



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:51 PM UTC

PDB ID : 7RTK / pdb_00007rtk
Title : Structure of the (NIAU)2 complex with N-terminal mutation of ISCU2 Y35D at 2.5 Å resolution
Authors : Boniecki, M.T.; Cygler, M.
Deposited on : 2021-08-13
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

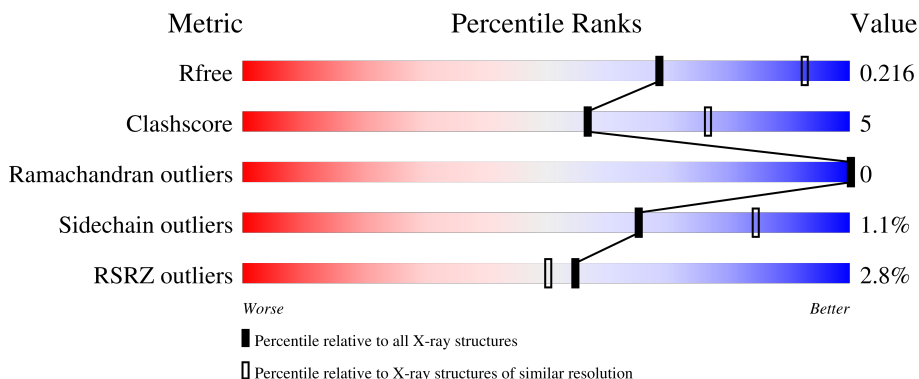
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

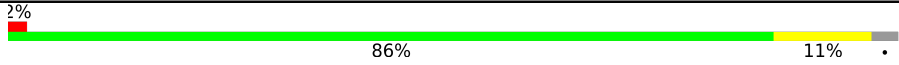



The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	 2% 86% 11%
2	B	91	 3% 84% 9% 8%
3	C	77	 5% 83% 14%
4	D	143	 2% 75% 12% 13%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 5798 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
			Total	C	N	O	S			
1	A	395	3071	1935	535	580	21	0	5	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	713	449	140	123	1	0	5	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	75	528	331	84	112	1	0	0	0

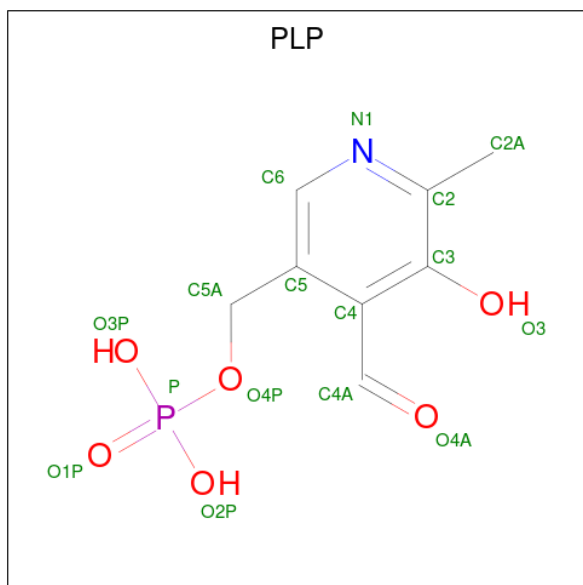
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	124	919	580	156	175	8	0	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	MET	-	initiating methionine	UNP Q9H1K1
D	34	ALA	-	expression tag	UNP Q9H1K1
D	35	ASP	TYR	conflict	UNP Q9H1K1
D	168	LEU	-	expression tag	UNP Q9H1K1
D	169	GLU	-	expression tag	UNP Q9H1K1
D	170	HIS	-	expression tag	UNP Q9H1K1
D	171	HIS	-	expression tag	UNP Q9H1K1
D	172	HIS	-	expression tag	UNP Q9H1K1
D	173	HIS	-	expression tag	UNP Q9H1K1
D	174	HIS	-	expression tag	UNP Q9H1K1
D	175	HIS	-	expression tag	UNP Q9H1K1

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



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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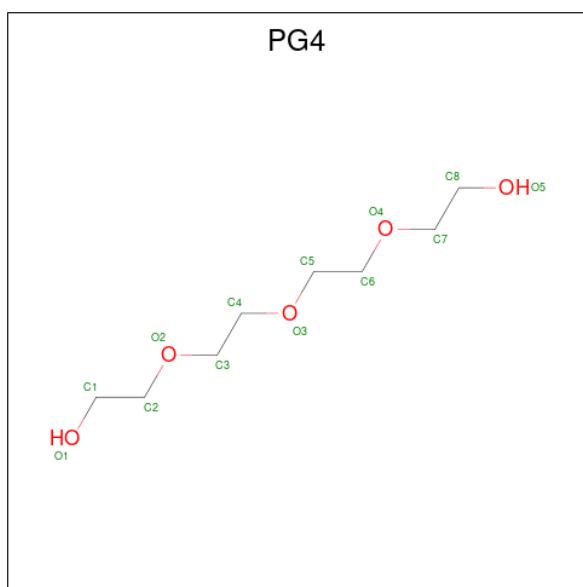
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



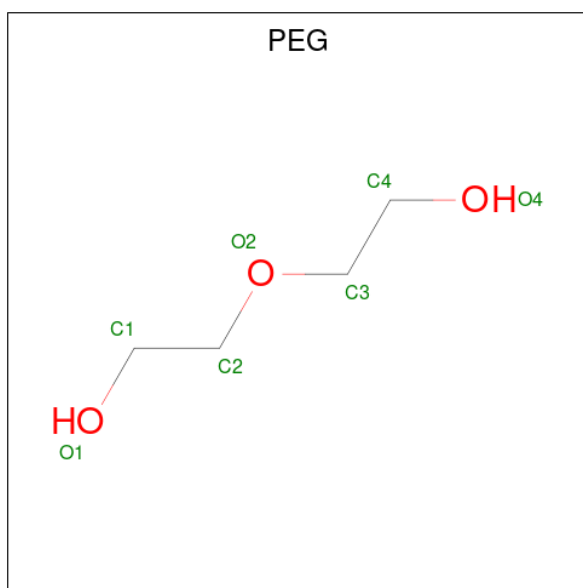
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



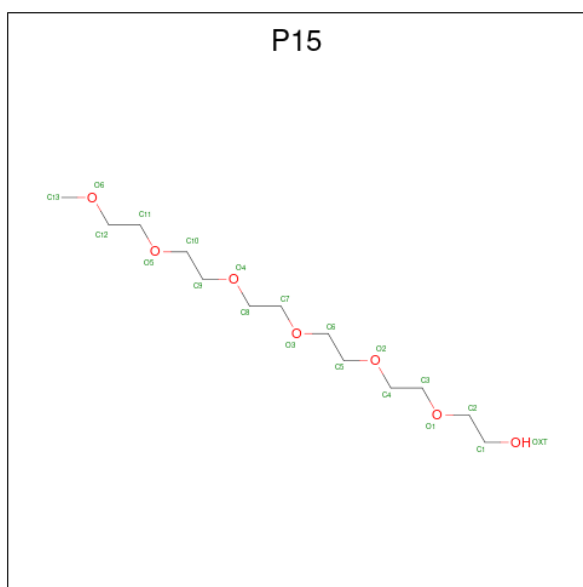
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



