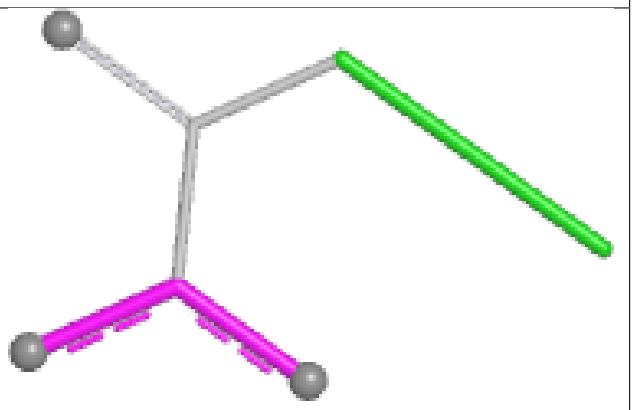


Rings

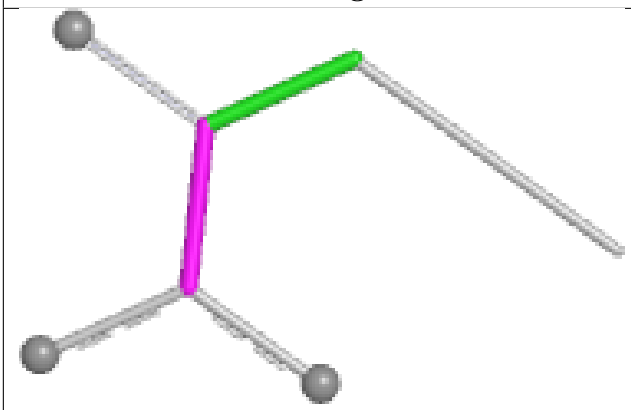
Ligand LPH A 504



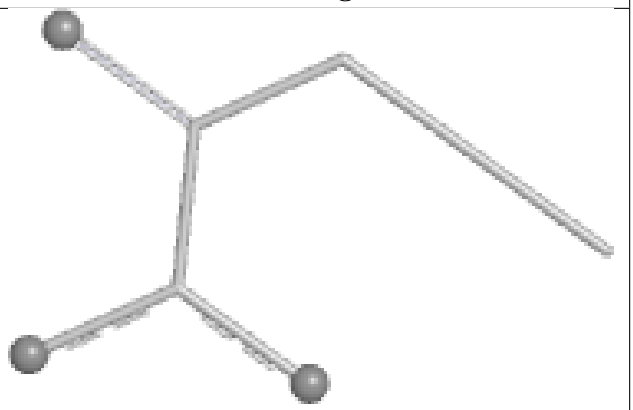
Bond lengths



Bond angles

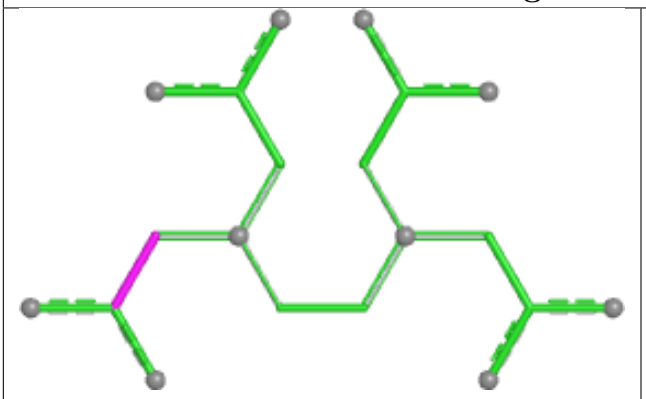


Torsions

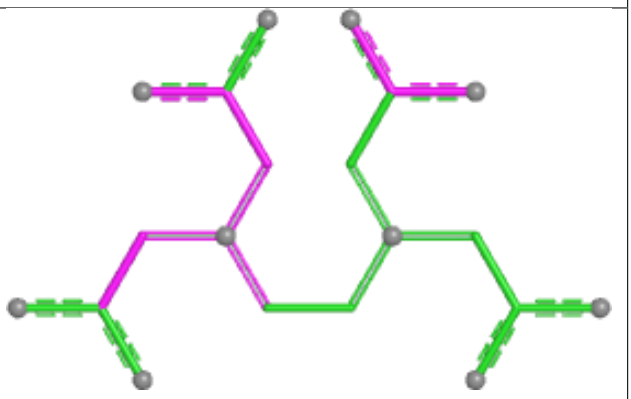


Rings

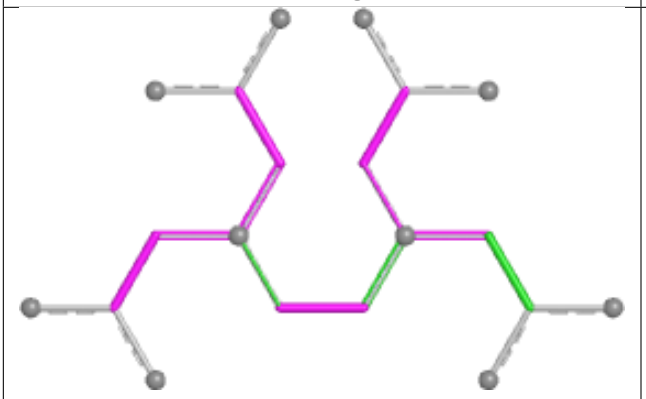
Ligand EDT B 108



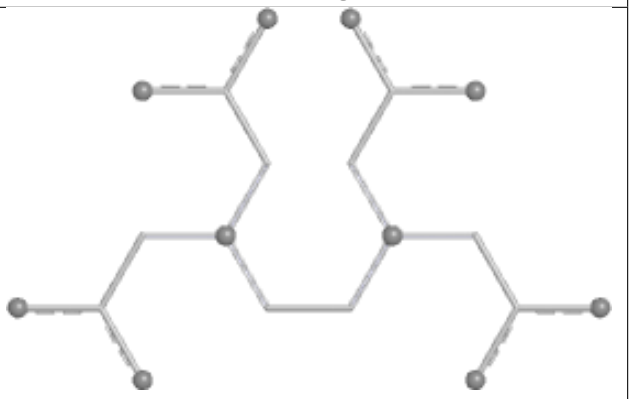
Bond lengths



Bond angles

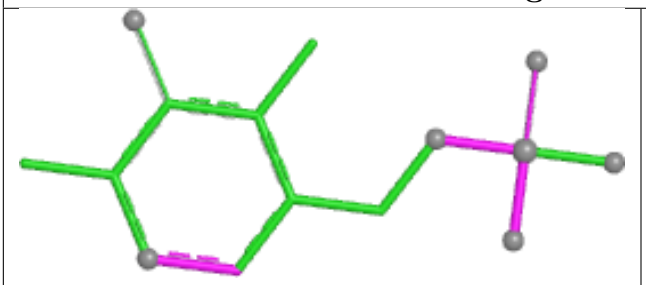


Torsions

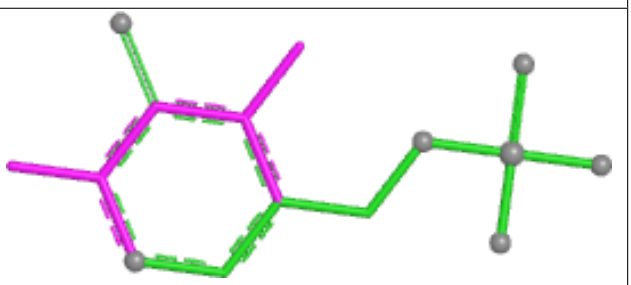


Rings

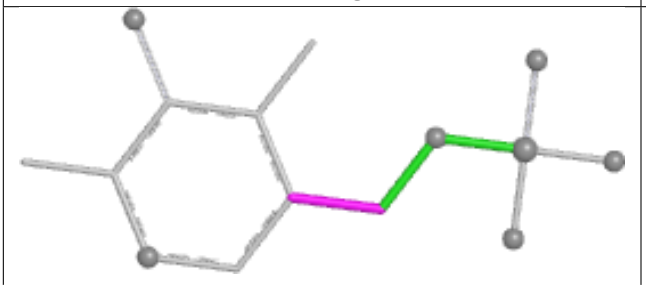
Ligand PLP A 503



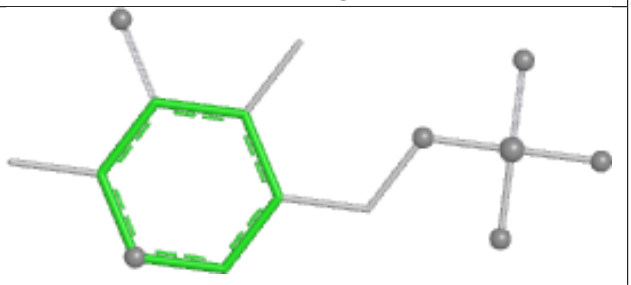
Bond lengths



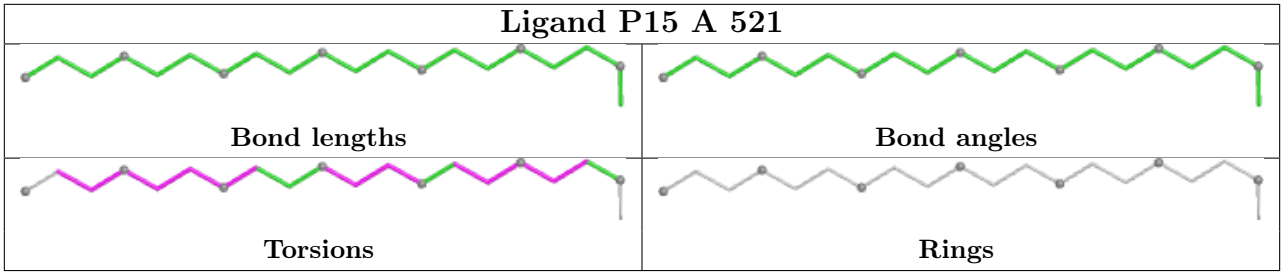