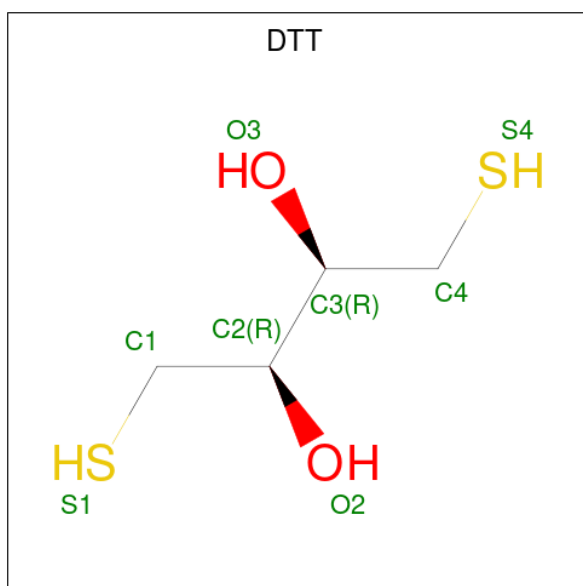
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0

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



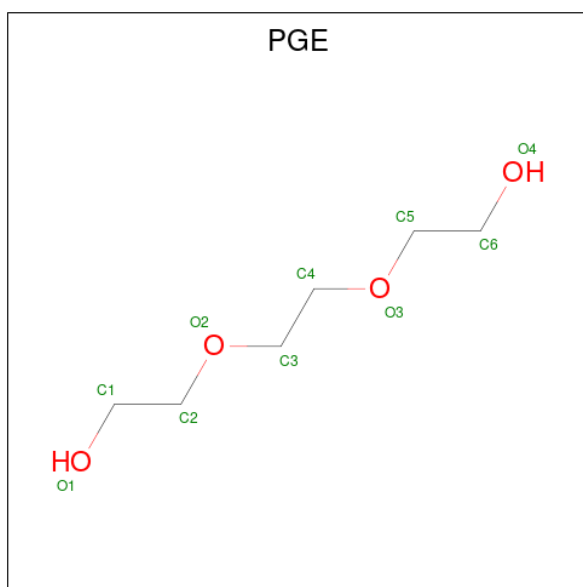
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			20	13	7		

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



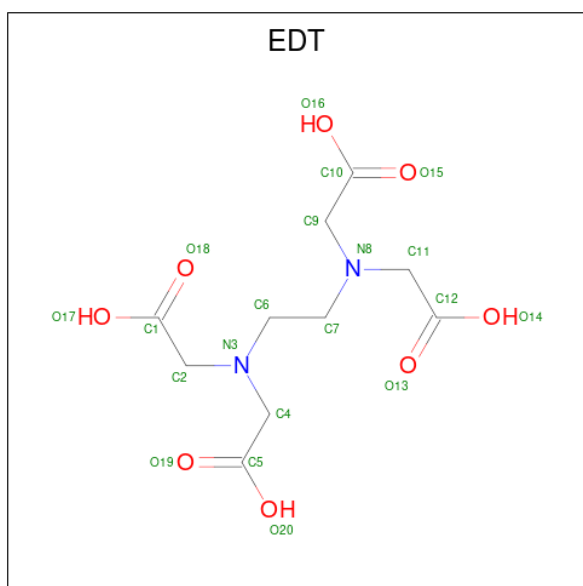
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			8	4	2	2		

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



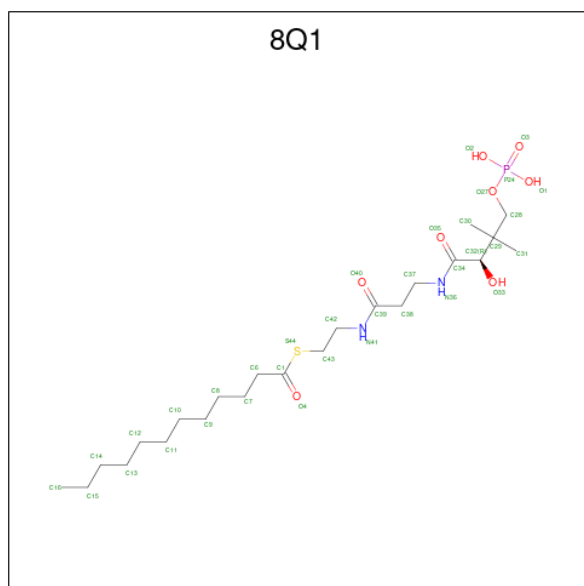
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 10 6 4	0	0
12	A	1	Total C O 10 6 4	0	0
12	A	1	Total C O 10 6 4	0	0

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



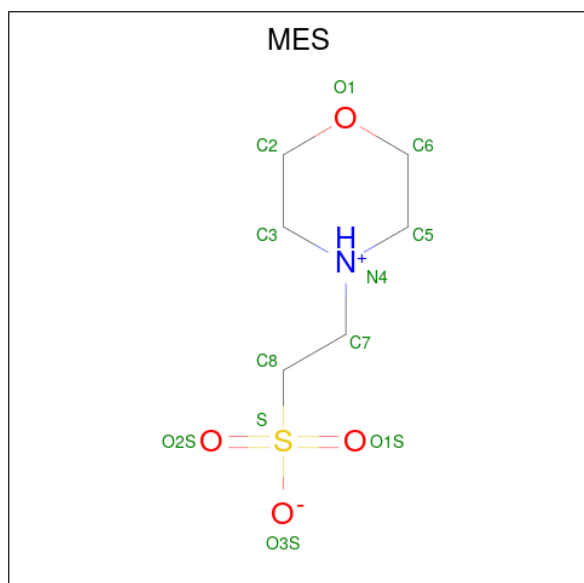
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	20	10	2	8	0	0

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



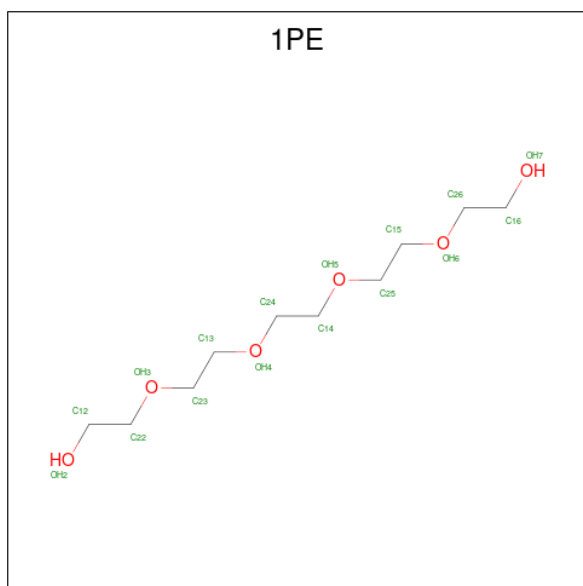
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
14	C	1	34	23	2	7	1	1	0	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 16 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

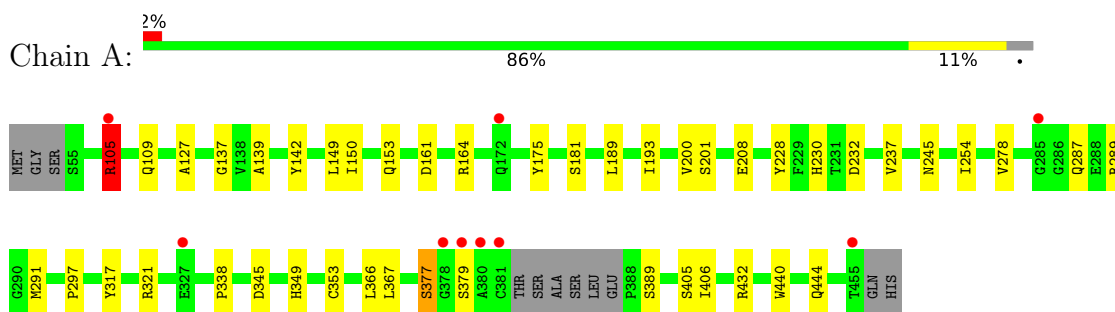
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	163	Total	O	0	0
			163	163		
17	B	30	Total	O	0	0
			30	30		
17	C	4	Total	O	0	0
			4	4		
17	D	12	Total	O	0	0
			12	12		

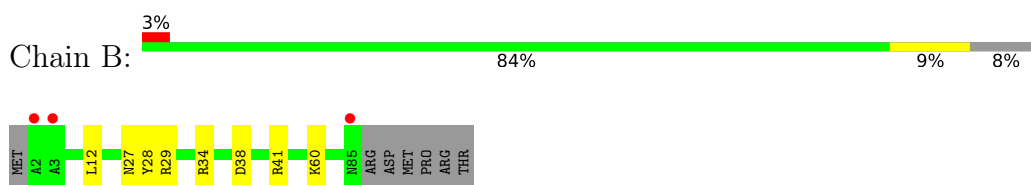
3 Residue-property plots [i](#)

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

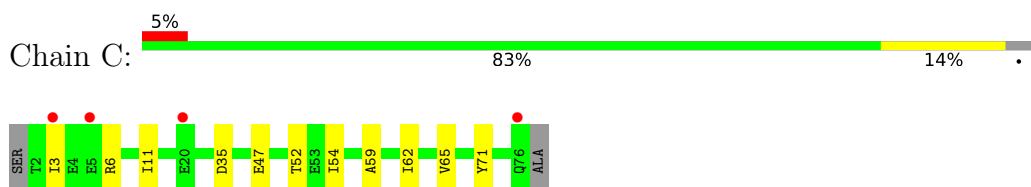
- Molecule 1: Cysteine desulfurase, mitochondrial



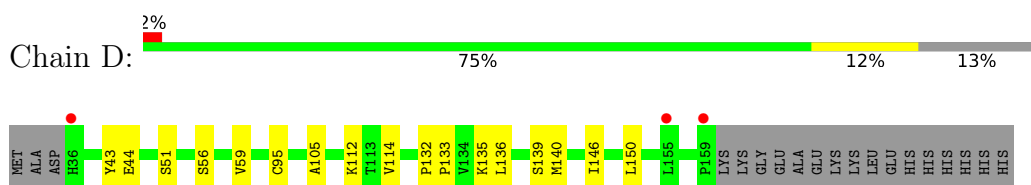
- Molecule 2: LYR motif-containing protein 4



- Molecule 3: Acyl carrier protein



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.35Å 86.35Å 246.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.50 49.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.00-2.50) 100.0 (49.00-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.169 , 0.214 0.171 , 0.216	Depositor DCC
R_{free} test set	1663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtrriage
Anisotropy	0.191	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5798	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P15, DTT, 1PE, PEG, EDT, 8Q1, MES, GOL, PLP, EDO, PG4, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	4/3142 (0.1%)	0.43	2/4251 (0.0%)
2	B	0.14	0/737	0.29	0/989
3	C	0.11	0/532	0.24	0/726
4	D	0.17	0/941	0.35	0/1273
All	All	0.25	4/5352 (0.1%)	0.39	2/7239 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105[A]	ARG	C-O	8.39	1.33	1.24
1	A	105[B]	ARG	C-O	8.39	1.33	1.24
1	A	105[A]	ARG	CA-C	5.14	1.59	1.52
1	A	105[B]	ARG	CA-C	5.14	1.59	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105[A]	ARG	CA-C-O	9.86	131.00	120.55
1	A	105[B]	ARG	CA-C-O	9.86	131.00	120.55

There are no chirality outliers.

There are no planarity outliers.

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	3071	0	3061	29	0
2	B	713	0	738	7	0
3	C	528	0	467	6	0
4	D	919	0	931	11	0
5	A	15	0	7	2	0
6	A	84	0	126	9	0
6	B	16	0	24	0	0
6	C	4	0	6	0	0
6	D	12	0	18	0	0
7	A	12	0	16	2	0
7	D	6	0	8	0	0
8	A	13	0	18	0	0
9	A	35	0	50	1	0
9	B	21	0	30	1	0
10	A	20	0	28	0	0
11	A	8	0	10	1	0
12	A	30	0	42	1	0
13	B	20	0	12	1	0
14	C	34	0	0	0	0
15	C	12	0	12	0	0
16	D	16	0	22	2	0
17	A	163	0	0	1	0
17	B	30	0	0	1	0
17	C	4	0	0	0	0
17	D	12	0	0	0	0
All	All	5798	0	5626	52	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 5.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ARG:HH21	13:B:108:EDT:H061	1.35	0.90
1:A:105[B]:ARG:NH1	17:A:601:HOH:O	2.23	0.71
1:A:245:ASN:HD21	11:A:523:DTT:H2	1.55	0.71
1:A:175:TYR:HD1	6:A:502:EDO:H22	1.56	0.70
1:A:208:GLU:OE2	1:A:389:SER:OG	2.12	0.67
4:D:112:LYS:HG2	16:D:202:1PE:H222	1.78	0.64
4:D:95:CYS:SG	4:D:135:LYS:NZ	2.60	0.64
1:A:237:VAL:HG21	1:A:254:ILE:HG12	1.80	0.63
3:C:11:ILE:HD13	3:C:65:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:114:VAL:HG13	4:D:150:LEU:HD22	1.81	0.63
4:D:112:LYS:HE3	16:D:202:1PE:H252	1.80	0.62
6:A:506:EDO:H11	4:D:44:GLU:HG2	1.83	0.60
1:A:287:GLN:HG3	6:A:532:EDO:H11	1.82	0.60
2:B:41:ARG:NH2	3:C:35:ASP:OD2	2.35	0.60
2:B:12:LEU:HD11	2:B:60:LYS:HG3	1.82	0.60
1:A:297:PRO:HD3	6:A:512:EDO:H21	1.87	0.57
2:B:34[B]:ARG:NE	17:B:202:HOH:O	2.38	0.56
1:A:321[B]:ARG:NH2	7:A:504:GOL:O2	2.37	0.56
1:A:366:LEU:HD23	1:A:406:ILE:HG13	1.86	0.56
1:A:109:GLN:HE22	12:A:528:PGE:H5	1.71	0.55
1:A:377:SER:HB2	1:A:405:SER:O	2.09	0.53
1:A:137:GLY:HA3	1:A:278:VAL:HG13	1.91	0.53
1:A:150:ILE:HB	1:A:200:VAL:HG22	1.89	0.53
1:A:139:ALA:HB2	1:A:149:LEU:HD21	1.91	0.52
1:A:201:SER:HA	1:A:230:HIS:O	2.10	0.52
4:D:133:PRO:HA	4:D:136:LEU:HG	1.91	0.51
1:A:161:ASP:OD1	1:A:164:ARG:NH2	2.41	0.51
1:A:367:LEU:HD11	1:A:377:SER:HB3	1.93	0.51
1:A:432[B]:ARG:HH12	6:A:505:EDO:H11	1.76	0.51
1:A:153:GLN:HG2	9:A:521:PEG:H21	1.93	0.50
7:A:504:GOL:H12	2:B:34[A]:ARG:HH21	1.76	0.50
3:C:47:GLU:HG2	3:C:52:THR:O	2.11	0.49
1:A:338:PRO:HD3	6:A:507:EDO:H11	1.95	0.48
3:C:54:ILE:HG12	3:C:71:TYR:CE2	2.49	0.48
1:A:317:TYR:HB2	6:A:513:EDO:H11	1.95	0.48
1:A:181:SER:HB2	1:A:345:ASP:HB2	1.95	0.48
6:A:506:EDO:H12	4:D:43:TYR:CE2	2.49	0.48
1:A:142:TYR:CE2	1:A:228:TYR:HE2	2.34	0.46
1:A:289:ARG:HB2	1:A:291[A]:MET:HE3	1.98	0.46
3:C:59:ALA:HA	3:C:62:ILE:HD12	1.97	0.45
4:D:132:PRO:HD2	4:D:135:LYS:HB2	1.99	0.44
1:A:127:ALA:HB3	5:A:501:PLP:O4P	2.17	0.44
3:C:3:ILE:O	3:C:6:ARG:HG3	2.18	0.43
2:B:27[B]:ASN:OD1	2:B:28:TYR:N	2.52	0.43
2:B:38:ASP:HB3	9:B:103:PEG:H21	2.00	0.43
4:D:56:SER:HB3	4:D:59:VAL:HB	2.02	0.42
6:A:506:EDO:H12	4:D:43:TYR:HE2	1.84	0.42
1:A:349:HIS:NE2	1:A:353:CYS:O	2.52	0.42
1:A:440:TRP:O	1:A:444:GLN:HG2	2.20	0.41
4:D:105:ALA:HB1	4:D:146:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:OD2	5:A:501:PLP:N1	2.54	0.41
1:A:189:LEU:O	1:A:193:ILE:HG13	2.21	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	396/406 (98%)	383 (97%)	13 (3%)	0	100	100
2	B	87/91 (96%)	86 (99%)	1 (1%)	0	100	100
3	C	73/77 (95%)	69 (94%)	4 (6%)	0	100	100
4	D	125/143 (87%)	125 (100%)	0	0	100	100
All	All	681/717 (95%)	663 (97%)	18 (3%)	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	330/346 (95%)	326 (99%)	4 (1%)	63	83
2	B	73/80 (91%)	73 (100%)	0	100	100
3	C	48/66 (73%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	98/118 (83%)	94 (96%)	4 (4%)	27	53
All	All	549/610 (90%)	541 (98%)	8 (2%)	65	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105[A]	ARG
1	A	105[B]	ARG
1	A	377	SER
1	A	379	SER
4	D	51	SER
4	D	139	SER
4	D	140[A]	MET
4	D	140[B]	MET