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	400/403 (99%)	-0.40	12 (3%)	52	51	10, 22, 50, 91	30 (7%)
2	B	84/91 (92%)	-0.27	3 (3%)	46	44	11, 26, 51, 73	7 (8%)
3	C	74/76 (97%)	1.04	8 (10%)	12	11	29, 56, 86, 95	0
4	D	126/135 (93%)	0.20	7 (5%)	31	29	13, 38, 64, 105	4 (3%)
All	All	684/705 (97%)	-0.11	30 (4%)	39	38	10, 27, 68, 105	41 (5%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	SER	9.4
1	A	380	ALA	8.4
1	A	382	THR	7.2
1	A	386	LEU	6.5
1	A	384	ALA	6.5
1	A	381	CYS	6.3
1	A	379	SER	5.8
4	D	35	TYR	4.9
2	B	2	ALA	4.8
1	A	385	SER	4.8
3	C	3	ILE	4.4
1	A	387	GLU	4.0
2	B	3	ALA	3.8
4	D	159	PRO	3.7
1	A	388	PRO	3.2
4	D	155	LEU	3.2
4	D	34	ALA	3.1
3	C	76	GLN	2.8
3	C	5	GLU	2.7
3	C	69	ILE	2.6
1	A	144	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	48	GLU	2.4
4	D	158	GLU	2.4