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	108	GLN
1	A	172	GLN
1	A	245	ASN
1	A	444	GLN
4	D	78	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

51 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
9	PEG	B	105	-	6,6,6	0.49	0	5,5,5	0.23	0
6	EDO	A	530	-	3,3,3	0.47	0	2,2,2	0.30	0
9	PEG	A	521	-	6,6,6	0.51	0	5,5,5	0.31	0
6	EDO	A	514	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	D	203	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	A	506	-	3,3,3	0.38	0	2,2,2	0.35	0
13	EDT	B	108	-	19,19,19	1.00	0	24,24,24	0.81	0
9	PEG	B	102	-	6,6,6	0.49	0	5,5,5	0.27	0
7	GOL	D	204	-	5,5,5	1.00	0	5,5,5	1.00	0
6	EDO	A	513	-	3,3,3	0.43	0	2,2,2	0.33	0
6	EDO	A	507	-	3,3,3	0.43	0	2,2,2	0.31	0
12	PGE	A	524	-	9,9,9	0.31	0	8,8,8	0.30	0
9	PEG	A	517	-	6,6,6	0.50	0	5,5,5	0.32	0
9	PEG	A	534	-	6,6,6	0.49	0	5,5,5	0.21	0
6	EDO	A	525	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	A	526	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	A	519	-	3,3,3	0.43	0	2,2,2	0.41	0
6	EDO	A	509	-	3,3,3	0.43	0	2,2,2	0.34	0
6	EDO	A	531	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	A	535	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	106	-	3,3,3	0.42	0	2,2,2	0.40	0
7	GOL	A	503	-	5,5,5	0.86	0	5,5,5	1.11	0
6	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.37	0
9	PEG	A	533	-	6,6,6	0.50	0	5,5,5	0.31	0
10	P15	A	520	-	19,19,19	0.56	0	18,18,18	0.25	0
6	EDO	A	512	-	3,3,3	0.41	0	2,2,2	0.29	0
6	EDO	A	527	-	3,3,3	0.44	0	2,2,2	0.29	0
9	PEG	A	522	-	6,6,6	0.52	0	5,5,5	0.25	0
6	EDO	B	104	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	D	201	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	A	515	-	3,3,3	0.45	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	532	-	3,3,3	0.46	0	2,2,2	0.36	0
16	1PE	D	202	-	15,15,15	0.55	0	14,14,14	0.22	0
7	GOL	A	504	-	5,5,5	0.90	0	5,5,5	1.09	0
6	EDO	A	510	-	3,3,3	0.39	0	2,2,2	0.45	0
5	PLP	A	501	1	15,15,16	1.09	2 (13%)	21,22,23	1.03	2 (9%)
6	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.33	0
12	PGE	A	529	-	9,9,9	0.13	0	8,8,8	0.11	0
15	MES	C	302	-	12,12,12	2.25	1 (8%)	15,16,16	1.81	4 (26%)
12	PGE	A	528	-	9,9,9	0.31	0	8,8,8	0.36	0
6	EDO	A	511	-	3,3,3	0.44	0	2,2,2	0.39	0
9	PEG	B	103	-	6,6,6	0.51	0	5,5,5	0.22	0
6	EDO	A	508	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	D	205	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	B	107	-	3,3,3	0.45	0	2,2,2	0.37	0
8	PG4	A	516	-	12,12,12	0.54	0	11,11,11	0.18	0
11	DTT	A	523	-	7,7,7	0.56	0	4,8,8	0.34	0
14	8Q1	C	301	3	28,33,34	2.28	8 (28%)	32,40,43	1.57	4 (12%)
6	EDO	B	101	-	3,3,3	0.44	0	2,2,2	0.38	0
6	EDO	A	518	-	3,3,3	0.41	0	2,2,2	0.41	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
9	PEG	B	105	-	-	4/4/4/4	-
6	EDO	A	530	-	-	0/1/1/1	-
9	PEG	A	521	-	-	1/4/4/4	-
6	EDO	A	514	-	-	1/1/1/1	-
6	EDO	D	203	-	-	0/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
13	EDT	B	108	-	-	7/21/21/21	-
9	PEG	B	102	-	-	1/4/4/4	-
7	GOL	D	204	-	-	0/4/4/4	-
6	EDO	A	513	-	-	0/1/1/1	-
6	EDO	A	507	-	-	0/1/1/1	-
12	PGE	A	524	-	-	3/7/7/7	-
9	PEG	A	517	-	-	0/4/4/4	-
9	PEG	A	534	-	-	0/4/4/4	-
6	EDO	A	525	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	526	-	-	0/1/1/1	-
6	EDO	C	303	-	-	0/1/1/1	-
6	EDO	A	519	-	-	0/1/1/1	-
6	EDO	A	509	-	-	0/1/1/1	-
6	EDO	A	531	-	-	0/1/1/1	-
6	EDO	A	535	-	-	0/1/1/1	-
6	EDO	B	106	-	-	0/1/1/1	-
7	GOL	A	503	-	-	0/4/4/4	-
6	EDO	A	505	-	-	0/1/1/1	-
9	PEG	A	533	-	-	3/4/4/4	-
10	P15	A	520	-	-	8/17/17/17	-
6	EDO	A	512	-	-	1/1/1/1	-
6	EDO	A	527	-	-	0/1/1/1	-
9	PEG	A	522	-	-	1/4/4/4	-
6	EDO	B	104	-	-	0/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	A	532	-	-	0/1/1/1	-
16	1PE	D	202	-	-	6/13/13/13	-
7	GOL	A	504	-	-	2/4/4/4	-
6	EDO	A	510	-	-	1/1/1/1	-
5	PLP	A	501	1	-	0/6/6/8	0/1/1/1
6	EDO	A	502	-	-	1/1/1/1	-
12	PGE	A	529	-	-	3/7/7/7	-
15	MES	C	302	-	-	2/6/14/14	0/1/1/1
12	PGE	A	528	-	-	2/7/7/7	-
6	EDO	A	511	-	-	0/1/1/1	-
9	PEG	B	103	-	-	1/4/4/4	-
6	EDO	A	508	-	-	0/1/1/1	-
6	EDO	D	205	-	-	0/1/1/1	-
6	EDO	B	107	-	-	0/1/1/1	-
8	PG4	A	516	-	-	7/10/10/10	-
11	DTT	A	523	-	-	5/8/8/8	-
14	8Q1	C	301	3	-	5/38/40/41	-
6	EDO	B	101	-	-	0/1/1/1	-
6	EDO	A	518	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	302	MES	C8-S	-7.52	1.67	1.77
14	C	301	8Q1	C39-N41	5.92	1.47	1.33
14	C	301	8Q1	C34-N36	5.86	1.47	1.33
14	C	301	8Q1	C6-C1	4.06	1.54	1.50
14	C	301	8Q1	C12-C13	-3.52	1.34	1.51
14	C	301	8Q1	C1-S44	3.11	1.83	1.76
14	C	301	8Q1	C15-C14	-2.89	1.33	1.51
5	A	501	PLP	C2-N1	2.46	1.38	1.33
14	C	301	8Q1	C28-C29	2.12	1.56	1.52
14	C	301	8Q1	O35-C34	-2.11	1.19	1.23
5	A	501	PLP	C6-N1	2.08	1.38	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	301	8Q1	C6-C1-S44	5.28	119.69	113.40
15	C	302	MES	C5-N4-C3	3.90	117.23	108.84
15	C	302	MES	C7-N4-C5	2.87	118.90	111.24
15	C	302	MES	C6-C5-N4	-2.74	105.96	110.12
14	C	301	8Q1	O4-C1-S44	-2.67	119.28	122.68
14	C	301	8Q1	O4-C1-C6	-2.57	121.02	123.98
15	C	302	MES	O1S-S-C8	2.21	110.07	106.73
5	A	501	PLP	C5-C6-N1	-2.12	120.38	123.83
5	A	501	PLP	C6-C5-C4	2.05	119.78	118.10
14	C	301	8Q1	C43-S44-C1	2.01	107.77	101.84

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	GOL	O1-C1-C2-O2
7	A	504	GOL	O1-C1-C2-C3
11	A	523	DTT	S1-C1-C2-C3
11	A	523	DTT	C2-C3-C4-S4
11	A	523	DTT	O3-C3-C4-S4
13	B	108	EDT	O17-C1-C2-N3
13	B	108	EDT	N8-C11-C12-O13
15	C	302	MES	C8-C7-N4-C5
12	A	529	PGE	C1-C2-O2-C3
13	B	108	EDT	O18-C1-C2-N3
13	B	108	EDT	O16-C10-C9-N8
13	B	108	EDT	O15-C10-C9-N8

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Mol	Chain	Res	Type	Atoms
13	B	108	EDT	N8-C11-C12-O14
16	D	202	1PE	OH4-C13-C23-OH3
10	A	520	P15	O2-C5-C6-O3
12	A	524	PGE	O2-C3-C4-O3
16	D	202	1PE	OH6-C15-C25-OH5
12	A	529	PGE	O2-C3-C4-O3
8	A	516	PG4	O2-C3-C4-O3
16	D	202	1PE	OH5-C14-C24-OH4
10	A	520	P15	O3-C7-C8-O4
8	A	516	PG4	O4-C7-C8-O5
10	A	520	P15	C6-C5-O2-C4
12	A	528	PGE	O3-C5-C6-O4
12	A	529	PGE	O1-C1-C2-O2
13	B	108	EDT	C1-C2-N3-C4
8	A	516	PG4	C3-C4-O3-C5
9	B	105	PEG	O2-C3-C4-O4
10	A	520	P15	OXT-C1-C2-O1
8	A	516	PG4	O1-C1-C2-O2
8	A	516	PG4	O3-C5-C6-O4
9	A	533	PEG	O2-C3-C4-O4
9	A	521	PEG	C1-C2-O2-C3
9	B	103	PEG	C1-C2-O2-C3
9	A	533	PEG	O1-C1-C2-O2
12	A	528	PGE	O2-C3-C4-O3
8	A	516	PG4	C1-C2-O2-C3
14	C	301	8Q1	C12-C13-C14-C15
10	A	520	P15	C8-C7-O3-C6
9	B	105	PEG	C1-C2-O2-C3
16	D	202	1PE	C14-C24-OH4-C13
11	A	523	DTT	S1-C1-C2-O2
8	A	516	PG4	C6-C5-O3-C4
10	A	520	P15	C12-C11-O5-C10
9	B	102	PEG	O1-C1-C2-O2
9	A	522	PEG	C1-C2-O2-C3
12	A	524	PGE	C3-C4-O3-C5
16	D	202	1PE	C13-C23-OH3-C22
10	A	520	P15	C10-C9-O4-C8
12	A	524	PGE	C1-C2-O2-C3
9	B	105	PEG	O1-C1-C2-O2
14	C	301	8Q1	O4-C1-S44-C43
9	A	533	PEG	C1-C2-O2-C3
6	A	510	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	512	EDO	O1-C1-C2-O2
6	A	515	EDO	O1-C1-C2-O2
14	C	301	8Q1	C10-C11-C12-C13
15	C	302	MES	C8-C7-N4-C3
16	D	202	1PE	C15-C25-OH5-C14
6	A	514	EDO	O1-C1-C2-O2
11	A	523	DTT	C1-C2-C3-C4
9	B	105	PEG	C4-C3-O2-C2
6	A	502	EDO	O1-C1-C2-O2
14	C	301	8Q1	O27-C28-C29-C30
14	C	301	8Q1	O27-C28-C29-C31
10	A	520	P15	C9-C10-O5-C11