3	C	22	VAL	2.3
3	C	26	ALA	2.3
4	D	36	HIS	2.2
3	C	70	ASP	2.1
2	B	85	ASN	2.1
1	A	378	GLY	2.0
4	D	114	VAL	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
9	PEG	A	535	7/7	0.65	0.22	63,64,75,76	0
5	EDO	A	528	4/4	0.70	0.17	62,70,72,77	0
5	EDO	A	502	4/4	0.71	0.17	50,59,62,65	0
5	EDO	B	102	4/4	0.74	0.19	44,49,57,64	0
5	EDO	A	527	4/4	0.75	0.15	48,55,55,66	4
10	PG4	A	517	13/13	0.75	0.21	34,42,61,61	13
5	EDO	B	109	4/4	0.76	0.20	52,63,67,69	0
14	EDT	B	108	20/20	0.76	0.22	30,48,61,66	20
5	EDO	B	106	4/4	0.77	0.15	49,70,75,78	0
5	EDO	A	515	4/4	0.78	0.18	43,51,59,62	0
9	PEG	A	534	7/7	0.79	0.17	46,58,70,73	0
5	EDO	D	204	4/4	0.79	0.16	62,64,65,73	0
10	PG4	A	518	13/13	0.80	0.17	36,50,66,71	13
5	EDO	A	520	4/4	0.81	0.18	37,38,39,43	4