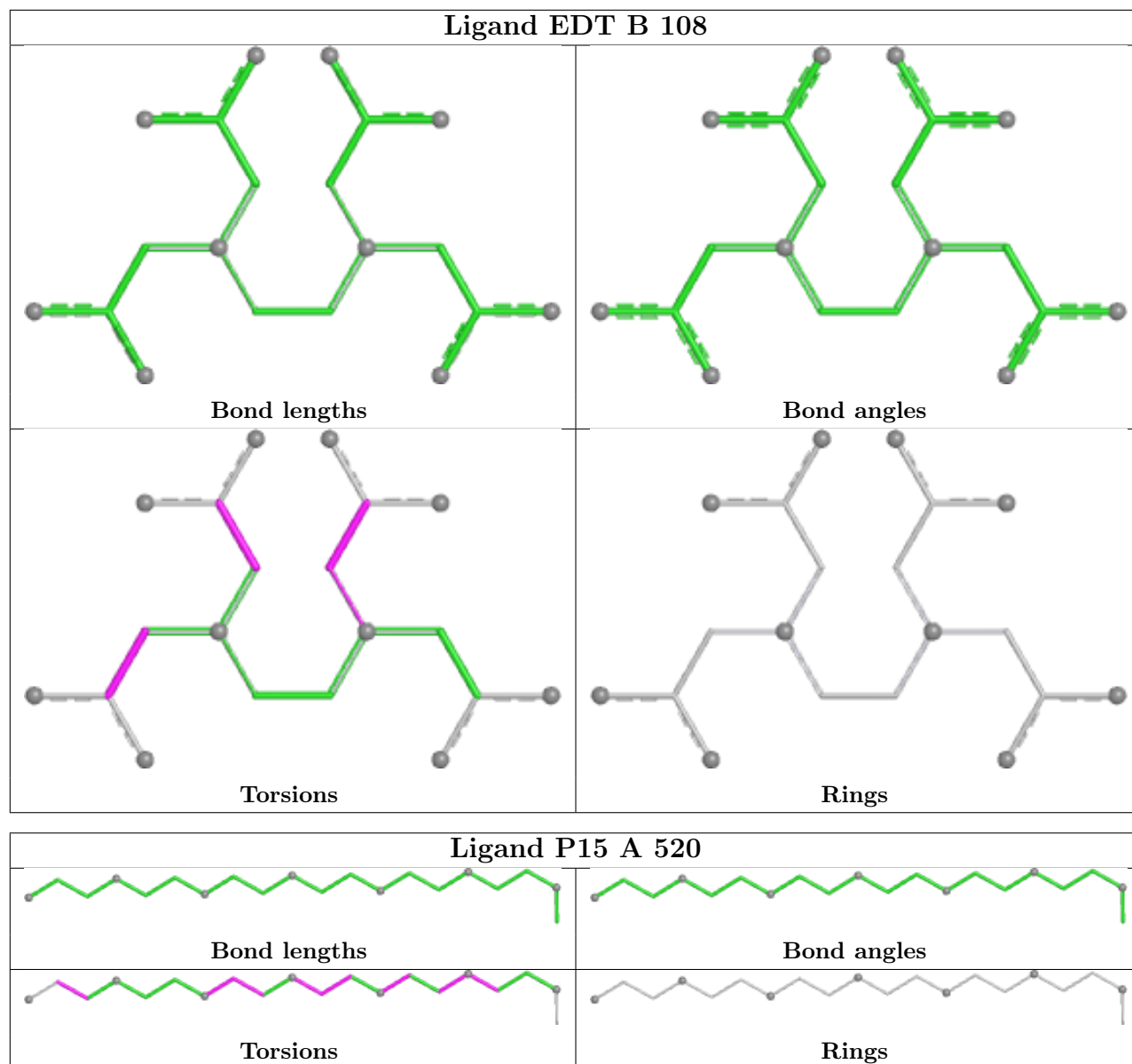
There are no ring outliers.

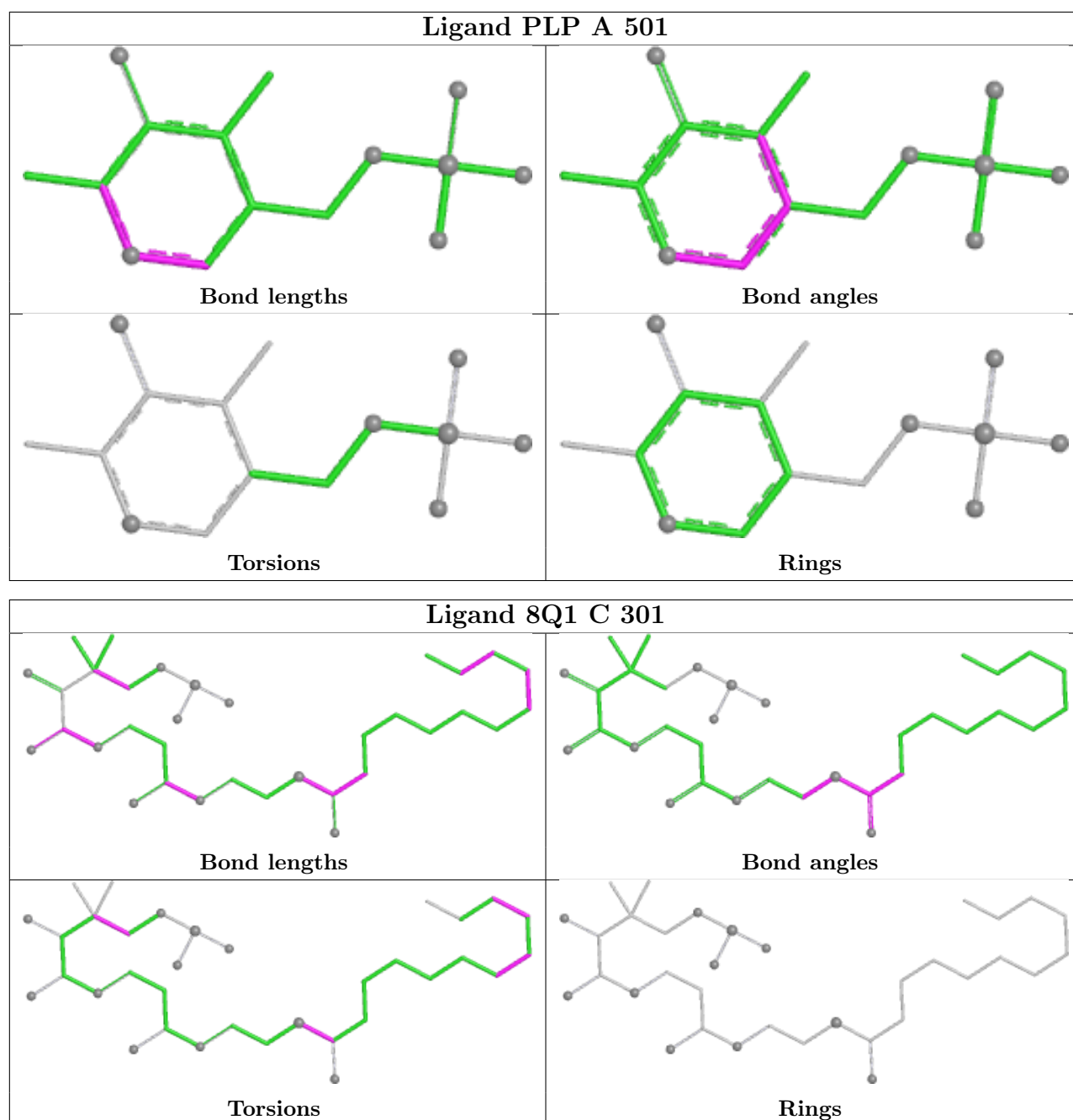
15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	521	PEG	1	0
6	A	506	EDO	3	0
13	B	108	EDT	1	0
6	A	513	EDO	1	0
6	A	507	EDO	1	0
6	A	505	EDO	1	0
6	A	512	EDO	1	0
6	A	532	EDO	1	0
16	D	202	1PE	2	0
7	A	504	GOL	2	0
5	A	501	PLP	2	0
6	A	502	EDO	1	0
12	A	528	PGE	1	0
9	B	103	PEG	1	0
11	A	523	DTT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/406 (97%)	-0.48	9 (2%) 61 57	21, 36, 69, 115	8 (2%)
2	B	84/91 (92%)	-0.30	3 (3%) 46 41	20, 40, 67, 100	5 (5%)
3	C	75/77 (97%)	0.43	4 (5%) 32 28	46, 78, 111, 124	0
4	D	124/143 (86%)	-0.14	3 (2%) 59 55	26, 57, 83, 131	3 (2%)
All	All	678/717 (94%)	-0.30	19 (2%) 55 50	20, 42, 86, 131	16 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	ALA	6.1
1	A	378	GLY	4.9
1	A	379	SER	4.4
1	A	381	CYS	4.2
1	A	455	THR	4.0
3	C	5	GLU	3.6
3	C	76	GLN	3.6
2	B	2	ALA	3.5
4	D	159	PRO	3.3
1	A	105[A]	ARG	3.0
4	D	36	HIS	2.8
1	A	285	GLY	2.7
3	C	3	ILE	2.7
2	B	3	ALA	2.4
2	B	85	ASN	2.3
4	D	155	LEU	2.3
1	A	172	GLN	2.2
3	C	20	GLU	2.1
1	A	327	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