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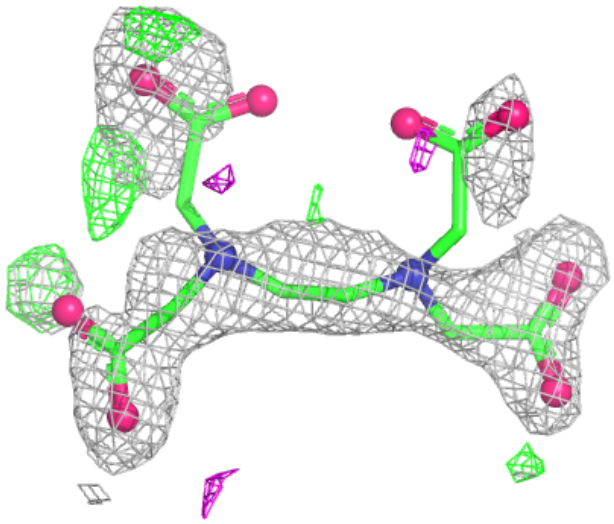
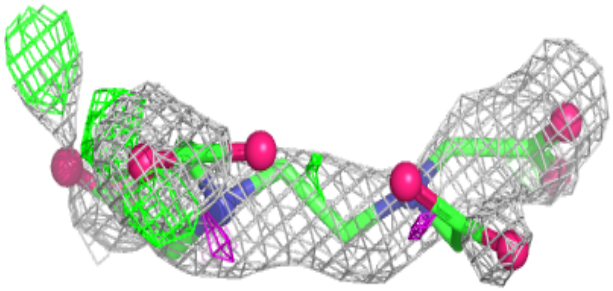
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	104	4/4	0.81	0.16	51,61,66,67	0
12	DTT	A	525	8/8	0.82	0.22	27,51,60,68	8
9	PEG	A	522	7/7	0.82	0.16	51,54,65,81	0
5	EDO	A	531	4/4	0.83	0.15	46,56,58,75	0
5	EDO	A	533	4/4	0.83	0.16	60,63,65,70	0
5	EDO	C	304	4/4	0.83	0.16	54,68,74,76	0
5	EDO	D	201	4/4	0.83	0.15	33,38,38,45	4
8	GOL	A	506	6/6	0.84	0.17	34,50,55,66	6
9	PEG	B	103	7/7	0.84	0.20	23,39,52,58	7
8	GOL	D	203	6/6	0.84	0.16	40,41,49,54	6
5	EDO	B	107	4/4	0.85	0.16	48,58,62,71	0
5	EDO	A	529	4/4	0.86	0.16	44,51,53,56	4
5	EDO	A	512	4/4	0.86	0.16	35,36,37,39	4
9	PEG	A	516	7/7	0.86	0.14	33,41,49,56	7
9	PEG	A	519	7/7	0.86	0.14	43,47,63,68	0
11	P15	A	521	20/20	0.86	0.17	13,41,58,63	20
5	EDO	C	303	4/4	0.86	0.17	38,39,39,41	4
13	PGE	A	530	10/10	0.86	0.17	22,41,50,53	10
8	GOL	A	505	6/6	0.86	0.14	28,56,62,69	0
5	EDO	A	526	4/4	0.87	0.16	40,56,62,70	0
5	EDO	A	509	4/4	0.87	0.11	42,45,53,58	0
9	PEG	B	105	7/7	0.87	0.17	32,33,51,52	7
5	EDO	A	507	4/4	0.88	0.15	43,47,49,58	4
5	EDO	A	523	4/4	0.88	0.16	29,30,30,48	4
5	EDO	A	510	4/4	0.88	0.16	49,57,57,61	0
17	1PE	D	202	16/16	0.88	0.12	45,61,76,78	0
5	EDO	A	511	4/4	0.89	0.12	34,34,35,37	4
16	MES	C	302	12/12	0.89	0.12	42,51,59,65	12
5	EDO	B	101	4/4	0.89	0.13	21,32,33,39	4
5	EDO	A	532	4/4	0.90	0.16	21,24,48,49	4
5	EDO	A	501	4/4	0.90	0.16	21,40,43,52	0
5	EDO	A	513	4/4	0.91	0.11	35,35,45,47	4
5	EDO	A	514	4/4	0.91	0.12	12,20,20,25	4
7	LPH	A	504	8/8	0.93	0.15	27,31,47,47	8
9	PEG	A	524	7/7	0.93	0.11	24,37,55,61	7
6	PLP	A	503	15/16	0.94	0.07	12,21,32,40	0
15	8Q1	C	301	34/35	0.95	0.08	22,30,40,44	0
5	EDO	A	508	4/4	0.96	0.12	14,14,23,27	4

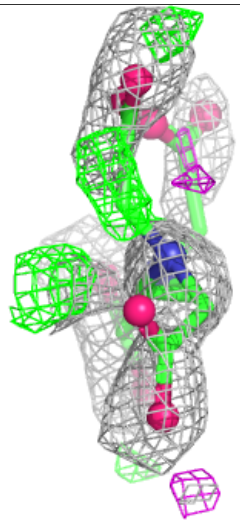
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

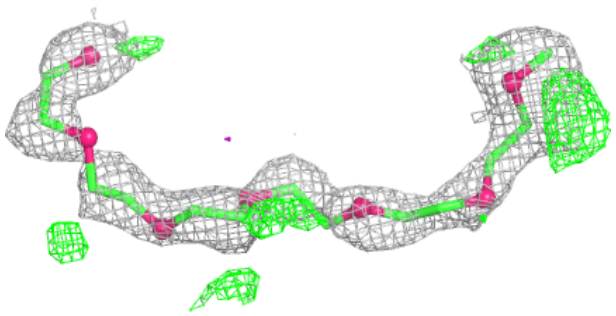


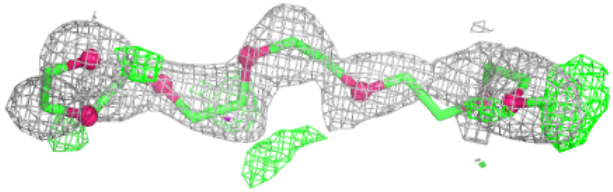


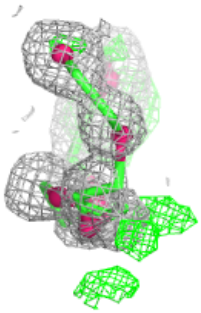


Electron density around P15 A 521:

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

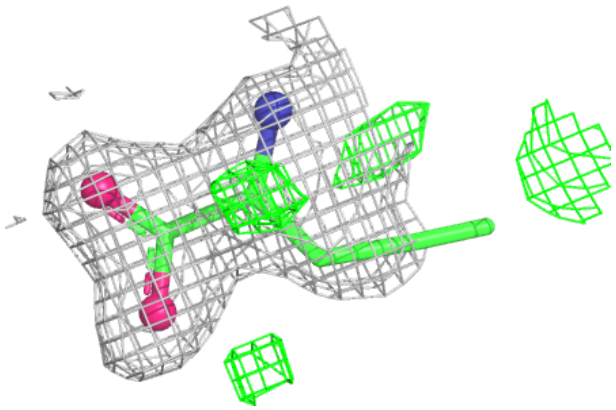


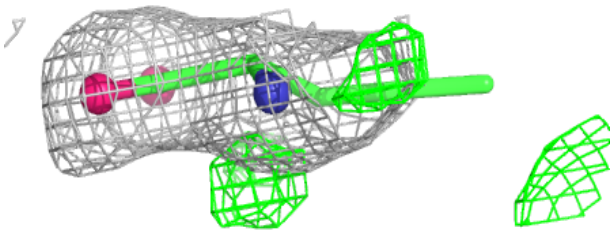


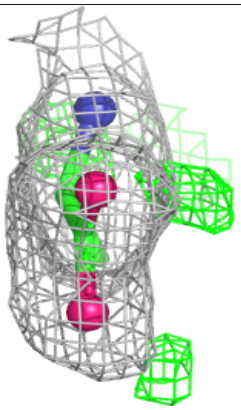


Electron density around LPH A 504:

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

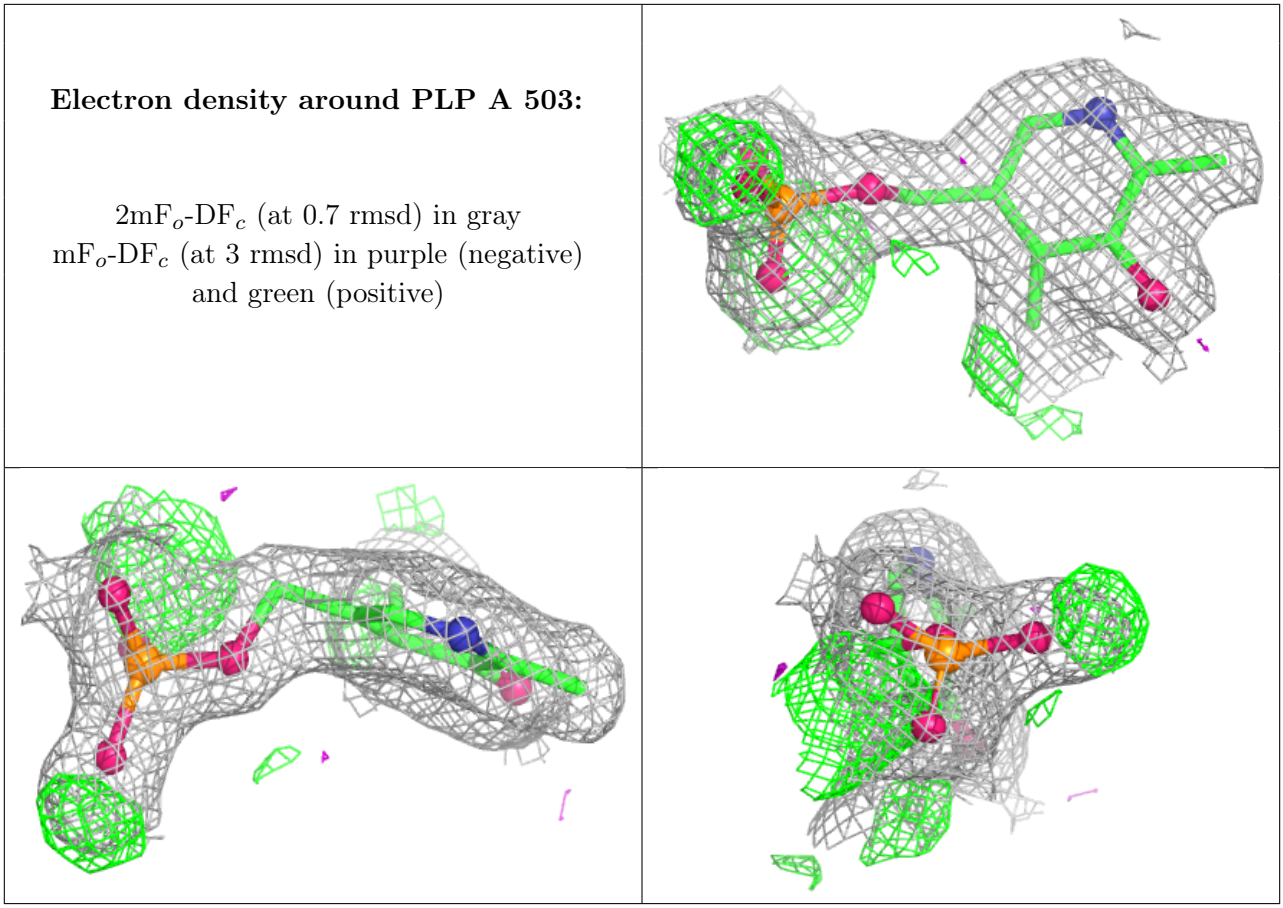