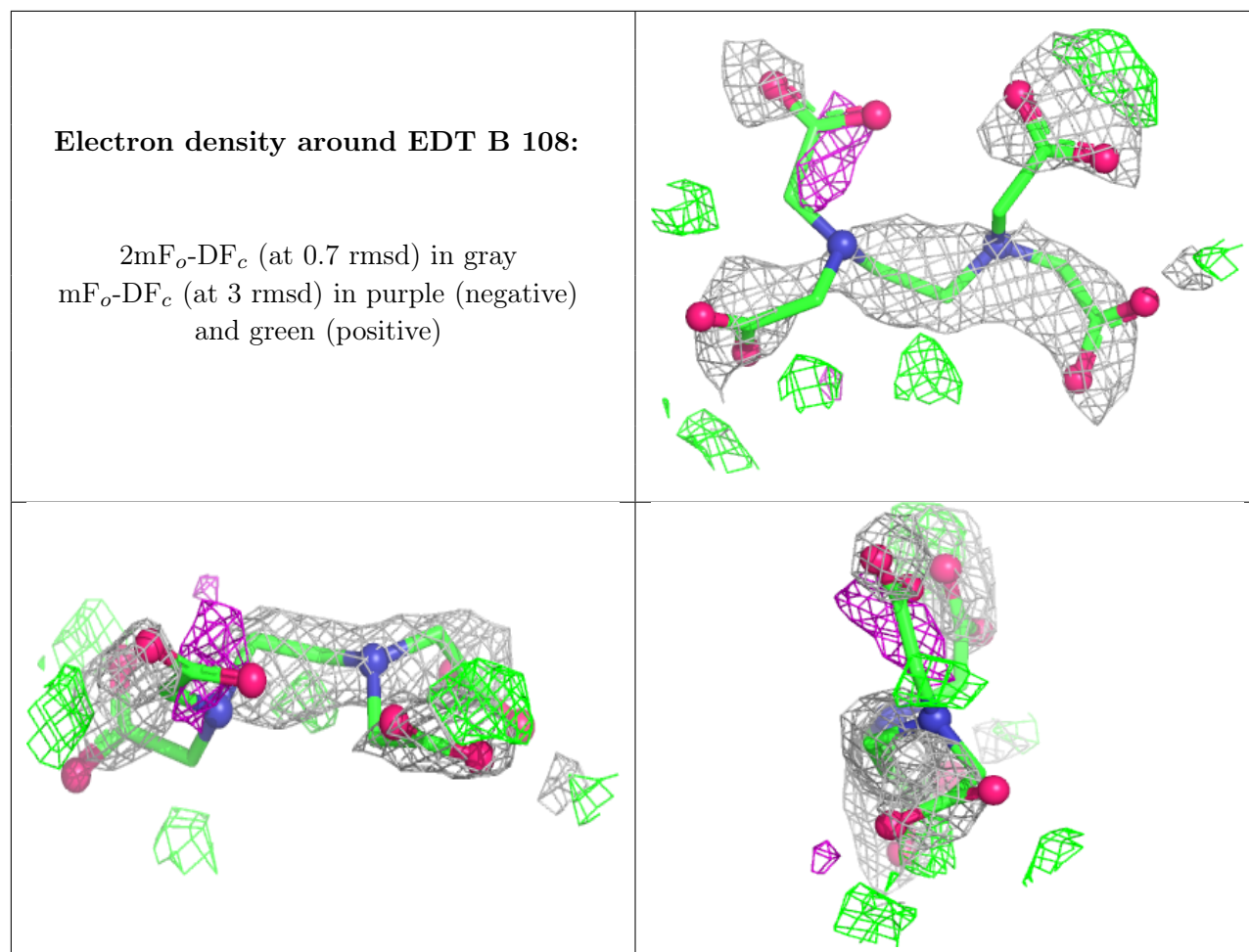
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	526	4/4	0.69	0.18	72,74,80,85	0
15	MES	C	302	12/12	0.70	0.21	63,85,103,105	12
9	PEG	A	522	7/7	0.71	0.25	64,71,81,95	0
6	EDO	D	205	4/4	0.73	0.20	73,77,82,95	0
6	EDO	A	514	4/4	0.73	0.24	42,52,60,69	4
6	EDO	D	201	4/4	0.73	0.16	68,74,82,85	0
6	EDO	A	519	4/4	0.74	0.19	52,54,58,65	4
6	EDO	D	203	4/4	0.74	0.20	74,74,80,85	0
6	EDO	A	510	4/4	0.74	0.21	38,40,43,49	4
6	EDO	B	101	4/4	0.74	0.25	56,59,77,82	0
13	EDT	B	108	20/20	0.74	0.23	44,61,76,79	20
6	EDO	B	106	4/4	0.74	0.14	73,77,78,94	0
8	PG4	A	516	13/13	0.75	0.21	41,63,77,80	13
10	P15	A	520	20/20	0.75	0.23	34,71,84,85	20
6	EDO	A	531	4/4	0.76	0.23	50,67,73,73	0
6	EDO	A	532	4/4	0.76	0.15	73,76,79,82	0
9	PEG	A	521	7/7	0.78	0.18	62,66,77,83	0
6	EDO	B	104	4/4	0.79	0.18	69,70,74,76	0
9	PEG	A	533	7/7	0.80	0.18	63,72,95,96	0
6	EDO	A	530	4/4	0.80	0.21	55,67,84,90	0
12	PGE	A	529	10/10	0.81	0.15	75,82,86,88	0
9	PEG	A	534	7/7	0.81	0.16	72,79,85,88	0
7	GOL	A	504	6/6	0.81	0.16	47,73,80,82	0
9	PEG	B	103	7/7	0.82	0.18	42,57,64,67	7
16	1PE	D	202	16/16	0.82	0.16	68,87,96,101	0
6	EDO	C	303	4/4	0.83	0.19	56,59,64,64	4
7	GOL	D	204	6/6	0.83	0.16	56,62,68,71	6