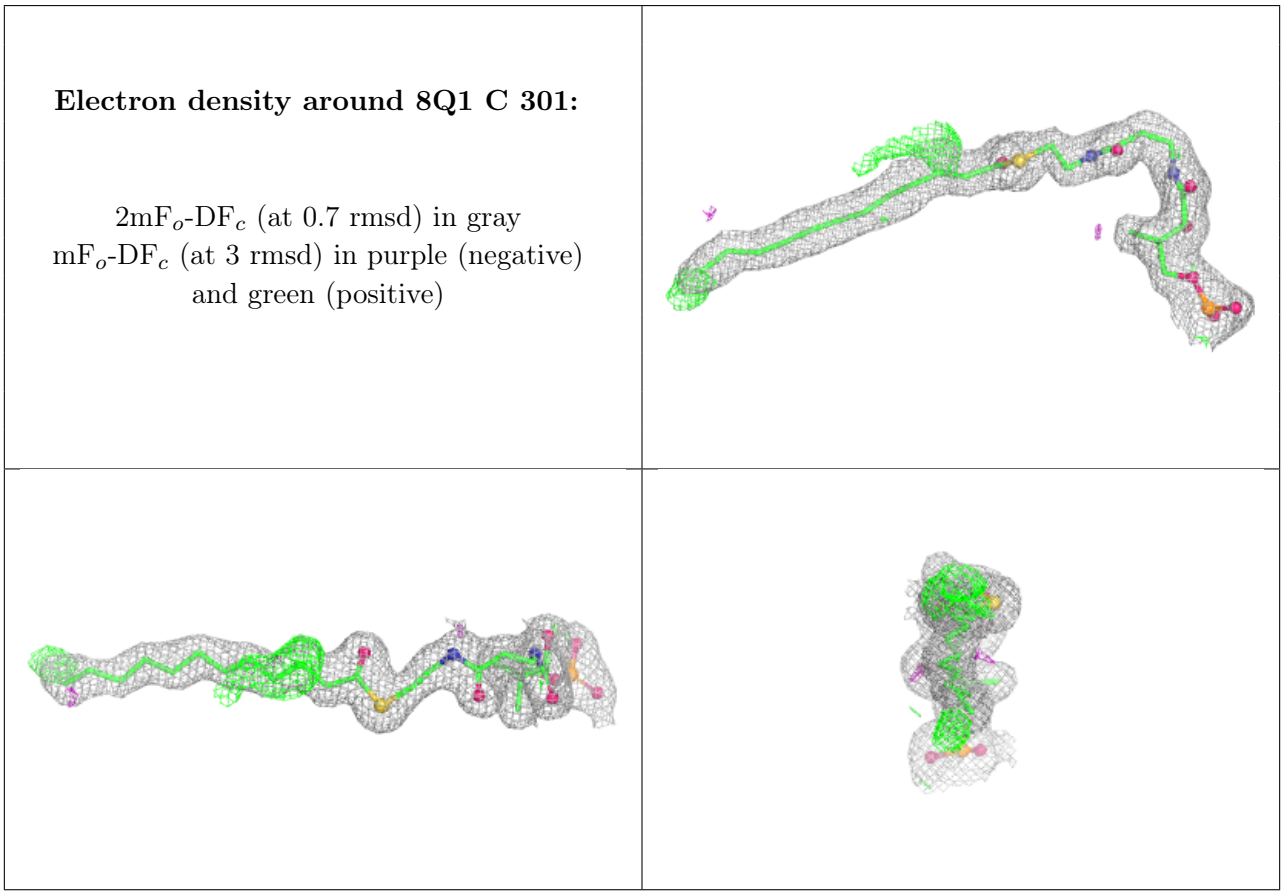
Electron density around PLP A 503:

$2mF_o$-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.