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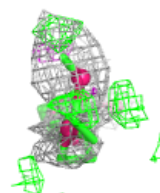
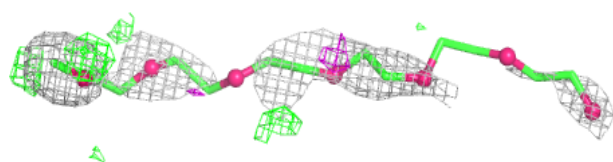
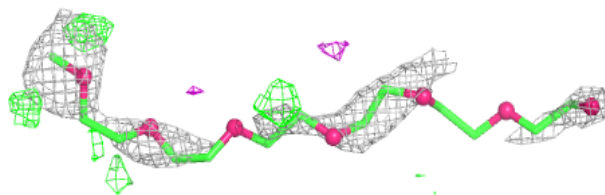
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	525	4/4	0.83	0.17	66,67,71,76	0
12	PGE	A	524	10/10	0.83	0.19	43,52,65,68	10
6	EDO	A	505	4/4	0.84	0.17	59,63,63,68	0
12	PGE	A	528	10/10	0.84	0.20	29,48,57,59	10
9	PEG	A	517	7/7	0.85	0.16	53,62,73,85	0
11	DTT	A	523	8/8	0.85	0.17	53,73,86,93	8
9	PEG	B	102	7/7	0.85	0.14	34,56,60,65	0
6	EDO	A	527	4/4	0.85	0.20	41,56,58,59	4
6	EDO	A	535	4/4	0.86	0.16	57,60,63,67	0
6	EDO	A	509	4/4	0.86	0.19	72,74,76,77	0
6	EDO	A	507	4/4	0.86	0.13	57,59,60,71	0
9	PEG	B	105	7/7	0.86	0.16	51,57,61,64	7
6	EDO	B	107	4/4	0.87	0.17	54,66,66,77	0
6	EDO	A	508	4/4	0.88	0.19	42,46,53,56	4
6	EDO	A	511	4/4	0.88	0.15	47,55,57,64	4
6	EDO	A	515	4/4	0.89	0.18	34,43,47,47	4
6	EDO	A	502	4/4	0.90	0.11	57,61,66,75	0
6	EDO	A	513	4/4	0.91	0.12	68,69,74,80	0
6	EDO	A	506	4/4	0.91	0.15	32,37,38,44	4
6	EDO	A	518	4/4	0.93	0.22	43,49,52,66	4
7	GOL	A	503	6/6	0.94	0.11	25,39,47,47	6
14	8Q1	C	301	34/35	0.94	0.08	35,44,58,59	0
6	EDO	A	512	4/4	0.97	0.10	28,33,35,45	4
5	PLP	A	501	15/16	0.99	0.05	29,33,41,42	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.

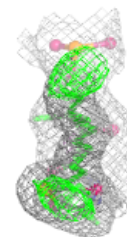
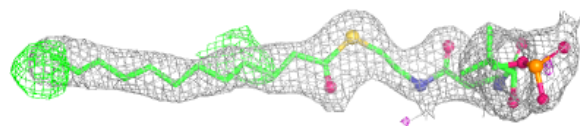
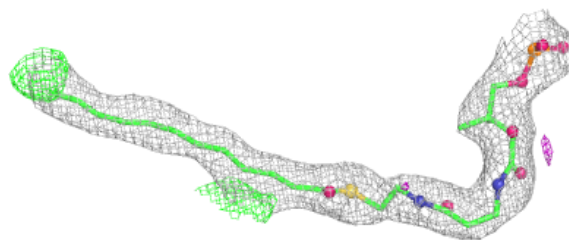


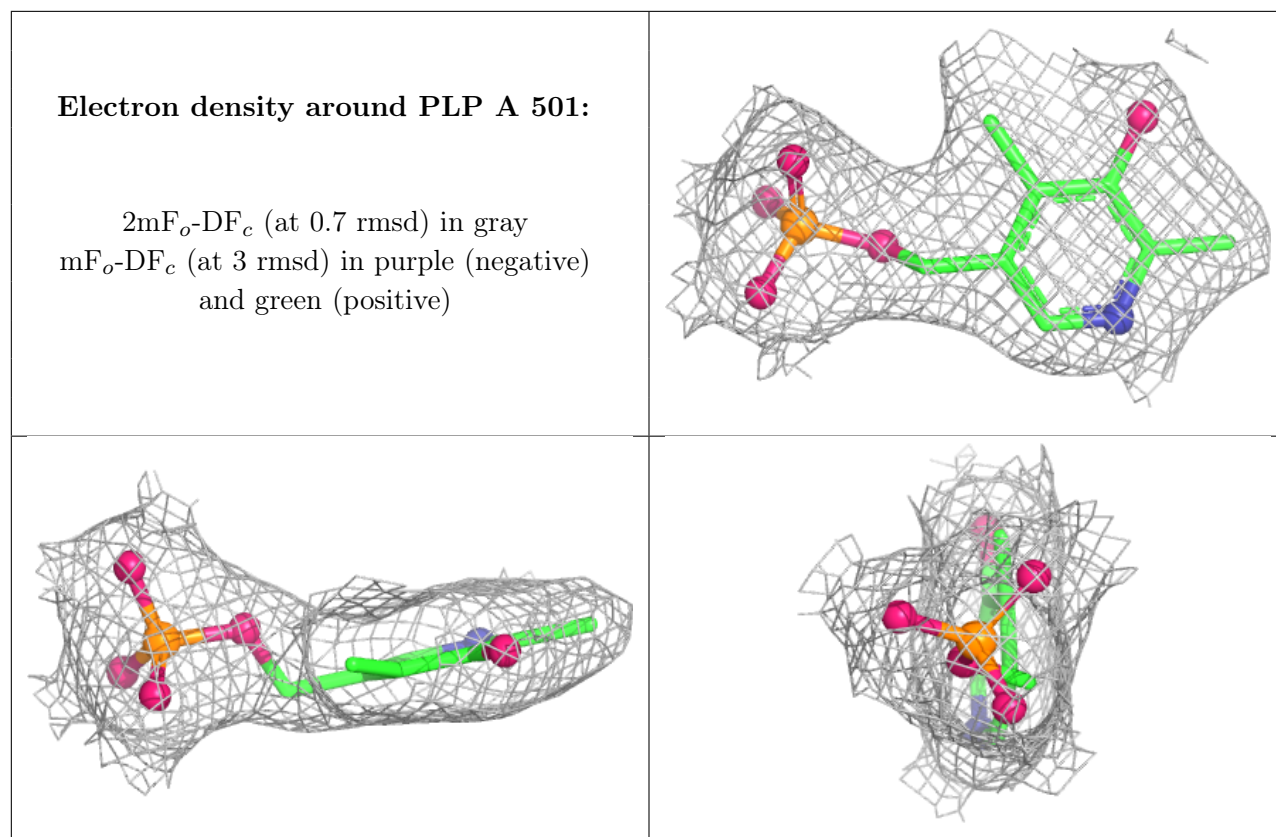
Electron density around P15 A 520:

$2mF_o-DF_c$ (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.